# Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:34 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 7XQP / pdb_00007xqp |
| EMDB ID | : | EMD-33401 |
| Title | : | PSI-LHCI-LHCII-Lhcb9 supercomplex of Physcomitrella patens |
| Authors | : | Zhang, S.; Tang, K.L.; Li, X.Y.; Wang, W.D.; Yan, Q.J.; Shen, L.L.; Kuang, T.Y.; Han, G.Y.; Shen, J.R.; Zhang, X. |
| Deposited on | : | 2022-05-08 |
| Resolution | : | 2.68 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:

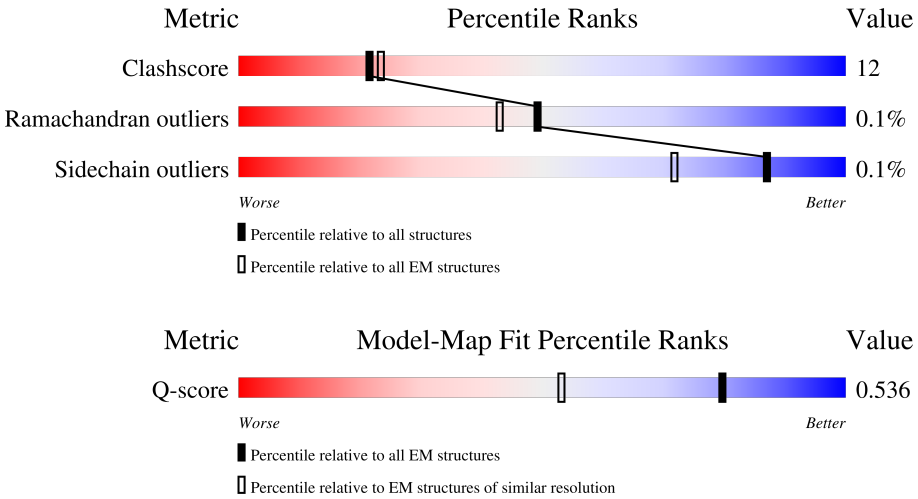
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 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

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

The reported resolution of this entry is 2.68 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 | 9255 ( 2.18 - 3.18 ) |

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 | 742 | 87% 13% |
| 2 | B | 733 | 86% 14% |
| 3 | C | 80 | 81% 19% |
| 4 | D | 141 | 87% 13% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 62 | 85% 15% |
| 6 | F | 159 | 89% 11% |
| 7 | G | 98 | 5% 85% 15% |
| 8 | H | 95 | 93% 7% |
| 9 | I | 34 | 79% 21% |
| 10 | J | 41 | 88% 12% |
| 11 | K | 81 | 90% 10% |
| 12 | L | 163 | 90% 10% |
| 13 | M | 32 | 84% 16% |
| 14 | O | 89 | 76% 24% |
| 15 | 1 | 192 | 84% 16% |
| 15 | 5 | 192 | 29% 66% 33% |
| 16 | 2 | 211 | 84% 16% |
| 16 | 6 | 211 | 36% 69% 28% |
| 17 | 3 | 216 | 89% 11% |
| 17 | 7 | 216 | 62% 67% 31% |
| 18 | 4 | 205 | 85% 15% |
| 18 | 8 | 205 | 32% 74% 25% |
| 19 | 9 | 225 | 75% 24% |
| 20 | a | 227 | 31% 70% 26% |
| 20 | b | 227 | 76% 20% |
| 20 | c | 227 | 11% 81% 19% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 1 | 303 | X | - | - | - |
| 21 | CLA | 1 | 304 | X | - | - | - |
| 21 | CLA | 1 | 305 | X | - | - | - |
| 21 | CLA | 1 | 306 | X | - | - | - |
| 21 | CLA | 1 | 308 | X | - | - | - |
| 21 | CLA | 1 | 309 | X | - | - | - |
| 21 | CLA | 1 | 310 | X | - | - | - |
| 21 | CLA | 1 | 311 | X | - | - | - |
| 21 | CLA | 1 | 312 | X | - | - | - |
| 21 | CLA | 1 | 313 | X | - | - | - |
| 21 | CLA | 1 | 314 | X | - | - | - |
| 21 | CLA | 1 | 315 | X | - | - | - |
| 21 | CLA | 1 | 316 | X | - | - | - |
| 21 | CLA | 2 | 603 | X | - | - | - |
| 21 | CLA | 2 | 604 | X | - | - | - |
| 21 | CLA | 2 | 608 | X | - | - | - |
| 21 | CLA | 2 | 609 | X | - | X | - |
| 21 | CLA | 2 | 610 | X | - | - | - |
| 21 | CLA | 2 | 611 | X | - | - | - |
| 21 | CLA | 2 | 612 | X | - | - | - |
| 21 | CLA | 2 | 613 | X | - | - | - |
| 21 | CLA | 3 | 401 | X | - | - | - |
| 21 | CLA | 3 | 402 | X | - | - | - |
| 21 | CLA | 3 | 403 | X | - | - | - |
| 21 | CLA | 3 | 404 | X | - | - | - |
| 21 | CLA | 3 | 405 | X | - | - | - |
| 21 | CLA | 3 | 406 | X | - | - | - |
| 21 | CLA | 3 | 408 | X | - | - | - |
| 21 | CLA | 3 | 409 | X | - | X | - |
| 21 | CLA | 3 | 410 | X | - | - | - |
| 21 | CLA | 3 | 411 | X | - | - | - |
| 21 | CLA | 3 | 412 | X | - | - | - |
| 21 | CLA | 3 | 413 | X | - | - | - |
| 21 | CLA | 3 | 414 | X | - | - | - |
| 21 | CLA | 3 | 415 | X | - | - | - |
| 21 | CLA | 4 | 601 | X | - | - | - |
| 21 | CLA | 4 | 602 | X | - | - | - |
| 21 | CLA | 4 | 603 | X | - | - | - |
| 21 | CLA | 4 | 604 | X | - | - | - |
| 21 | CLA | 4 | 608 | X | - | - | - |
| 21 | CLA | 4 | 610 | X | - | - | - |
| 21 | CLA | 4 | 611 | X | - | - | - |
| 21 | CLA | 4 | 612 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 4 | 613 | X | - | - | - |
| 21 | CLA | 5 | 602 | X | - | - | - |
| 21 | CLA | 5 | 603 | X | - | - | - |
| 21 | CLA | 5 | 604 | X | - | - | - |
| 21 | CLA | 5 | 605 | X | - | - | - |
| 21 | CLA | 5 | 607 | X | - | - | - |
| 21 | CLA | 5 | 608 | 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 | 6 | 603 | X | - | - | - |
| 21 | CLA | 6 | 604 | X | - | - | - |
| 21 | CLA | 6 | 608 | X | - | - | - |
| 21 | CLA | 6 | 609 | X | - | - | - |
| 21 | CLA | 6 | 610 | X | - | - | - |
| 21 | CLA | 6 | 611 | X | - | - | - |
| 21 | CLA | 6 | 612 | X | - | - | - |
| 21 | CLA | 6 | 613 | X | - | - | - |
| 21 | CLA | 7 | 401 | X | - | - | - |
| 21 | CLA | 7 | 402 | X | - | - | - |
| 21 | CLA | 7 | 403 | X | - | - | - |
| 21 | CLA | 7 | 404 | X | - | - | - |
| 21 | CLA | 7 | 405 | X | - | - | - |
| 21 | CLA | 7 | 408 | X | - | - | - |
| 21 | CLA | 7 | 409 | X | - | - | - |
| 21 | CLA | 7 | 410 | X | - | - | - |
| 21 | CLA | 7 | 411 | X | - | - | - |
| 21 | CLA | 7 | 412 | X | - | - | - |
| 21 | CLA | 7 | 413 | X | - | - | - |
| 21 | CLA | 7 | 414 | X | - | - | - |
| 21 | CLA | 8 | 601 | X | - | - | - |
| 21 | CLA | 8 | 602 | X | - | - | - |
| 21 | CLA | 8 | 603 | X | - | - | - |
| 21 | CLA | 8 | 604 | X | - | - | - |
| 21 | CLA | 8 | 608 | X | - | - | - |
| 21 | CLA | 8 | 609 | X | - | X | - |
| 21 | CLA | 8 | 610 | X | - | - | - |
| 21 | CLA | 8 | 611 | X | - | - | - |
| 21 | CLA | 8 | 612 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 8 | 618 | X | - | - | - |
| 21 | CLA | 9 | 602 | X | - | - | - |
| 21 | CLA | 9 | 603 | X | - | - | - |
| 21 | CLA | 9 | 604 | X | - | - | - |
| 21 | CLA | 9 | 610 | X | - | - | - |
| 21 | CLA | 9 | 611 | X | - | - | - |
| 21 | CLA | 9 | 612 | X | - | - | - |
| 21 | CLA | 9 | 613 | X | - | - | - |
| 21 | CLA | A | 802 | X | - | - | - |
| 21 | CLA | A | 803 | X | - | - | - |
| 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 | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 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 | 852 | X | - | - | - |
| 21 | CLA | B | 801 | 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 | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 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 | F | 302 | X | - | - | - |
| 21 | CLA | F | 304 | X | - | - | - |
| 21 | CLA | F | 305 | X | - | - | - |
| 21 | CLA | G | 202 | X | - | - | - |
| 21 | CLA | G | 203 | X | - | - | - |
| 21 | CLA | G | 204 | X | - | - | - |
| 21 | CLA | H | 201 | X | - | - | - |
| 21 | CLA | J | 102 | X | - | - | - |
| 21 | CLA | K | 201 | X | - | - | - |
| 21 | CLA | K | 202 | X | - | - | - |
| 21 | CLA | K | 203 | X | - | - | - |
| 21 | CLA | K | 204 | X | - | - | - |
| 21 | CLA | L | 302 | X | - | - | - |
| 21 | CLA | L | 303 | X | - | - | - |
| 21 | CLA | L | 304 | X | - | - | - |
| 21 | CLA | O | 201 | X | - | - | - |
| 21 | CLA | O | 202 | X | - | - | - |
| 21 | CLA | O | 203 | X | - | - | - |
| 21 | CLA | O | 204 | X | - | - | - |
| 21 | CLA | a | 602 | X | - | - | - |
| 21 | CLA | a | 603 | X | - | - | - |
| 21 | CLA | a | 604 | X | - | - | - |
| 21 | CLA | a | 610 | X | - | - | - |
| 21 | CLA | a | 611 | X | - | - | - |
| 21 | CLA | a | 612 | X | - | - | - |
| 21 | CLA | a | 613 | X | - | - | - |
| 21 | CLA | a | 614 | X | - | - | - |
| 21 | CLA | b | 303 | X | - | - | - |
| 21 | CLA | b | 304 | X | - | - | - |
| 21 | CLA | b | 305 | X | - | - | - |
| 21 | CLA | b | 311 | X | - | - | - |
| 21 | CLA | b | 312 | X | - | - | - |
| 21 | CLA | b | 313 | X | - | - | - |
| 21 | CLA | b | 314 | X | - | - | - |
| 21 | CLA | b | 315 | X | - | - | - |
| 21 | CLA | c | 602 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | c | 603 | X | - | - | - |
| 21 | CLA | c | 604 | X | - | - | - |
| 21 | CLA | c | 610 | X | - | - | - |
| 21 | CLA | c | 611 | X | - | - | - |
| 21 | CLA | c | 612 | X | - | - | - |
| 21 | CLA | c | 613 | X | - | - | - |
| 21 | CLA | c | 614 | X | - | - | - |
| 24 | BCR | K | 205 | - | - | X | - |
| 29 | CHL | 1 | 302 | X | - | - | - |
| 29 | CHL | 1 | 307 | X | - | - | - |
| 29 | CHL | 2 | 601 | X | - | - | - |
| 29 | CHL | 2 | 602 | X | - | - | - |
| 29 | CHL | 2 | 605 | X | - | - | - |
| 29 | CHL | 2 | 606 | X | - | - | - |
| 29 | CHL | 2 | 607 | X | - | - | - |
| 29 | CHL | 2 | 614 | X | - | - | - |
| 29 | CHL | 3 | 407 | X | - | - | - |
| 29 | CHL | 4 | 605 | X | - | - | - |
| 29 | CHL | 4 | 606 | X | - | - | - |
| 29 | CHL | 4 | 607 | X | - | - | - |
| 29 | CHL | 4 | 614 | X | - | - | - |
| 29 | CHL | 5 | 601 | X | - | - | - |
| 29 | CHL | 5 | 606 | X | - | - | - |
| 29 | CHL | 6 | 601 | X | - | - | - |
| 29 | CHL | 6 | 602 | X | - | - | - |
| 29 | CHL | 6 | 605 | X | - | - | - |
| 29 | CHL | 6 | 606 | X | - | - | - |
| 29 | CHL | 6 | 607 | X | - | - | - |
| 29 | CHL | 6 | 614 | X | - | - | - |
| 29 | CHL | 7 | 406 | X | - | - | - |
| 29 | CHL | 8 | 605 | X | - | - | - |
| 29 | CHL | 8 | 606 | X | - | - | - |
| 29 | CHL | 8 | 607 | X | - | - | - |
| 29 | CHL | 8 | 613 | X | - | - | - |
| 29 | CHL | 9 | 601 | X | - | - | - |
| 29 | CHL | 9 | 605 | X | - | - | - |
| 29 | CHL | 9 | 606 | X | - | - | - |
| 29 | CHL | 9 | 607 | X | - | - | - |
| 29 | CHL | 9 | 608 | X | - | - | - |
| 29 | CHL | 9 | 609 | X | - | - | - |
| 29 | CHL | a | 601 | X | - | - | - |
| 29 | CHL | a | 605 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 29 | CHL | a | 606 | X | - | - | - |
| 29 | CHL | a | 607 | X | - | - | - |
| 29 | CHL | a | 608 | X | - | - | - |
| 29 | CHL | a | 609 | X | - | - | - |
| 29 | CHL | b | 302 | X | - | - | - |
| 29 | CHL | b | 306 | X | - | - | - |
| 29 | CHL | b | 307 | X | - | - | - |
| 29 | CHL | b | 308 | X | - | - | - |
| 29 | CHL | b | 309 | X | - | - | - |
| 29 | CHL | b | 310 | X | - | - | - |
| 29 | CHL | c | 601 | X | - | - | - |
| 29 | CHL | c | 605 | X | - | - | - |
| 29 | CHL | c | 606 | X | - | - | - |
| 29 | CHL | c | 607 | X | - | - | - |
| 29 | CHL | c | 608 | X | - | - | - |
| 29 | CHL | c | 609 | X | - | - | - |

# 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 56417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 742 | Total | C | N | O | S | 0 | 0 |
| | | | 5836 | 3827 | 993 | 997 | 19 | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 595 | 365 | 103 | 116 | 11 | | |

- Molecule 4 is a protein called Predicted protein PsaD.

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

- Molecule 5 is a protein called PsaE.

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

- Molecule 6 is a protein called PSI-F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1230 | 796 | 210 | 221 | 3 | | |

- Molecule 7 is a protein called PSI-G.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 476 | 125 | 138 | 1 | | |

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

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

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

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

- Molecule 11 is a protein called PsaK.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 566 | 356 | 98 | 109 | 3 | | |

- Molecule 12 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1229 | 808 | 197 | 222 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 238 | 155 | 38 | 44 | 1 | | |

- Molecule 14 is a protein called PsaO.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | O | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 702 | 472 | 115 | 114 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | 1 | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1478 | 965 | 247 | 265 | 1 | | |
| 15 | 5 | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1475 | 962 | 247 | 265 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | 2 | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1632 | 1062 | 274 | 292 | 4 | | |
| 16 | 6 | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1587 | 1035 | 265 | 283 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 3 | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1670 | 1094 | 269 | 300 | 7 | | |
| 17 | 7 | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1644 | 1076 | 265 | 296 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | 4 | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1592 | 1033 | 266 | 288 | 5 | | |
| 18 | 8 | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1585 | 1029 | 265 | 286 | 5 | | |

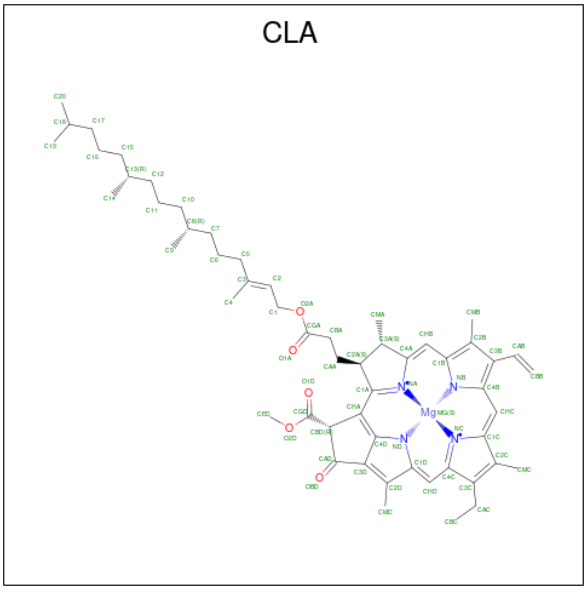
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | 9 | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1747 | 1139 | 287 | 312 | 9 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | a | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1651 | 1069 | 268 | 309 | 5 | | |
| 20 | b | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1651 | 1069 | 268 | 309 | 5 | | |
| 20 | c | 227 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1727 | 1110 | 284 | 327 | 1 | 5 | | |

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 64 | 54 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 63 | 53 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 35 | 1 | 4 | 3 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 64 | 54 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | F | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 21 | F | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | F | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 21 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | J | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 36 | 1 | 4 | 5 | |
| 21 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 30 | 1 | 4 | 3 | |
| 21 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 42 | 1 | 4 | 3 | |
| 21 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 33 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 30 | 1 | 4 | 3 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 30 | 1 | 4 | 3 | |
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 33 | 1 | 4 | 5 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 42 | 1 | 4 | 4 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 32 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 35 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 36 | 30 | 1 | 4 | 1 | |
| 21 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 35 | 1 | 4 | 3 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 49 | 39 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 33 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 30 | 1 | 4 | 3 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 38 | 30 | 1 | 4 | 3 | |
| 21 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 33 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 32 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 35 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 36 | 30 | 1 | 4 | 1 | |
| 21 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 45 | 1 | 4 | 4 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 35 | 1 | 4 | 3 | |
| 21 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |

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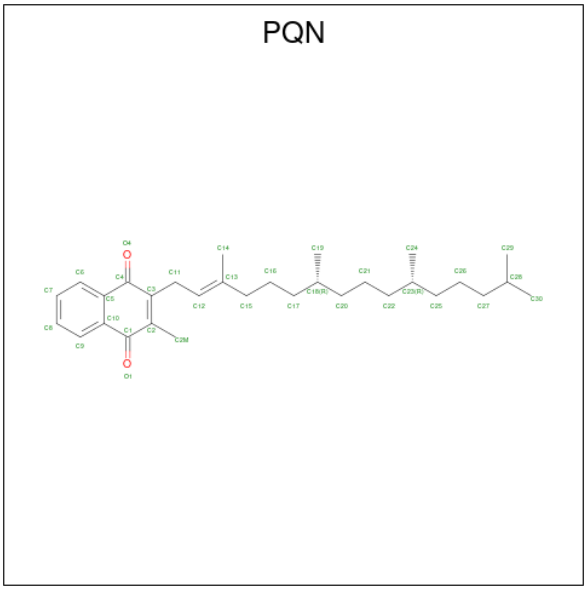
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 21 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 33 | 1 | 4 | 3 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 59 | 49 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 21 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 35 | 1 | 4 | 4 | |

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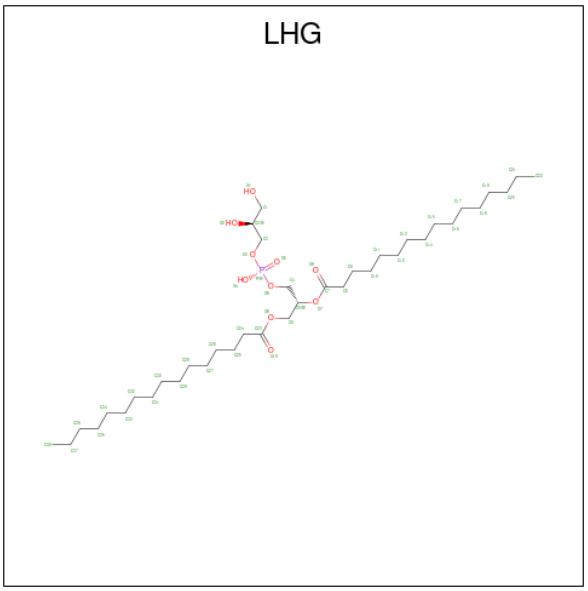
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 21 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 22 | A | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 22 | B | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



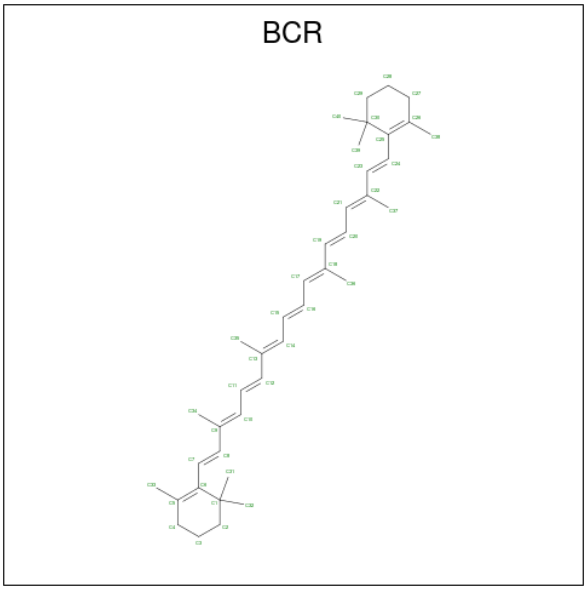

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 23 | A | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 23 | A | 1 | Total | C | O | P | 0 |
| | | | 27 | 16 | 10 | 1 | |
| 23 | A | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 23 | 1 | 1 | Total | C | O | P | 0 |
| | | | 23 | 12 | 10 | 1 | |
| 23 | 1 | 1 | Total | C | O | P | 0 |
| | | | 28 | 17 | 10 | 1 | |
| 23 | 2 | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 23 | 4 | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 23 | 4 | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 23 | 5 | 1 | Total | C | O | P | 0 |
| | | | 28 | 17 | 10 | 1 | |
| 23 | 6 | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 23 | 8 | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 23 | 9 | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 23 | a | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 23 | b | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 23 | c | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).




| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 24 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | A | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | B | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | B | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | B | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 24 | B | 1 | Total | C | 0 |
| | | | 40 | 40 | |

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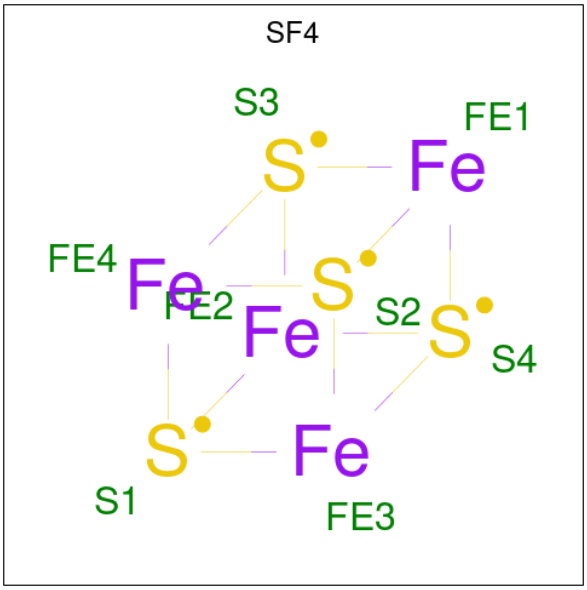
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 24 | B | 1 | Total C<br>40 40 | 0 |
| 24 | F | 1 | Total C<br>40 40 | 0 |
| 24 | F | 1 | Total C<br>40 40 | 0 |
| 24 | G | 1 | Total C<br>40 40 | 0 |
| 24 | G | 1 | Total C<br>40 40 | 0 |
| 24 | I | 1 | Total C<br>40 40 | 0 |
| 24 | J | 1 | Total C<br>40 40 | 0 |
| 24 | J | 1 | Total C<br>40 40 | 0 |
| 24 | J | 1 | Total C<br>40 40 | 0 |
| 24 | K | 1 | Total C<br>40 40 | 0 |
| 24 | L | 1 | Total C<br>40 40 | 0 |
| 24 | L | 1 | Total C<br>40 40 | 0 |
| 24 | L | 1 | Total C<br>40 40 | 0 |
| 24 | M | 1 | Total C<br>40 40 | 0 |
| 24 | O | 1 | Total C<br>40 40 | 0 |
| 24 | 2 | 1 | Total C<br>40 40 | 0 |
| 24 | 3 | 1 | Total C<br>40 40 | 0 |
| 24 | 3 | 1 | Total C<br>40 40 | 0 |
| 24 | 4 | 1 | Total C<br>40 40 | 0 |
| 24 | 6 | 1 | Total C<br>40 40 | 0 |
| 24 | 7 | 1 | Total C<br>40 40 | 0 |

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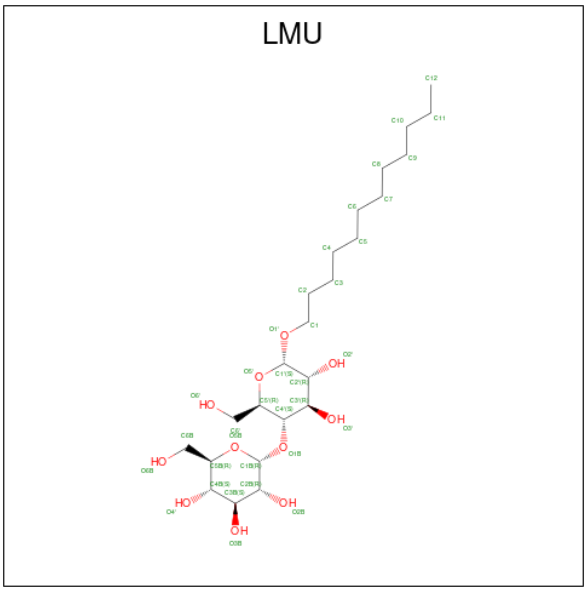
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 24 | 7 | 1 | Total C<br>40 40 | 0 |
| 24 | 8 | 1 | Total C<br>40 40 | 0 |

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: $Fe_4S_4$).



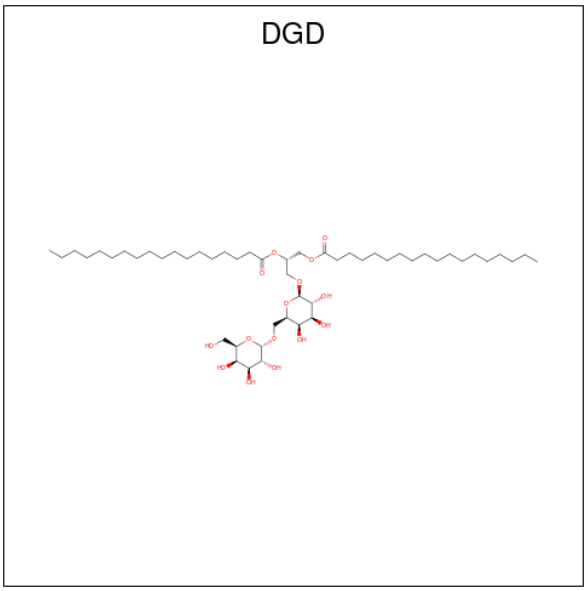

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 25 | A | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | C | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | C | 1 | Total Fe S<br>8 4 4 | 0 |

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



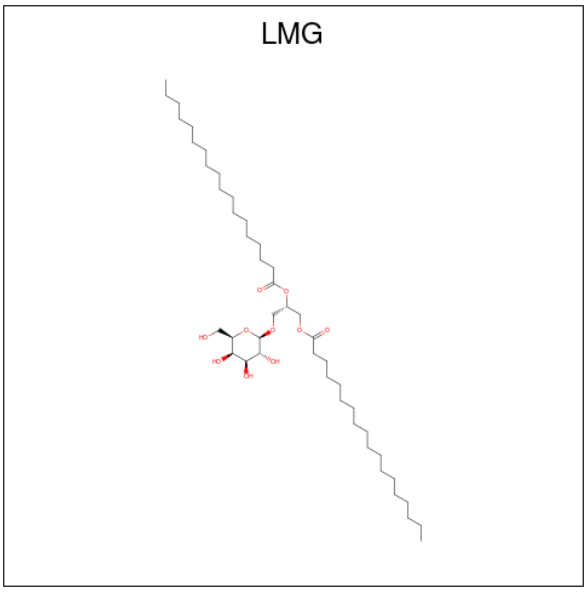

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 26 | A | 1 | Total C O<br>35 24 11 | 0 |
| 26 | A | 1 | Total C O<br>35 24 11 | 0 |
| 26 | O | 1 | Total C O<br>35 24 11 | 0 |
| 26 | 3 | 1 | Total C O<br>35 24 11 | 0 |
| 26 | b | 1 | Total C O<br>35 24 11 | 0 |

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




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

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



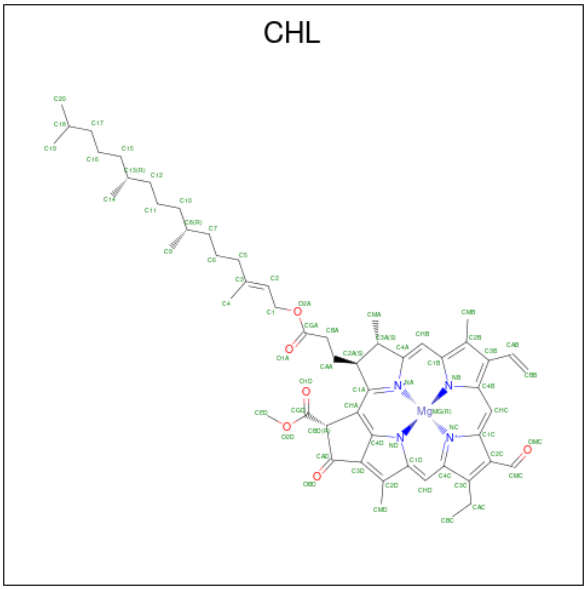

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 28 | G | 1 | Total | C | O | 0 |
| | | | 55 | 45 | 10 | |
| 28 | J | 1 | Total | C | O | 0 |
| | | | 30 | 20 | 10 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 28 | 2 | 1 | Total C O<br>13 7 6 | 0 |
| 28 | 6 | 1 | Total C O<br>13 7 6 | 0 |

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




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 29 | 1 | 1 | Total C Mg N O<br>51 40 1 4 6 | 0 |
| 29 | 1 | 1 | Total C Mg N O<br>51 40 1 4 6 | 0 |
| 29 | 2 | 1 | Total C Mg N O<br>53 42 1 4 6 | 0 |
| 29 | 2 | 1 | Total C Mg N O<br>53 42 1 4 6 | 0 |
| 29 | 2 | 1 | Total C Mg N O<br>46 35 1 4 6 | 0 |
| 29 | 2 | 1 | Total C Mg N O<br>46 35 1 4 6 | 0 |
| 29 | 2 | 1 | Total C Mg N O<br>51 40 1 4 6 | 0 |
| 29 | 2 | 1 | Total C Mg N O<br>46 35 1 4 6 | 0 |
| 29 | 3 | 1 | Total C Mg N O<br>40 32 1 4 3 | 0 |

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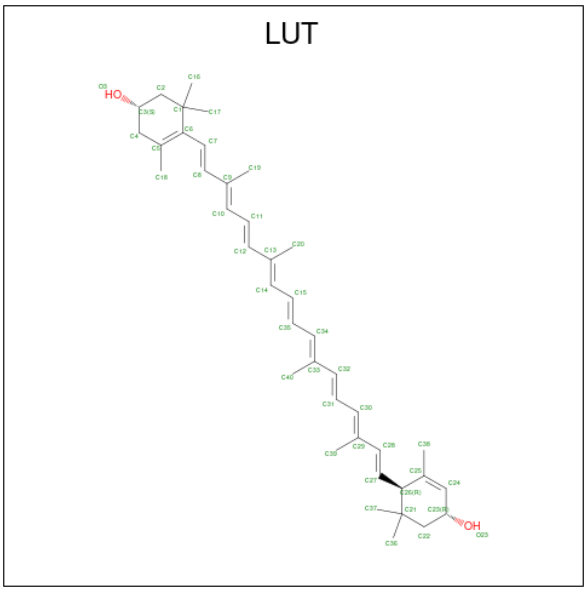
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |
| 29 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 34 | 1 | 4 | 5 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 42 | 1 | 4 | 6 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 40 | 32 | 1 | 4 | 3 | |
| 29 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 41 | 32 | 1 | 4 | 4 | |
| 29 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 40 | 1 | 4 | 6 | |
| 29 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 33 | 1 | 4 | 4 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 34 | 1 | 4 | 6 | |
| 29 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 29 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 42 | 1 | 4 | 6 | |
| 29 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 49 | 38 | 1 | 4 | 6 | |
| 29 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 41 | 1 | 4 | 6 | |
| 29 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 49 | 38 | 1 | 4 | 6 | |
| 29 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 29 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 46 | 35 | 1 | 4 | 6 | |
| 29 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 44 | 33 | 1 | 4 | 6 | |

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



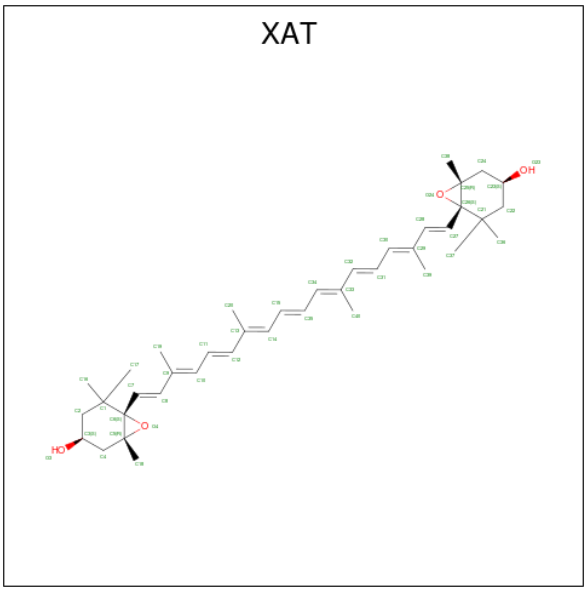

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 30 | 1 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 2 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 3 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 4 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 5 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 6 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 7 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 8 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 9 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | 9 | 1 | Total C O<br>42 40 2 | 0 |
| 30 | a | 1 | Total C O<br>42 40 2 | 0 |
| 30 | a | 1 | Total C O<br>42 40 2 | 0 |
| 30 | b | 1 | Total C O<br>42 40 2 | 0 |
| 30 | b | 1 | Total C O<br>42 40 2 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 30 | c | 1 | Total C O<br>42 40 2 | 0 |
| 30 | c | 1 | Total C O<br>42 40 2 | 0 |

- 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: $C_{40}H_{56}O_4$).



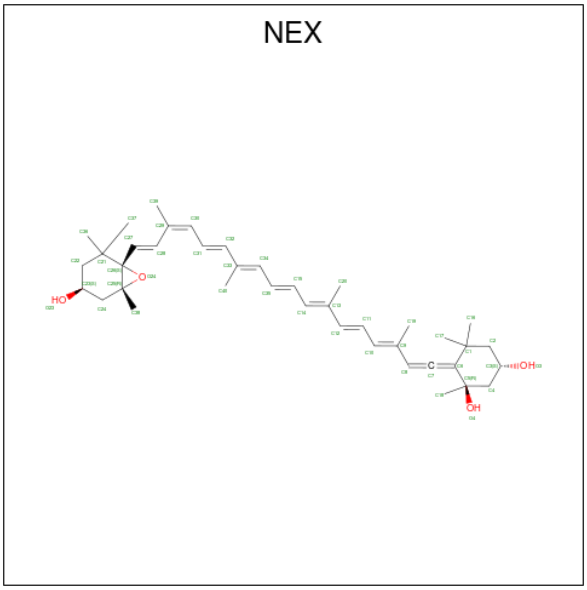

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 31 | 1 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 2 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 3 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 4 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 5 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 6 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 7 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 8 | 1 | Total C O<br>44 40 4 | 0 |
| 31 | 9 | 1 | Total C O<br>44 40 4 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 31 | a | 1 | Total C O<br>44 40 4 | 0 |
| 31 | c | 1 | Total C O<br>44 40 4 | 0 |

- 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: $C_{40}H_{56}O_4$).



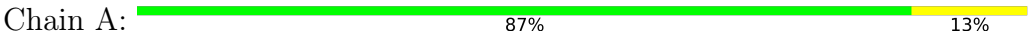

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 32 | 9 | 1 | Total C O<br>44 40 4 | 0 |
| 32 | b | 1 | Total C O<br>44 40 4 | 0 |
| 32 | c | 1 | Total C O<br>44 40 4 | 0 |

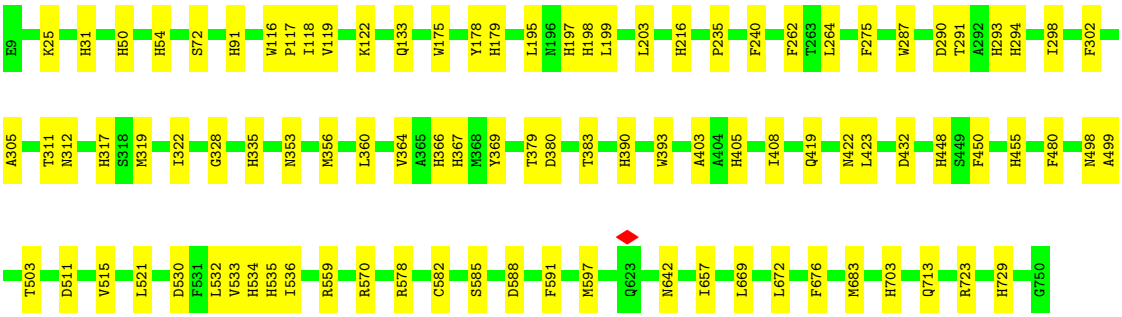
# 3 Residue-property plots (i)

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

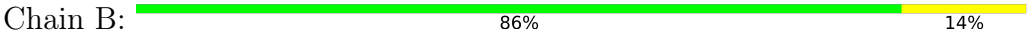
Chain A:

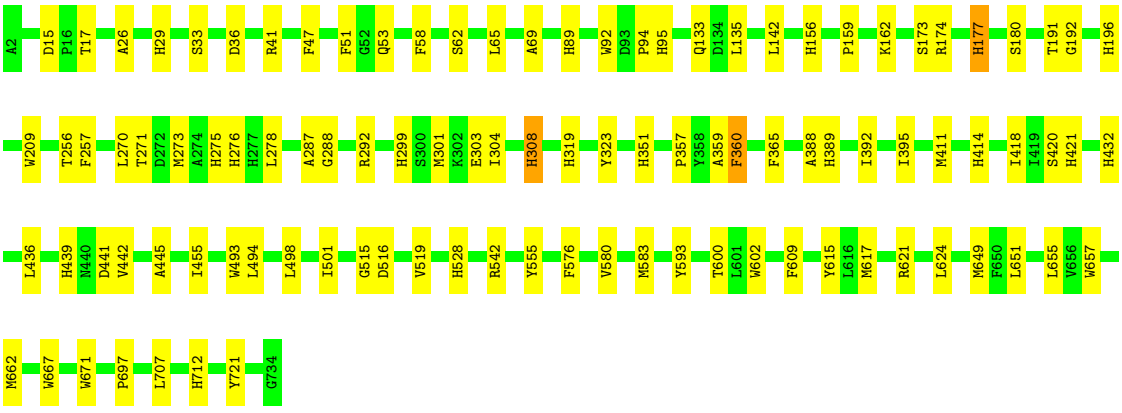



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

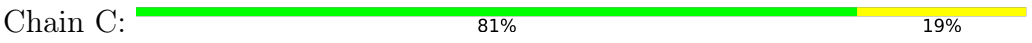
Chain B:

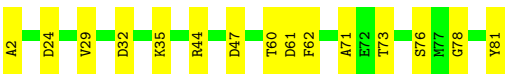



• Molecule 3: Photosystem I iron-sulfur center

Chain C:

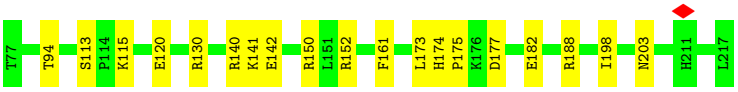


• Molecule 4: Predicted protein PsaD

Chain D:

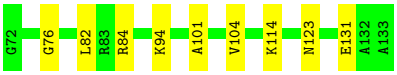



• Molecule 5: PsaE

Chain E:




• Molecule 6: PSI-F

Chain F:



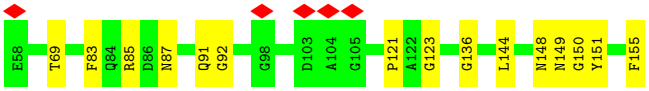




• Molecule 7: PSI-G

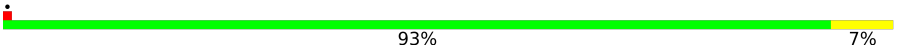
Chain G:




• Molecule 8: PsaH photosystem I reaction center subunit

Chain H:



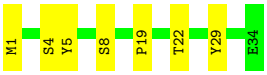




• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:

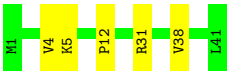



• Molecule 10: Photosystem I reaction center subunit IX

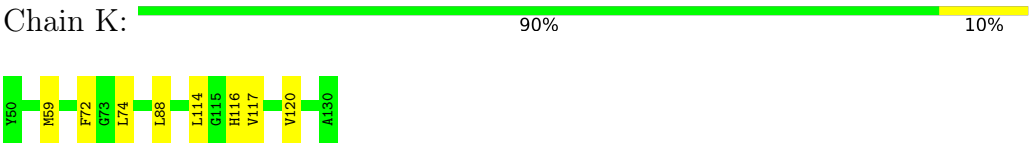
Chain J:



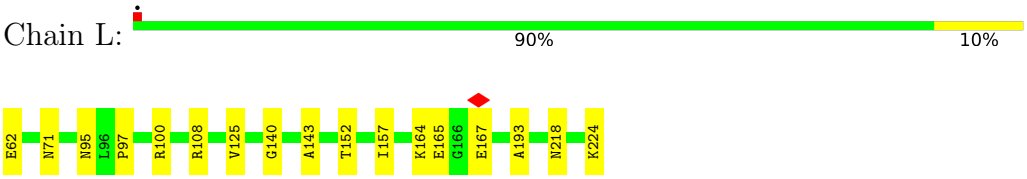
• Molecule 11: PsaK

Chain K:



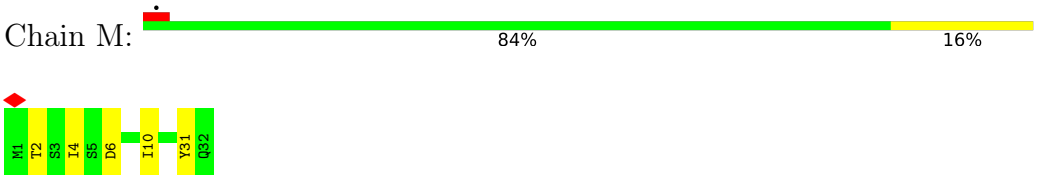

• Molecule 12: PSI subunit V

Chain L:



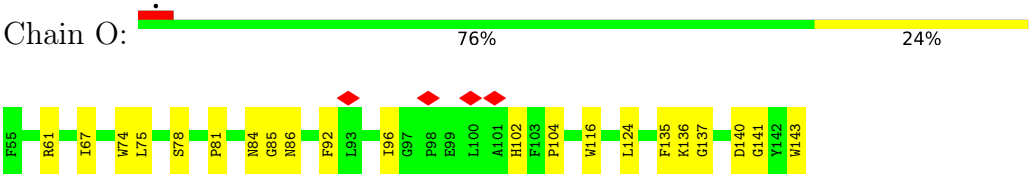

• Molecule 13: Photosystem I reaction center subunit XII

Chain M:



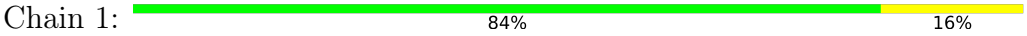

• Molecule 14: PsaO

Chain O:




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

Chain 1:



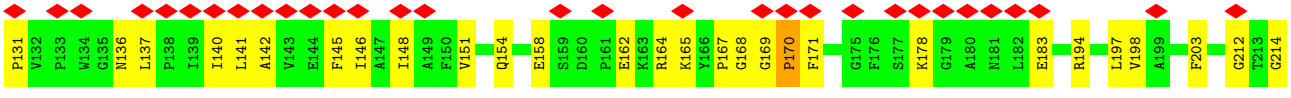

• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

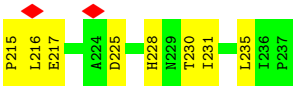
Chain 5:





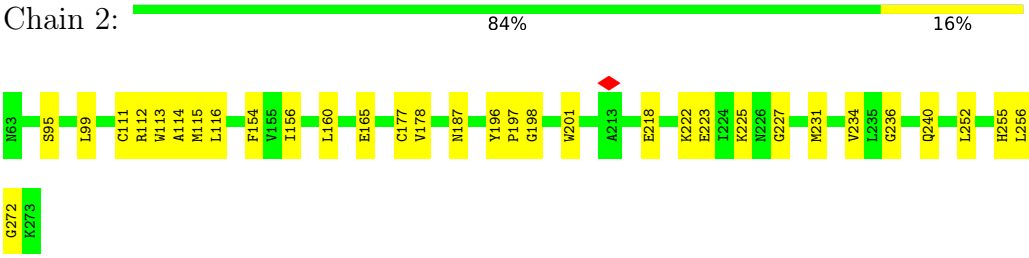




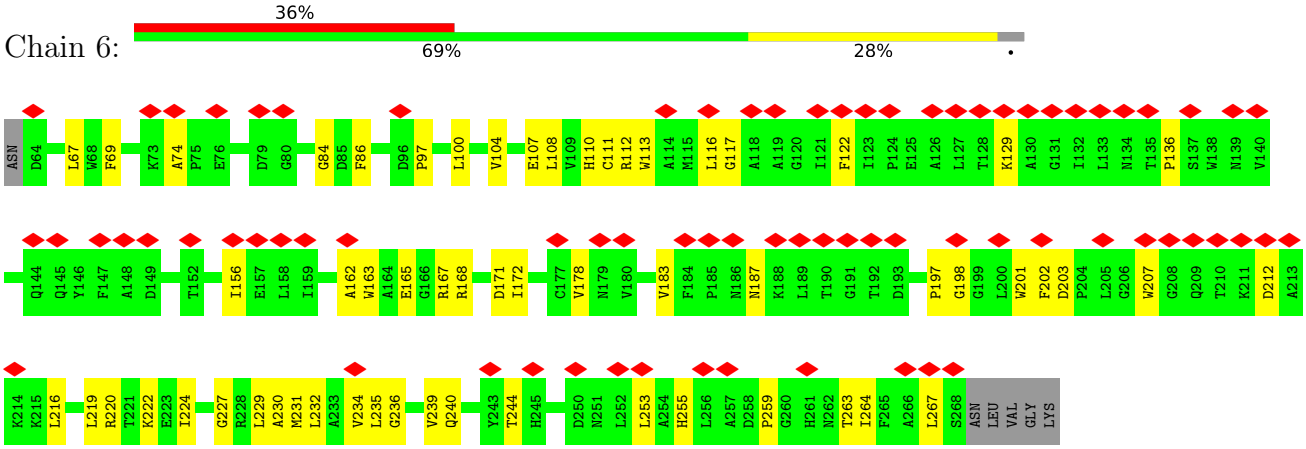
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



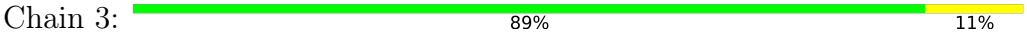

• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



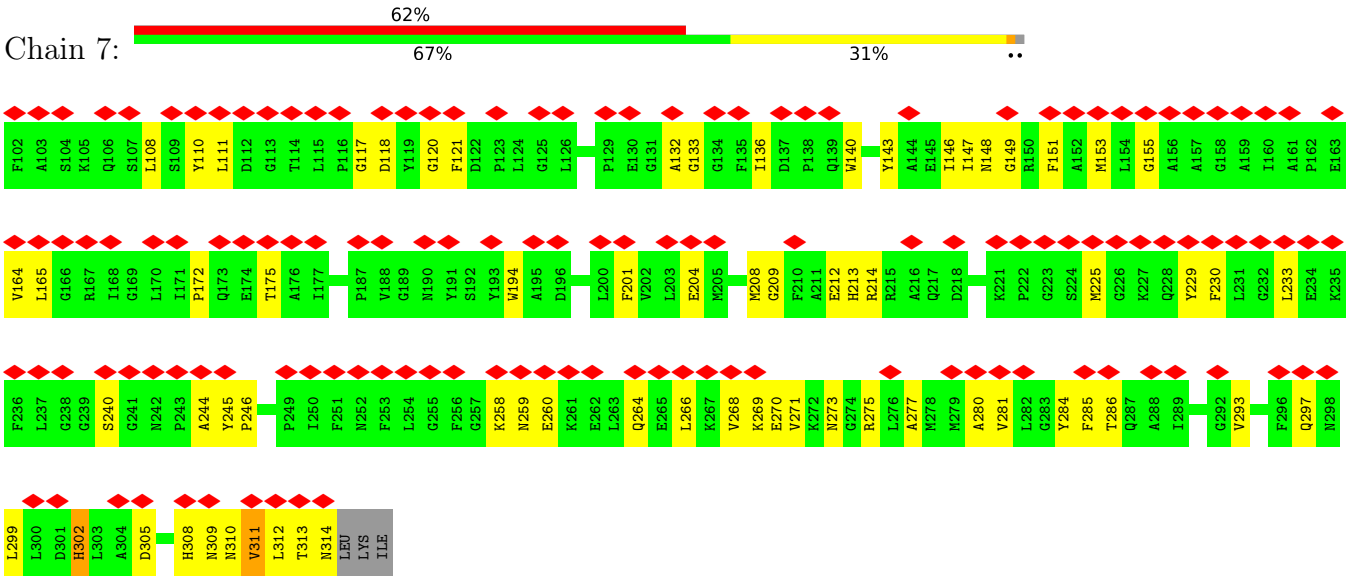

• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



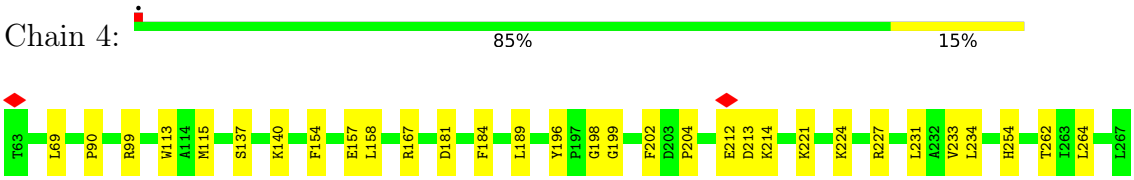

• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



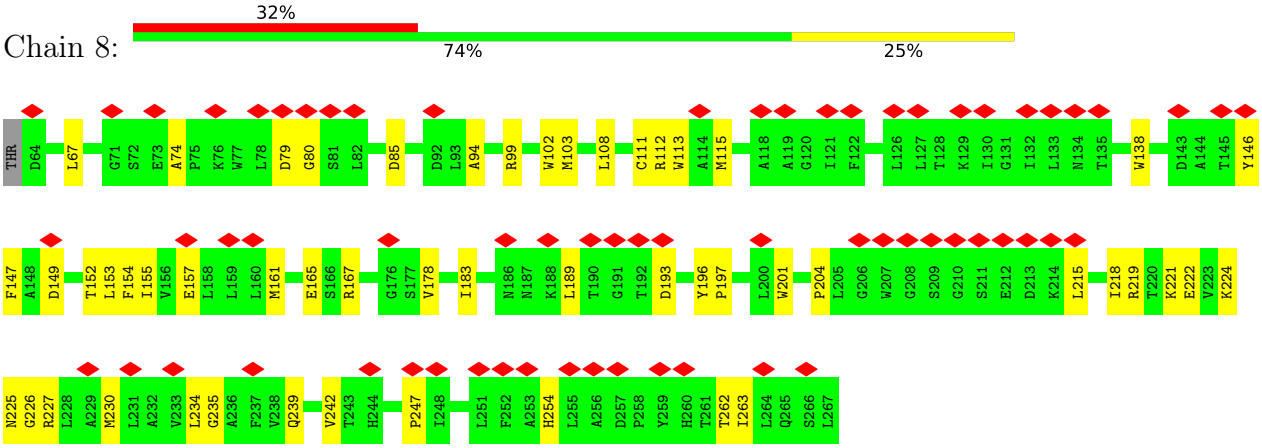
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



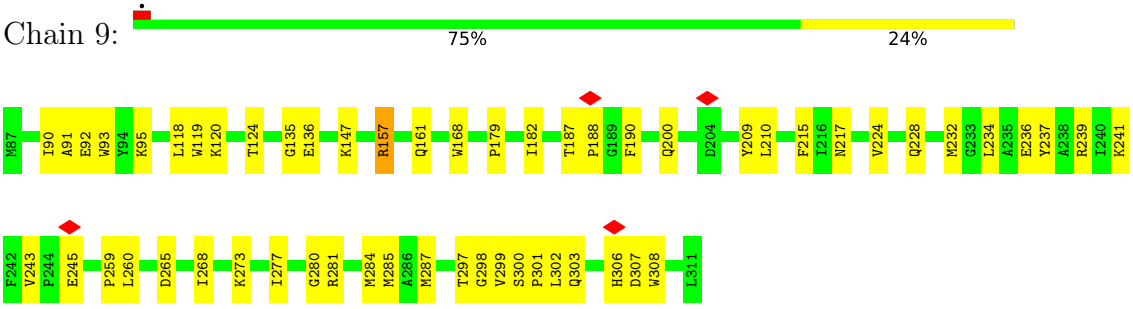

• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



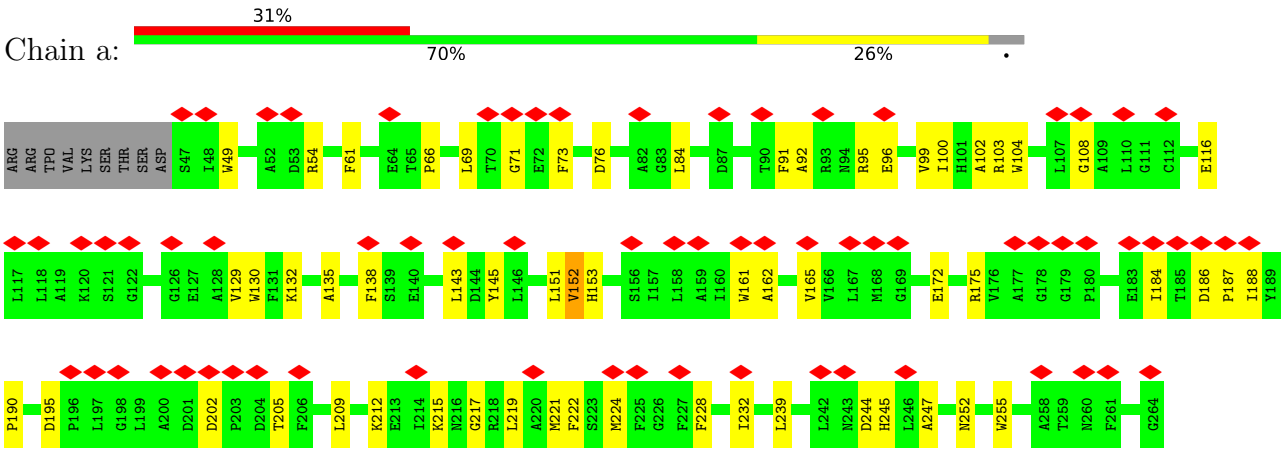

• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 9:



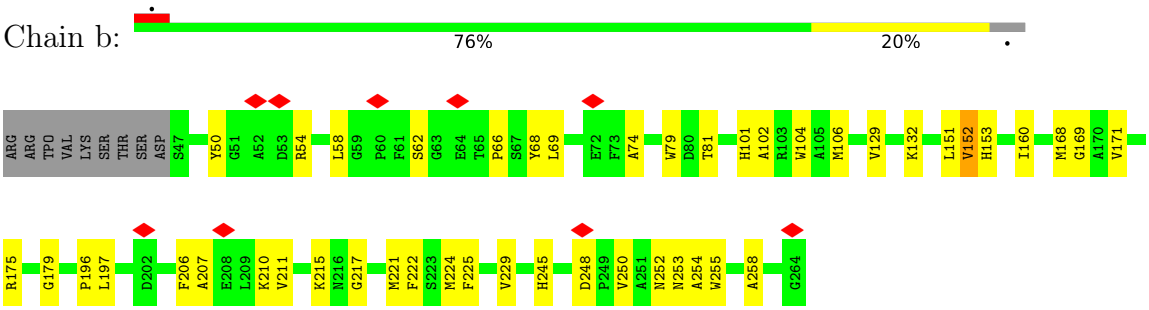

• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain a:



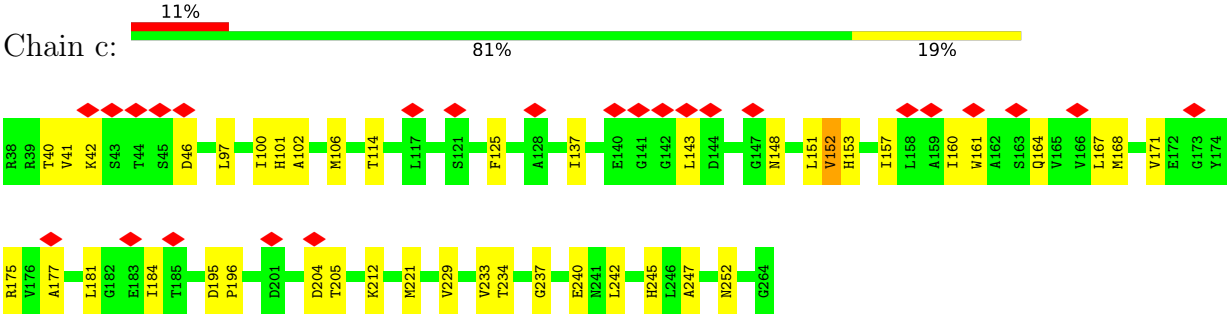

• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain b:




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

Chain c:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 83777 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 78 | Depositor |
| Minimum defocus (nm) | 1600 | Depositor |
| Maximum defocus (nm) | 1900 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 4.400 | Depositor |
| Minimum map value | -1.758 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.105 | Depositor |
| Recommended contour level | 0.45 | Depositor |
| Map size (Å) | 486.72003, 486.72003, 486.72003 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.014, 1.014, 1.014 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.18 | 0/6031 | 0.33 | 0/8227 |
| 2 | B | 0.26 | 2/6063 (0.0%) | 0.38 | 1/8274 (0.0%) |
| 3 | C | 0.19 | 0/605 | 0.41 | 0/821 |
| 4 | D | 0.13 | 0/1132 | 0.38 | 1/1532 (0.1%) |
| 5 | E | 0.12 | 0/498 | 0.23 | 0/677 |
| 6 | F | 0.15 | 0/1255 | 0.29 | 0/1696 |
| 7 | G | 0.20 | 0/767 | 0.38 | 0/1046 |
| 8 | H | 0.12 | 0/758 | 0.26 | 0/1022 |
| 9 | I | 0.15 | 0/273 | 0.37 | 0/373 |
| 10 | J | 0.14 | 0/334 | 0.25 | 0/457 |
| 11 | K | 0.13 | 0/572 | 0.23 | 0/773 |
| 12 | L | 0.14 | 0/1264 | 0.28 | 0/1727 |
| 13 | M | 0.24 | 0/239 | 0.26 | 0/322 |
| 14 | O | 0.17 | 0/729 | 0.37 | 0/997 |
| 15 | 1 | 0.20 | 0/1527 | 0.34 | 0/2088 |
| 15 | 5 | 0.18 | 0/1524 | 0.43 | 1/2084 (0.0%) |
| 16 | 2 | 0.22 | 0/1683 | 0.41 | 0/2300 |
| 16 | 6 | 0.13 | 0/1638 | 0.31 | 0/2241 |
| 17 | 3 | 0.21 | 0/1721 | 0.40 | 0/2335 |
| 17 | 7 | 0.18 | 0/1695 | 0.39 | 0/2302 |
| 18 | 4 | 0.15 | 0/1641 | 0.29 | 0/2244 |
| 18 | 8 | 0.16 | 0/1634 | 0.31 | 0/2234 |
| 19 | 9 | 0.26 | 1/1801 (0.1%) | 0.43 | 0/2451 |
| 20 | a | 0.18 | 0/1700 | 0.37 | 0/2316 |
| 20 | b | 0.15 | 0/1700 | 0.31 | 0/2316 |
| 20 | c | 0.14 | 0/1764 | 0.35 | 0/2399 |
| All | All | 0.19 | 3/40548 (0.0%) | 0.35 | 3/55254 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | 9 | 157 | ARG | C-O | -6.48 | 1.16 | 1.24 |
| 2 | B | 177 | HIS | CA-C | -5.34 | 1.46 | 1.52 |
| 2 | B | 308 | HIS | CA-C | -5.26 | 1.45 | 1.52 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 360 | PHE | CB-CA-C | 9.86 | 119.59 | 109.83 |
| 4 | D | 173 | LEU | N-CA-C | 5.43 | 120.41 | 113.18 |
| 15 | 5 | 171 | PHE | N-CA-C | -5.28 | 106.17 | 113.18 |

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 | 5836 | 0 | 5725 | 105 | 0 |
| 2 | B | 5849 | 0 | 5623 | 116 | 0 |
| 3 | C | 595 | 0 | 573 | 12 | 0 |
| 4 | D | 1104 | 0 | 1112 | 16 | 0 |
| 5 | E | 487 | 0 | 480 | 8 | 0 |
| 6 | F | 1230 | 0 | 1282 | 14 | 0 |
| 7 | G | 749 | 0 | 729 | 12 | 0 |
| 8 | H | 740 | 0 | 727 | 7 | 0 |
| 9 | I | 266 | 0 | 274 | 4 | 0 |
| 10 | J | 325 | 0 | 341 | 5 | 0 |
| 11 | K | 566 | 0 | 587 | 8 | 0 |
| 12 | L | 1229 | 0 | 1242 | 13 | 0 |
| 13 | M | 238 | 0 | 263 | 3 | 0 |
| 14 | O | 702 | 0 | 697 | 12 | 0 |
| 15 | 1 | 1478 | 0 | 1455 | 27 | 0 |
| 15 | 5 | 1475 | 0 | 1447 | 51 | 0 |
| 16 | 2 | 1632 | 0 | 1603 | 34 | 0 |
| 16 | 6 | 1587 | 0 | 1556 | 57 | 0 |
| 17 | 3 | 1670 | 0 | 1633 | 21 | 0 |
| 17 | 7 | 1644 | 0 | 1599 | 65 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 18 | 4 | 1592 | 0 | 1561 | 31 | 0 |
| 18 | 8 | 1585 | 0 | 1555 | 63 | 0 |
| 19 | 9 | 1747 | 0 | 1721 | 44 | 0 |
| 20 | a | 1651 | 0 | 1586 | 61 | 0 |
| 20 | b | 1651 | 0 | 1585 | 46 | 0 |
| 20 | c | 1727 | 0 | 1661 | 49 | 0 |
| 21 | 1 | 587 | 0 | 420 | 22 | 0 |
| 21 | 2 | 366 | 0 | 281 | 33 | 0 |
| 21 | 3 | 642 | 0 | 487 | 37 | 0 |
| 21 | 4 | 472 | 0 | 362 | 27 | 0 |
| 21 | 5 | 531 | 0 | 369 | 24 | 0 |
| 21 | 6 | 347 | 0 | 253 | 19 | 0 |
| 21 | 7 | 551 | 0 | 377 | 35 | 0 |
| 21 | 8 | 460 | 0 | 348 | 46 | 0 |
| 21 | 9 | 352 | 0 | 290 | 12 | 0 |
| 21 | A | 2422 | 0 | 2311 | 116 | 0 |
| 21 | B | 2312 | 0 | 2267 | 108 | 0 |
| 21 | F | 147 | 0 | 123 | 3 | 0 |
| 21 | G | 139 | 0 | 102 | 3 | 0 |
| 21 | H | 45 | 0 | 33 | 2 | 0 |
| 21 | J | 42 | 0 | 31 | 0 | 0 |
| 21 | K | 185 | 0 | 135 | 16 | 0 |
| 21 | L | 132 | 0 | 97 | 3 | 0 |
| 21 | O | 170 | 0 | 116 | 2 | 0 |
| 21 | a | 383 | 0 | 304 | 20 | 0 |
| 21 | b | 391 | 0 | 316 | 20 | 0 |
| 21 | c | 417 | 0 | 367 | 18 | 0 |
| 22 | A | 33 | 0 | 46 | 0 | 0 |
| 22 | B | 33 | 0 | 46 | 3 | 0 |
| 23 | 1 | 51 | 0 | 42 | 0 | 0 |
| 23 | 2 | 35 | 0 | 40 | 1 | 0 |
| 23 | 4 | 86 | 0 | 118 | 6 | 0 |
| 23 | 5 | 28 | 0 | 26 | 1 | 0 |
| 23 | 6 | 35 | 0 | 40 | 3 | 0 |
| 23 | 8 | 37 | 0 | 44 | 3 | 0 |
| 23 | 9 | 49 | 0 | 74 | 4 | 0 |
| 23 | A | 125 | 0 | 172 | 8 | 0 |
| 23 | a | 49 | 0 | 74 | 2 | 0 |
| 23 | b | 49 | 0 | 74 | 9 | 0 |
| 23 | c | 49 | 0 | 74 | 2 | 0 |
| 24 | 2 | 40 | 0 | 56 | 6 | 0 |
| 24 | 3 | 80 | 0 | 112 | 7 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 24 | 4 | 40 | 0 | 56 | 0 | 0 |
| 24 | 6 | 40 | 0 | 56 | 14 | 0 |
| 24 | 7 | 80 | 0 | 112 | 10 | 0 |
| 24 | 8 | 40 | 0 | 56 | 8 | 0 |
| 24 | A | 240 | 0 | 336 | 21 | 0 |
| 24 | B | 200 | 0 | 280 | 39 | 0 |
| 24 | F | 80 | 0 | 112 | 2 | 0 |
| 24 | G | 80 | 0 | 112 | 5 | 0 |
| 24 | I | 40 | 0 | 56 | 1 | 0 |
| 24 | J | 120 | 0 | 168 | 15 | 0 |
| 24 | K | 40 | 0 | 56 | 24 | 0 |
| 24 | L | 120 | 0 | 168 | 8 | 0 |
| 24 | M | 40 | 0 | 56 | 3 | 0 |
| 24 | O | 40 | 0 | 56 | 1 | 0 |
| 25 | A | 8 | 0 | 0 | 0 | 0 |
| 25 | C | 16 | 0 | 0 | 0 | 0 |
| 26 | 3 | 35 | 0 | 46 | 3 | 0 |
| 26 | A | 70 | 0 | 92 | 2 | 0 |
| 26 | O | 35 | 0 | 46 | 4 | 0 |
| 26 | b | 35 | 0 | 46 | 4 | 0 |
| 27 | B | 66 | 0 | 96 | 7 | 0 |
| 28 | 2 | 13 | 0 | 11 | 0 | 0 |
| 28 | 6 | 13 | 0 | 11 | 1 | 0 |
| 28 | G | 55 | 0 | 86 | 2 | 0 |
| 28 | J | 30 | 0 | 30 | 0 | 0 |
| 29 | 1 | 102 | 0 | 74 | 7 | 0 |
| 29 | 2 | 295 | 0 | 212 | 15 | 0 |
| 29 | 3 | 40 | 0 | 23 | 1 | 0 |
| 29 | 4 | 180 | 0 | 116 | 6 | 0 |
| 29 | 5 | 92 | 0 | 62 | 6 | 0 |
| 29 | 6 | 286 | 0 | 196 | 17 | 0 |
| 29 | 7 | 40 | 0 | 23 | 2 | 0 |
| 29 | 8 | 180 | 0 | 116 | 15 | 0 |
| 29 | 9 | 273 | 0 | 184 | 9 | 0 |
| 29 | a | 272 | 0 | 181 | 15 | 0 |
| 29 | b | 292 | 0 | 206 | 13 | 0 |
| 29 | c | 274 | 0 | 178 | 10 | 0 |
| 30 | 1 | 42 | 0 | 56 | 2 | 0 |
| 30 | 2 | 42 | 0 | 56 | 8 | 0 |
| 30 | 3 | 42 | 0 | 56 | 12 | 0 |
| 30 | 4 | 42 | 0 | 56 | 7 | 0 |
| 30 | 5 | 42 | 0 | 56 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 30 | 6 | 42 | 0 | 56 | 6 | 0 |
| 30 | 7 | 42 | 0 | 56 | 12 | 0 |
| 30 | 8 | 42 | 0 | 56 | 5 | 0 |
| 30 | 9 | 84 | 0 | 112 | 10 | 0 |
| 30 | a | 84 | 0 | 112 | 11 | 0 |
| 30 | b | 84 | 0 | 112 | 11 | 0 |
| 30 | c | 84 | 0 | 112 | 7 | 0 |
| 31 | 1 | 44 | 0 | 56 | 2 | 0 |
| 31 | 2 | 44 | 0 | 56 | 2 | 0 |
| 31 | 3 | 44 | 0 | 56 | 4 | 0 |
| 31 | 4 | 44 | 0 | 56 | 4 | 0 |
| 31 | 5 | 44 | 0 | 56 | 5 | 0 |
| 31 | 6 | 44 | 0 | 56 | 6 | 0 |
| 31 | 7 | 44 | 0 | 56 | 5 | 0 |
| 31 | 8 | 44 | 0 | 56 | 4 | 0 |
| 31 | 9 | 44 | 0 | 56 | 2 | 0 |
| 31 | a | 44 | 0 | 56 | 6 | 0 |
| 31 | c | 44 | 0 | 56 | 3 | 0 |
| 32 | 9 | 44 | 0 | 56 | 4 | 0 |
| 32 | b | 44 | 0 | 56 | 1 | 0 |
| 32 | c | 44 | 0 | 56 | 3 | 0 |
| All | All | 56417 | 0 | 54439 | 1292 | 0 |

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

All (1292) 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) |
|---|---|---|---|
| 21:3:409:CLA:C4 | 30:3:416:LUT:H28 | 1.47 | 1.43 |
| 21:A:852:CLA:O1D | 21:B:801:CLA:H61 | 1.31 | 1.22 |
| 21:2:609:CLA:H43 | 30:2:616:LUT:H7 | 1.25 | 1.13 |
| 21:K:203:CLA:HMC2 | 24:K:205:BCR:H312 | 1.27 | 1.10 |
| 21:2:609:CLA:HBC2 | 21:2:609:CLA:HHD | 1.30 | 1.10 |
| 21:K:203:CLA:CMC | 24:K:205:BCR:H312 | 1.82 | 1.09 |
| 20:a:152:VAL:HG23 | 20:a:153:HIS:H | 1.03 | 1.08 |
| 2:B:411:MET:HE2 | 24:B:844:BCR:H403 | 1.28 | 1.07 |
| 21:3:409:CLA:H43 | 30:3:416:LUT:H28 | 1.15 | 1.06 |
| 21:2:609:CLA:CHB | 21:2:609:CLA:H11 | 1.85 | 1.06 |
| 21:3:409:CLA:C4 | 30:3:416:LUT:C28 | 2.32 | 1.06 |
| 18:8:224:LYS:HG3 | 21:8:609:CLA:CMD | 1.90 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:A:854:BCR:H353 | 24:K:205:BCR:H323 | 1.38 | 1.01 |
| 16:2:196:TYR:HD1 | 21:2:609:CLA:O1D | 1.45 | 1.00 |
| 21:K:203:CLA:HMC2 | 24:K:205:BCR:C31 | 1.92 | 0.99 |
| 21:4:609:CLA:H41 | 30:4:615:LUT:H28 | 1.39 | 0.99 |
| 20:a:143:LEU:O | 20:a:152:VAL:HG23 | 1.64 | 0.97 |
| 21:3:409:CLA:H43 | 30:3:416:LUT:C28 | 1.94 | 0.97 |
| 24:6:618:BCR:H312 | 21:8:609:CLA:HBB2 | 1.46 | 0.97 |
| 17:7:299:LEU:HD21 | 30:7:415:LUT:H163 | 1.44 | 0.96 |
| 21:A:802:CLA:HBB1 | 21:A:852:CLA:C4B | 1.97 | 0.95 |
| 21:b:311:CLA:HAB | 30:b:316:LUT:H32 | 1.50 | 0.94 |
| 21:4:609:CLA:C4 | 30:4:615:LUT:H28 | 1.97 | 0.94 |
| 18:8:224:LYS:CG | 21:8:609:CLA:HMD1 | 1.99 | 0.93 |
| 20:a:152:VAL:HG23 | 20:a:153:HIS:N | 1.85 | 0.92 |
| 18:8:224:LYS:HG3 | 21:8:609:CLA:HMD1 | 1.52 | 0.91 |
| 20:a:152:VAL:CG2 | 20:a:153:HIS:H | 1.84 | 0.90 |
| 21:K:203:CLA:CMC | 24:K:205:BCR:C31 | 2.49 | 0.90 |
| 21:1:309:CLA:HHC | 21:1:309:CLA:CBB | 1.99 | 0.90 |
| 2:B:411:MET:CE | 24:B:844:BCR:H403 | 2.03 | 0.89 |
| 24:A:854:BCR:H353 | 24:K:205:BCR:C32 | 2.03 | 0.88 |
| 21:2:609:CLA:C4 | 30:2:616:LUT:H7 | 2.04 | 0.88 |
| 1:A:390:HIS:HE1 | 21:A:828:CLA:ND | 1.71 | 0.87 |
| 20:a:172:GLU:OE1 | 20:a:175:ARG:CZ | 2.22 | 0.87 |
| 1:A:311:THR:HG22 | 1:A:312:ASN:H | 1.40 | 0.86 |
| 21:2:609:CLA:H41 | 30:2:616:LUT:H10 | 1.56 | 0.85 |
| 21:1:309:CLA:HHC | 21:1:309:CLA:HBB1 | 1.56 | 0.85 |
| 18:8:224:LYS:HG3 | 21:8:609:CLA:HMD3 | 1.58 | 0.84 |
| 20:b:221:MET:HE1 | 21:b:303:CLA:HAB | 1.59 | 0.84 |
| 21:A:852:CLA:O1D | 21:B:801:CLA:C6 | 2.24 | 0.84 |
| 16:2:196:TYR:CD1 | 21:2:609:CLA:O1D | 2.31 | 0.83 |
| 17:7:212:GLU:HG3 | 21:7:407:CLA:C3B | 2.08 | 0.83 |
| 24:6:618:BCR:C31 | 21:8:609:CLA:HBB2 | 2.09 | 0.82 |
| 20:c:106:MET:HE1 | 21:c:610:CLA:HAB | 1.60 | 0.82 |
| 18:4:227:ARG:HB3 | 21:4:602:CLA:HBC3 | 1.59 | 0.82 |
| 21:2:609:CLA:HHD | 21:2:609:CLA:CBC | 2.10 | 0.82 |
| 21:3:409:CLA:CHB | 21:3:409:CLA:H11 | 2.10 | 0.81 |
| 21:2:609:CLA:CHB | 21:2:609:CLA:C1 | 2.59 | 0.81 |
| 24:6:618:BCR:HC22 | 21:8:609:CLA:HAB | 1.63 | 0.81 |
| 17:7:212:GLU:HG3 | 21:7:407:CLA:C2B | 2.11 | 0.80 |
| 17:7:212:GLU:HG3 | 21:7:407:CLA:C4B | 2.13 | 0.79 |
| 21:A:842:CLA:HMD3 | 24:B:846:BCR:H383 | 1.66 | 0.78 |
| 24:A:854:BCR:C13 | 24:K:205:BCR:H321 | 2.14 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:7:402:CLA:HBC1 | 21:7:407:CLA:HAC1 | 1.67 | 0.77 |
| 24:A:854:BCR:C12 | 24:K:205:BCR:H321 | 2.14 | 0.77 |
| 21:H:201:CLA:HBB2 | 24:L:306:BCR:H392 | 1.67 | 0.77 |
| 16:6:219:LEU:HA | 16:6:222:LYS:HE3 | 1.67 | 0.76 |
| 21:a:610:CLA:HAB | 30:a:615:LUT:H32 | 1.67 | 0.76 |
| 21:1:309:CLA:HBB1 | 21:1:309:CLA:CHC | 2.11 | 0.76 |
| 21:3:409:CLA:H42 | 30:3:416:LUT:H28 | 1.63 | 0.76 |
| 18:8:224:LYS:HD3 | 21:8:609:CLA:C3D | 2.16 | 0.76 |
| 20:a:143:LEU:O | 20:a:152:VAL:CG2 | 2.34 | 0.76 |
| 21:2:609:CLA:C4 | 30:2:616:LUT:H10 | 2.15 | 0.75 |
| 24:6:618:BCR:H312 | 21:8:609:CLA:CBB | 2.15 | 0.75 |
| 19:9:303:GLN:HB2 | 21:9:613:CLA:HED2 | 1.69 | 0.75 |
| 2:B:142:LEU:HD11 | 24:B:843:BCR:C40 | 2.16 | 0.74 |
| 2:B:142:LEU:HD11 | 24:B:843:BCR:H403 | 1.69 | 0.74 |
| 21:a:602:CLA:H2 | 30:a:616:LUT:H26 | 1.70 | 0.74 |
| 15:5:194:ARG:HB3 | 21:5:602:CLA:HBC3 | 1.68 | 0.74 |
| 17:7:281:VAL:HG11 | 31:7:416:XAT:H12 | 1.67 | 0.74 |
| 17:7:311:VAL:HG13 | 17:7:312:LEU:H | 1.52 | 0.74 |
| 21:7:402:CLA:CBC | 21:7:407:CLA:HAC1 | 2.16 | 0.74 |
| 30:8:614:LUT:H30 | 21:8:618:CLA:HAB | 1.69 | 0.74 |
| 20:a:172:GLU:OE1 | 20:a:175:ARG:NH2 | 2.20 | 0.74 |
| 21:A:842:CLA:CMD | 24:B:846:BCR:H383 | 2.17 | 0.73 |
| 21:3:409:CLA:H41 | 30:3:416:LUT:C28 | 2.14 | 0.73 |
| 10:J:31:ARG:HD3 | 24:J:101:BCR:H312 | 1.70 | 0.73 |
| 16:6:201:TRP:HH2 | 29:6:614:CHL:NB | 1.85 | 0.73 |
| 21:B:807:CLA:H72 | 24:B:846:BCR:H321 | 1.71 | 0.73 |
| 15:1:194:ARG:HB3 | 21:1:303:CLA:HBC2 | 1.71 | 0.73 |
| 19:9:236:GLU:OE1 | 19:9:239:ARG:NH1 | 2.22 | 0.73 |
| 24:2:618:BCR:HC42 | 23:4:618:LHG:HC81 | 1.71 | 0.72 |
| 18:8:224:LYS:CG | 21:8:609:CLA:CMD | 2.62 | 0.72 |
| 10:J:5:LYS:HD3 | 16:2:99:LEU:HD11 | 1.70 | 0.72 |
| 2:B:301:MET:HE2 | 21:B:823:CLA:HBC3 | 1.73 | 0.71 |
| 18:8:227:ARG:HB3 | 21:8:602:CLA:HBC2 | 1.71 | 0.71 |
| 18:4:233:VAL:HG11 | 31:4:616:XAT:H12 | 1.70 | 0.71 |
| 20:b:196:PRO:HD2 | 30:b:316:LUT:H23 | 1.72 | 0.71 |
| 1:A:455:HIS:HE1 | 21:A:834:CLA:NA | 1.86 | 0.71 |
| 2:B:257:PHE:HE2 | 2:B:493:TRP:HE3 | 1.39 | 0.71 |
| 2:B:712:HIS:HE1 | 21:B:839:CLA:ND | 1.88 | 0.71 |
| 21:3:409:CLA:H11 | 21:3:409:CLA:C1B | 2.21 | 0.71 |
| 2:B:26:ALA:HB2 | 27:B:847:DGD:HA42 | 1.71 | 0.71 |
| 18:8:111:CYS:HB2 | 18:8:226:GLY:HA3 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:9:602:CLA:H52 | 30:9:615:LUT:H28 | 1.73 | 0.71 |
| 18:8:113:TRP:CE2 | 29:8:607:CHL:HED2 | 2.26 | 0.70 |
| 2:B:624:LEU:HD22 | 21:B:801:CLA:HMD2 | 1.73 | 0.70 |
| 19:9:287:MET:HE2 | 30:9:615:LUT:H10 | 1.72 | 0.70 |
| 21:A:822:CLA:HMB1 | 21:A:823:CLA:H2 | 1.73 | 0.70 |
| 21:B:822:CLA:HBB1 | 21:B:837:CLA:H152 | 1.72 | 0.70 |
| 15:1:148:ILE:HG21 | 21:1:309:CLA:HMC3 | 1.74 | 0.70 |
| 21:6:604:CLA:NC | 24:6:618:BCR:H272 | 2.04 | 0.70 |
| 5:E:84:ARG:HH21 | 6:F:244:SER:H | 1.40 | 0.70 |
| 21:A:818:CLA:HHC | 21:A:818:CLA:HBB1 | 1.71 | 0.70 |
| 20:c:233:VAL:HG13 | 20:c:234:THR:HG23 | 1.73 | 0.70 |
| 1:A:294:HIS:HB2 | 21:A:818:CLA:C1B | 2.22 | 0.69 |
| 20:c:175:ARG:HH22 | 29:c:608:CHL:HMA3 | 1.57 | 0.69 |
| 15:5:167:PRO:HG3 | 21:5:607:CLA:HMD2 | 1.72 | 0.69 |
| 29:5:606:CHL:HAB | 31:5:616:XAT:H7 | 1.74 | 0.69 |
| 18:4:196:TYR:HD1 | 21:4:609:CLA:O1D | 1.75 | 0.69 |
| 15:1:126:THR:H | 15:1:131:PRO:HA | 1.57 | 0.69 |
| 5:E:84:ARG:HG3 | 6:F:243:VAL:HG22 | 1.75 | 0.69 |
| 15:5:137:LEU:O | 15:5:141:LEU:HB2 | 1.92 | 0.69 |
| 15:5:225:ASP:OD1 | 15:5:228:HIS:ND1 | 2.26 | 0.69 |
| 15:5:137:LEU:HA | 15:5:141:LEU:HD23 | 1.74 | 0.69 |
| 17:7:117:GLY:HA3 | 17:7:271:VAL:HG11 | 1.74 | 0.69 |
| 18:8:113:TRP:CZ2 | 18:8:161:MET:HE1 | 2.27 | 0.69 |
| 21:5:602:CLA:HAB | 31:5:616:XAT:H32 | 1.75 | 0.69 |
| 21:A:840:CLA:H2 | 21:B:831:CLA:H42 | 1.76 | 0.68 |
| 1:A:403:ALA:HB2 | 24:A:849:BCR:H323 | 1.76 | 0.68 |
| 1:A:117:PRO:HB3 | 1:A:122:LYS:HD2 | 1.73 | 0.68 |
| 18:8:221:LYS:HG2 | 21:8:609:CLA:OBD | 1.92 | 0.68 |
| 20:b:151:LEU:O | 20:b:153:HIS:N | 2.26 | 0.68 |
| 1:A:683:MET:HB2 | 21:A:802:CLA:C1C | 2.23 | 0.68 |
| 31:a:618:XAT:H161 | 20:b:254:ALA:HB1 | 1.74 | 0.68 |
| 17:7:305:ASP:HB3 | 17:7:308:HIS:HB2 | 1.75 | 0.68 |
| 15:5:121:PRO:HA | 15:5:137:LEU:HD21 | 1.75 | 0.68 |
| 2:B:257:PHE:CE2 | 2:B:493:TRP:HE3 | 2.10 | 0.67 |
| 2:B:439:HIS:HE1 | 21:B:832:CLA:NA | 1.88 | 0.67 |
| 16:6:236:GLY:O | 16:6:240:GLN:HG3 | 1.95 | 0.67 |
| 1:A:50:HIS:HE1 | 21:A:804:CLA:ND | 1.93 | 0.67 |
| 15:5:126:THR:HG22 | 15:5:131:PRO:HB3 | 1.76 | 0.67 |
| 16:6:197:PRO:HG2 | 16:6:202:PHE:HD2 | 1.59 | 0.67 |
| 17:7:212:GLU:HG3 | 21:7:407:CLA:C1B | 2.23 | 0.67 |
| 18:8:224:LYS:CD | 21:8:609:CLA:HMD1 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:118:ILE:HG23 | 1:A:119:VAL:HG22 | 1.77 | 0.67 |
| 15:5:197:LEU:HD23 | 21:5:602:CLA:HMC3 | 1.77 | 0.67 |
| 21:1:310:CLA:HAB | 30:1:317:LUT:H32 | 1.77 | 0.67 |
| 16:6:156:ILE:HG12 | 21:8:612:CLA:HAA2 | 1.77 | 0.67 |
| 4:D:152:ARG:NH2 | 4:D:182:GLU:OE2 | 2.28 | 0.67 |
| 12:L:164:LYS:NZ | 12:L:167:GLU:OE1 | 2.28 | 0.67 |
| 23:b:319:LHG:HC91 | 23:b:319:LHG:H321 | 1.77 | 0.66 |
| 1:A:703:HIS:HE1 | 21:A:840:CLA:ND | 1.92 | 0.66 |
| 2:B:455:ILE:CD1 | 24:J:104:BCR:C32 | 2.74 | 0.66 |
| 21:B:837:CLA:H141 | 24:B:844:BCR:H15C | 1.78 | 0.66 |
| 21:K:203:CLA:HMC1 | 24:K:205:BCR:H312 | 1.73 | 0.66 |
| 6:F:227:GLY:O | 18:4:99:ARG:NH2 | 2.29 | 0.66 |
| 11:K:117:VAL:HG22 | 24:K:205:BCR:H333 | 1.76 | 0.66 |
| 14:O:75:LEU:HD22 | 14:O:86:ASN:HD22 | 1.59 | 0.66 |
| 24:6:618:BCR:HC22 | 21:8:609:CLA:CAB | 2.25 | 0.66 |
| 16:6:86:PHE:HB2 | 29:6:602:CHL:HMD1 | 1.78 | 0.66 |
| 18:8:239:GLN:NE2 | 21:8:611:CLA:O1D | 2.29 | 0.66 |
| 2:B:174:ARG:HB2 | 21:B:812:CLA:HBC2 | 1.78 | 0.65 |
| 17:7:164:VAL:HG21 | 24:7:418:BCR:H291 | 1.78 | 0.65 |
| 21:2:609:CLA:H43 | 30:2:616:LUT:C7 | 2.17 | 0.65 |
| 17:7:299:LEU:HD11 | 30:7:415:LUT:H172 | 1.77 | 0.65 |
| 20:c:160:ILE:HG13 | 20:c:161:TRP:HD1 | 1.62 | 0.65 |
| 24:A:854:BCR:C11 | 24:K:205:BCR:C32 | 2.73 | 0.65 |
| 2:B:275:HIS:HE1 | 21:B:815:CLA:C4D | 2.10 | 0.65 |
| 3:C:62:PHE:HD2 | 4:D:198:ILE:HG21 | 1.62 | 0.65 |
| 18:8:153:LEU:O | 18:8:157:GLU:HG2 | 1.97 | 0.65 |
| 19:9:299:VAL:HG22 | 19:9:300:SER:H | 1.61 | 0.65 |
| 6:F:182:ILE:HG12 | 21:F:304:CLA:ND | 2.12 | 0.65 |
| 18:8:230:MET:HE1 | 21:8:602:CLA:HAB | 1.78 | 0.65 |
| 2:B:159:PRO:HA | 2:B:162:LYS:HE2 | 1.79 | 0.65 |
| 2:B:542:ARG:NH2 | 4:D:203:ASN:OD1 | 2.30 | 0.65 |
| 16:2:234:VAL:HG11 | 31:2:617:XAT:H12 | 1.78 | 0.65 |
| 2:B:389:HIS:HE1 | 21:B:828:CLA:NA | 1.93 | 0.65 |
| 20:b:54:ARG:NH2 | 20:b:69:LEU:O | 2.27 | 0.65 |
| 16:6:235:LEU:HD21 | 21:6:603:CLA:HAB | 1.77 | 0.65 |
| 17:3:132:ALA:HB1 | 17:3:138:PRO:HD3 | 1.77 | 0.64 |
| 21:3:409:CLA:H41 | 30:3:416:LUT:H30 | 1.79 | 0.64 |
| 21:B:813:CLA:HBA1 | 24:B:843:BCR:H393 | 1.79 | 0.64 |
| 15:5:48:LEU:HD11 | 29:5:601:CHL:HED3 | 1.78 | 0.64 |
| 19:9:188:PRO:O | 19:9:200:GLN:NE2 | 2.28 | 0.64 |
| 20:c:100:ILE:HG13 | 29:c:609:CHL:HMD2 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:8:67:LEU:HD11 | 18:8:74:ALA:HB2 | 1.79 | 0.64 |
| 29:8:605:CHL:C4A | 24:8:616:BCR:H383 | 2.22 | 0.64 |
| 15:5:167:PRO:HG2 | 21:5:609:CLA:HMD1 | 1.80 | 0.64 |
| 17:3:281:VAL:HG11 | 31:3:417:XAT:H12 | 1.79 | 0.64 |
| 24:6:618:BCR:C31 | 21:8:609:CLA:CBB | 2.75 | 0.64 |
| 2:B:256:THR:H | 2:B:271:THR:HB | 1.63 | 0.64 |
| 17:3:256:PHE:HB2 | 21:3:409:CLA:HBA1 | 1.80 | 0.64 |
| 20:a:202:ASP:HB3 | 20:a:205:THR:HG22 | 1.79 | 0.64 |
| 4:D:174:HIS:HB3 | 4:D:175:PRO:HD3 | 1.78 | 0.64 |
| 20:b:224:MET:HE2 | 30:b:317:LUT:H10 | 1.80 | 0.64 |
| 2:B:411:MET:HE2 | 24:B:844:BCR:C40 | 2.16 | 0.64 |
| 8:H:46:LYS:NZ | 12:L:71:ASN:O | 2.31 | 0.64 |
| 21:6:610:CLA:HAB | 24:7:417:BCR:H313 | 1.79 | 0.64 |
| 18:8:204:PRO:HD2 | 30:8:614:LUT:H23 | 1.80 | 0.64 |
| 21:B:827:CLA:H101 | 24:B:842:BCR:H19C | 1.80 | 0.63 |
| 19:9:302:LEU:O | 19:9:303:GLN:HG2 | 1.98 | 0.63 |
| 6:F:182:ILE:HG12 | 21:F:304:CLA:C4D | 2.28 | 0.63 |
| 21:6:604:CLA:C1B | 24:6:618:BCR:H282 | 2.29 | 0.63 |
| 20:a:161:TRP:O | 20:a:165:VAL:HG13 | 1.99 | 0.63 |
| 15:1:230:THR:HG23 | 15:1:232:ALA:H | 1.63 | 0.63 |
| 16:6:229:LEU:HD22 | 30:6:616:LUT:H402 | 1.81 | 0.63 |
| 2:B:142:LEU:CD1 | 24:B:843:BCR:H403 | 2.29 | 0.62 |
| 14:O:81:PRO:HB2 | 14:O:84:ASN:HB2 | 1.81 | 0.62 |
| 1:A:455:HIS:HE1 | 21:A:834:CLA:C1A | 2.11 | 0.62 |
| 24:A:854:BCR:C11 | 24:K:205:BCR:H322 | 2.29 | 0.62 |
| 21:K:203:CLA:HMC1 | 24:K:205:BCR:C31 | 2.28 | 0.62 |
| 16:2:112:ARG:NH1 | 29:2:607:CHL:OBD | 2.31 | 0.62 |
| 21:c:610:CLA:HBB1 | 21:c:612:CLA:H3A | 1.81 | 0.62 |
| 20:c:102:ALA:O | 20:c:106:MET:HG3 | 1.98 | 0.62 |
| 21:K:202:CLA:HBA1 | 21:K:202:CLA:HBD | 1.80 | 0.62 |
| 14:O:67:ILE:HG23 | 21:O:202:CLA:HBB2 | 1.82 | 0.62 |
| 1:A:419:GLN:HG3 | 1:A:422:ASN:HD21 | 1.63 | 0.62 |
| 24:B:844:BCR:H291 | 24:B:845:BCR:H383 | 1.81 | 0.62 |
| 21:2:604:CLA:HBA2 | 24:2:618:BCR:H292 | 1.81 | 0.62 |
| 19:9:120:LYS:HB2 | 19:9:124:THR:HA | 1.80 | 0.62 |
| 17:3:184:VAL:HG11 | 31:3:417:XAT:H172 | 1.81 | 0.62 |
| 21:2:609:CLA:H11 | 21:2:609:CLA:C4A | 2.29 | 0.62 |
| 20:c:152:VAL:HG13 | 20:c:153:HIS:H | 1.64 | 0.62 |
| 22:B:841:PQN:H301 | 24:L:305:BCR:H343 | 1.80 | 0.62 |
| 16:2:165:GLU:HG3 | 21:2:608:CLA:C4B | 2.30 | 0.62 |
| 16:2:198:GLY:HA2 | 21:2:609:CLA:HED3 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5:97:ILE:HG13 | 15:5:203:PHE:HE2 | 1.64 | 0.61 |
| 16:6:183:VAL:HG22 | 21:8:609:CLA:CBB | 2.29 | 0.61 |
| 16:6:234:VAL:HG21 | 31:6:617:XAT:H14 | 1.81 | 0.61 |
| 1:A:390:HIS:HE1 | 21:A:828:CLA:C1D | 2.13 | 0.61 |
| 2:B:65:LEU:HD11 | 24:B:843:BCR:C40 | 2.30 | 0.61 |
| 2:B:303:GLU:HG3 | 7:G:91:GLN:HA | 1.83 | 0.61 |
| 17:7:281:VAL:HG12 | 17:7:285:PHE:HE2 | 1.65 | 0.61 |
| 18:8:224:LYS:HD3 | 21:8:609:CLA:HMD1 | 1.82 | 0.61 |
| 17:7:212:GLU:CG | 21:7:407:CLA:C1B | 2.78 | 0.61 |
| 23:9:618:LHG:H272 | 23:9:618:LHG:H102 | 1.83 | 0.61 |
| 21:c:602:CLA:HAB | 30:c:616:LUT:H32 | 1.83 | 0.61 |
| 1:A:588:ASP:OD2 | 1:A:723:ARG:NH1 | 2.34 | 0.61 |
| 18:4:90:PRO:HB3 | 23:4:619:LHG:HC61 | 1.82 | 0.61 |
| 20:c:196:PRO:HD2 | 30:c:615:LUT:H23 | 1.83 | 0.61 |
| 1:A:50:HIS:HE1 | 21:A:804:CLA:C4D | 2.13 | 0.61 |
| 17:7:280:ALA:HB1 | 30:7:415:LUT:H8 | 1.83 | 0.61 |
| 21:9:612:CLA:HHC | 21:9:612:CLA:HBB1 | 1.82 | 0.61 |
| 20:c:237:GLY:N | 20:c:240:GLU:OE2 | 2.32 | 0.61 |
| 21:K:201:CLA:NA | 24:K:205:BCR:C40 | 2.63 | 0.61 |
| 18:8:201:TRP:HH2 | 29:8:613:CHL:NB | 1.98 | 0.61 |
| 14:O:61:ARG:O | 14:O:136:LYS:NZ | 2.34 | 0.60 |
| 15:5:90:ALA:HA | 15:5:197:LEU:HD13 | 1.82 | 0.60 |
| 20:c:171:VAL:O | 20:c:175:ARG:HD3 | 2.01 | 0.60 |
| 21:A:803:CLA:C4B | 21:B:802:CLA:HBB1 | 2.22 | 0.60 |
| 15:5:81:ARG:NH1 | 21:5:603:CLA:O1A | 2.31 | 0.60 |
| 16:6:244:THR:HG22 | 16:6:267:LEU:HG | 1.81 | 0.60 |
| 17:7:277:ALA:HB2 | 30:7:415:LUT:H202 | 1.81 | 0.60 |
| 15:1:149:ALA:CA | 21:1:309:CLA:HAB | 2.31 | 0.60 |
| 23:5:617:LHG:HC92 | 24:8:616:BCR:H313 | 1.83 | 0.60 |
| 1:A:317:HIS:HB3 | 1:A:322:ILE:HD11 | 1.82 | 0.60 |
| 18:4:198:GLY:CA | 21:4:609:CLA:HED3 | 2.31 | 0.60 |
| 17:7:111:LEU:HD13 | 17:7:118:ASP:OD1 | 2.01 | 0.60 |
| 2:B:65:LEU:HD11 | 24:B:843:BCR:H402 | 1.83 | 0.60 |
| 29:b:307:CHL:HBB1 | 30:b:317:LUT:H161 | 1.84 | 0.60 |
| 29:2:601:CHL:H2 | 21:3:415:CLA:HMA2 | 1.84 | 0.60 |
| 17:3:188:VAL:HG13 | 26:3:420:LMU:H5' | 1.82 | 0.60 |
| 18:8:224:LYS:CD | 21:8:609:CLA:CMD | 2.79 | 0.60 |
| 21:3:409:CLA:C4 | 30:3:416:LUT:H30 | 2.32 | 0.59 |
| 17:7:120:GLY:N | 21:7:401:CLA:OBD | 2.35 | 0.59 |
| 3:C:2:ALA:N | 3:C:71:ALA:O | 2.35 | 0.59 |
| 21:3:409:CLA:H41 | 30:3:416:LUT:C30 | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:a:103:ARG:NH1 | 29:a:608:CHL:OBD | 2.33 | 0.59 |
| 21:A:805:CLA:H2 | 21:A:812:CLA:H92 | 1.83 | 0.59 |
| 20:a:184:ILE:HG13 | 20:a:190:PRO:HB3 | 1.84 | 0.59 |
| 12:L:95:ASN:HB3 | 21:L:302:CLA:HAC1 | 1.84 | 0.59 |
| 17:7:280:ALA:CB | 30:7:415:LUT:H8 | 2.32 | 0.59 |
| 19:9:302:LEU:HD22 | 19:9:306:HIS:HB2 | 1.85 | 0.59 |
| 20:b:215:LYS:NZ | 23:b:319:LHG:O4 | 2.35 | 0.59 |
| 17:7:140:TRP:HZ3 | 21:7:402:CLA:HBA1 | 1.68 | 0.59 |
| 16:6:67:LEU:HD11 | 16:6:74:ALA:HB2 | 1.84 | 0.59 |
| 16:6:220:ARG:HD2 | 21:6:609:CLA:HMA3 | 1.84 | 0.59 |
| 19:9:285:MET:HG3 | 23:9:618:LHG:H281 | 1.84 | 0.59 |
| 20:a:222:PHE:HE2 | 21:a:613:CLA:HAB | 1.67 | 0.59 |
| 21:a:611:CLA:HED3 | 21:a:611:CLA:H2A | 1.85 | 0.59 |
| 21:9:602:CLA:H61 | 30:9:615:LUT:H371 | 1.83 | 0.59 |
| 21:B:831:CLA:HHC | 21:B:831:CLA:HBB1 | 1.84 | 0.59 |
| 1:A:729:HIS:HE1 | 21:A:841:CLA:ND | 2.00 | 0.59 |
| 17:3:187:PRO:HG3 | 21:3:401:CLA:HMD1 | 1.85 | 0.59 |
| 1:A:293:HIS:HE1 | 21:A:817:CLA:C4D | 2.16 | 0.58 |
| 17:3:261:LYS:O | 17:3:265:GLU:HG2 | 2.03 | 0.58 |
| 2:B:299:HIS:HB3 | 2:B:304:ILE:HD11 | 1.85 | 0.58 |
| 29:2:601:CHL:HHC | 29:2:601:CHL:HBB1 | 1.85 | 0.58 |
| 29:8:605:CHL:NB | 24:8:616:BCR:H382 | 2.13 | 0.58 |
| 5:E:76:GLY:HA2 | 5:E:94:LYS:NZ | 2.17 | 0.58 |
| 17:7:258:LYS:HD2 | 17:7:259:ASN:HB2 | 1.83 | 0.58 |
| 20:c:137:ILE:HD12 | 20:c:157:ILE:HG12 | 1.85 | 0.58 |
| 20:c:242:LEU:HD12 | 30:c:615:LUT:H163 | 1.85 | 0.58 |
| 21:c:611:CLA:NA | 23:c:619:LHG:O4 | 2.36 | 0.58 |
| 6:F:128:ASN:O | 6:F:132:GLU:HG2 | 2.03 | 0.58 |
| 18:4:198:GLY:HA2 | 21:4:609:CLA:HED3 | 1.86 | 0.58 |
| 20:a:244:ASP:O | 20:a:252:ASN:ND2 | 2.32 | 0.58 |
| 1:A:335:HIS:CD2 | 21:A:824:CLA:ND | 2.72 | 0.58 |
| 1:A:353:ASN:ND2 | 21:A:806:CLA:OBD | 2.33 | 0.58 |
| 12:L:125:VAL:HG22 | 12:L:140:GLY:HA3 | 1.84 | 0.58 |
| 21:5:609:CLA:HAB | 30:5:615:LUT:H32 | 1.85 | 0.58 |
| 17:7:111:LEU:HD11 | 17:7:120:GLY:HA2 | 1.85 | 0.58 |
| 1:A:379:THR:HG21 | 1:A:515:VAL:HB | 1.86 | 0.58 |
| 21:2:609:CLA:C1 | 21:2:609:CLA:C1B | 2.81 | 0.58 |
| 18:4:262:THR:HG23 | 18:4:264:LEU:H | 1.69 | 0.58 |
| 16:6:232:LEU:HD11 | 23:6:619:LHG:H272 | 1.86 | 0.58 |
| 18:4:221:LYS:HD3 | 21:4:611:CLA:HBA1 | 1.84 | 0.58 |
| 17:7:286:THR:HG21 | 21:7:411:CLA:HAC2 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:7:417:BCR:H403 | 24:7:418:BCR:H351 | 1.85 | 0.58 |
| 20:c:151:LEU:O | 20:c:153:HIS:N | 2.37 | 0.58 |
| 2:B:142:LEU:CD1 | 24:B:843:BCR:C40 | 2.82 | 0.58 |
| 2:B:275:HIS:HE1 | 21:B:815:CLA:ND | 1.98 | 0.58 |
| 26:O:206:LMU:O2' | 26:b:301:LMU:O2' | 2.21 | 0.58 |
| 19:9:297:THR:HG22 | 19:9:298:GLY:H | 1.69 | 0.58 |
| 20:a:129:VAL:HB | 20:a:132:LYS:HB2 | 1.85 | 0.58 |
| 20:a:247:ALA:O | 20:a:252:ASN:ND2 | 2.37 | 0.58 |
| 29:b:302:CHL:HAC2 | 23:b:319:LHG:HC41 | 1.86 | 0.58 |
| 2:B:292:ARG:NH1 | 7:G:92:GLY:O | 2.37 | 0.57 |
| 21:a:602:CLA:HAB | 30:a:616:LUT:H32 | 1.86 | 0.57 |
| 23:A:855:LHG:H251 | 23:A:855:LHG:HC92 | 1.84 | 0.57 |
| 7:G:155:PHE:HB2 | 15:1:119:ALA:HB1 | 1.86 | 0.57 |
| 19:9:90:ILE:HG13 | 19:9:260:LEU:HD23 | 1.86 | 0.57 |
| 16:6:207:TRP:HE3 | 30:6:616:LUT:H22 | 1.69 | 0.57 |
| 2:B:133:GLN:HE21 | 13:M:2:THR:HB | 1.70 | 0.57 |
| 7:G:144:LEU:O | 7:G:148:ASN:ND2 | 2.36 | 0.57 |
| 29:6:602:CHL:HBA1 | 31:6:617:XAT:H241 | 1.86 | 0.57 |
| 2:B:442:VAL:HG21 | 21:B:832:CLA:HAC2 | 1.85 | 0.57 |
| 18:8:183:ILE:HG13 | 24:8:616:BCR:H332 | 1.86 | 0.57 |
| 18:8:218:ILE:O | 18:8:222:GLU:HG2 | 2.05 | 0.57 |
| 1:A:198:HIS:CD2 | 21:A:814:CLA:NB | 2.72 | 0.57 |
| 21:B:827:CLA:H43 | 24:B:842:BCR:H393 | 1.85 | 0.57 |
| 16:2:154:PHE:HB2 | 29:2:606:CHL:HBC1 | 1.85 | 0.57 |
| 21:2:609:CLA:CGA | 30:2:616:LUT:H41 | 2.34 | 0.57 |
| 15:5:89:HIS:CD2 | 21:5:603:CLA:NB | 2.73 | 0.57 |
| 1:A:294:HIS:NE2 | 21:A:818:CLA:NC | 2.52 | 0.57 |
| 21:A:819:CLA:H92 | 21:A:829:CLA:H91 | 1.87 | 0.57 |
| 29:5:601:CHL:HHC | 29:5:601:CHL:HBB1 | 1.86 | 0.57 |
| 21:5:605:CLA:HMC1 | 31:5:616:XAT:H183 | 1.86 | 0.57 |
| 17:7:153:MET:HE1 | 17:7:273:ASN:HB3 | 1.87 | 0.57 |
| 21:7:404:CLA:HAA1 | 24:7:417:BCR:H21C | 1.86 | 0.57 |
| 20:a:145:TYR:HD2 | 20:a:151:LEU:HD23 | 1.70 | 0.57 |
| 18:8:112:ARG:NH1 | 29:8:607:CHL:OBD | 2.34 | 0.57 |
| 20:a:255:TRP:CD2 | 20:c:161:TRP:HZ3 | 2.23 | 0.57 |
| 1:A:683:MET:HB2 | 21:A:802:CLA:NC | 2.19 | 0.57 |
| 21:A:810:CLA:HBB1 | 24:J:103:BCR:H23C | 1.86 | 0.57 |
| 24:A:846:BCR:H362 | 24:A:847:BCR:H21C | 1.87 | 0.57 |
| 28:G:206:LMG:H301 | 29:1:307:CHL:H11 | 1.87 | 0.57 |
| 21:K:201:CLA:HED1 | 24:K:205:BCR:C38 | 2.35 | 0.57 |
| 29:1:302:CHL:HHC | 29:1:302:CHL:HBB1 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:8:224:LYS:HD3 | 21:8:609:CLA:C2D | 2.34 | 0.57 |
| 1:A:199:LEU:HD12 | 1:A:203:LEU:HD12 | 1.87 | 0.56 |
| 1:A:405:HIS:HE1 | 21:A:830:CLA:NA | 2.01 | 0.56 |
| 2:B:65:LEU:CD1 | 24:B:843:BCR:H401 | 2.35 | 0.56 |
| 18:4:189:LEU:HD22 | 18:4:199:GLY:HA3 | 1.87 | 0.56 |
| 21:A:806:CLA:H61 | 24:A:847:BCR:HC8 | 1.86 | 0.56 |
| 18:8:224:LYS:HD3 | 21:8:609:CLA:CAD | 2.35 | 0.56 |
| 21:a:610:CLA:HAB | 30:a:615:LUT:C32 | 2.35 | 0.56 |
| 2:B:36:ASP:O | 2:B:41:ARG:NH1 | 2.39 | 0.56 |
| 16:6:84:GLY:HA3 | 16:6:224:ILE:HD11 | 1.87 | 0.56 |
| 20:b:168:MET:HA | 20:b:171:VAL:HG22 | 1.87 | 0.56 |
| 16:2:252:LEU:HD13 | 21:2:613:CLA:HBC2 | 1.87 | 0.56 |
| 20:a:222:PHE:CE2 | 21:a:613:CLA:HAB | 2.41 | 0.56 |
| 7:G:85:ARG:NH2 | 7:G:123:GLY:O | 2.39 | 0.56 |
| 18:4:196:TYR:CD1 | 21:4:609:CLA:O1D | 2.56 | 0.56 |
| 16:6:235:LEU:HD13 | 31:6:617:XAT:H401 | 1.87 | 0.56 |
| 21:c:613:CLA:H2 | 21:c:614:CLA:HMD1 | 1.88 | 0.56 |
| 1:A:91:HIS:HE1 | 21:A:808:CLA:NA | 1.99 | 0.56 |
| 1:A:360:LEU:HD11 | 21:A:819:CLA:H71 | 1.87 | 0.56 |
| 21:B:824:CLA:HMB1 | 21:B:837:CLA:HBA1 | 1.88 | 0.56 |
| 26:O:206:LMU:H82 | 26:b:301:LMU:H52 | 1.88 | 0.56 |
| 29:a:608:CHL:HHC | 29:a:608:CHL:HBB1 | 1.88 | 0.56 |
| 2:B:439:HIS:HE1 | 21:B:832:CLA:C1A | 2.19 | 0.56 |
| 21:2:610:CLA:HBC3 | 23:2:619:LHG:H242 | 1.88 | 0.56 |
| 16:6:97:PRO:HA | 16:6:100:LEU:HD13 | 1.88 | 0.56 |
| 2:B:455:ILE:CD1 | 24:J:104:BCR:H321 | 2.36 | 0.55 |
| 6:F:202:LYS:NZ | 6:F:207:ASP:OD2 | 2.38 | 0.55 |
| 32:9:617:NEX:H192 | 32:9:617:NEX:H183 | 1.89 | 0.55 |
| 21:b:304:CLA:HED3 | 30:c:616:LUT:H363 | 1.89 | 0.55 |
| 21:A:852:CLA:HHB | 21:B:801:CLA:H202 | 1.87 | 0.55 |
| 24:A:854:BCR:C12 | 24:K:205:BCR:C32 | 2.85 | 0.55 |
| 15:1:149:ALA:HB2 | 21:1:309:CLA:HAB | 1.88 | 0.55 |
| 1:A:54:HIS:HE1 | 21:A:805:CLA:C1C | 2.19 | 0.55 |
| 17:3:245:TYR:HD1 | 21:3:409:CLA:O1D | 1.90 | 0.55 |
| 18:4:204:PRO:HD2 | 30:4:615:LUT:H23 | 1.88 | 0.55 |
| 20:a:219:LEU:HA | 23:a:617:LHG:H261 | 1.87 | 0.55 |
| 29:a:607:CHL:HBC2 | 20:b:255:TRP:HH2 | 1.71 | 0.55 |
| 20:c:245:HIS:CD2 | 21:c:614:CLA:NC | 2.74 | 0.55 |
| 15:5:85:SER:OG | 21:5:603:CLA:HAA1 | 2.07 | 0.55 |
| 2:B:600:THR:HG21 | 2:B:609:PHE:HB2 | 1.87 | 0.55 |
| 18:8:221:LYS:HD3 | 21:8:610:CLA:HBA2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:a:618:XAT:H193 | 20:b:254:ALA:HB3 | 1.89 | 0.55 |
| 29:3:407:CHL:HHC | 29:3:407:CHL:HBB1 | 1.88 | 0.55 |
| 21:9:611:CLA:HBC1 | 23:9:618:LHG:H292 | 1.88 | 0.55 |
| 30:5:615:LUT:H12 | 30:5:615:LUT:H191 | 1.88 | 0.54 |
| 17:7:151:PHE:CD1 | 21:7:407:CLA:HBC3 | 2.41 | 0.54 |
| 20:a:151:LEU:O | 20:a:152:VAL:HG22 | 2.06 | 0.54 |
| 18:4:214:LYS:O | 18:4:214:LYS:NZ | 2.32 | 0.54 |
| 20:a:151:LEU:O | 20:a:153:HIS:N | 2.40 | 0.54 |
| 20:c:160:ILE:HG22 | 29:c:605:CHL:HAC1 | 1.89 | 0.54 |
| 29:a:607:CHL:HHC | 29:a:607:CHL:HBB1 | 1.90 | 0.54 |
| 21:3:409:CLA:H41 | 30:3:416:LUT:H28 | 1.62 | 0.54 |
| 15:5:112:VAL:HG21 | 15:5:212:GLY:H | 1.71 | 0.54 |
| 21:7:404:CLA:HBB1 | 21:7:407:CLA:HMC1 | 1.89 | 0.54 |
| 1:A:302:PHE:HE1 | 21:A:821:CLA:HAB | 1.72 | 0.54 |
| 1:A:703:HIS:HE1 | 21:A:840:CLA:C4D | 2.20 | 0.54 |
| 21:A:840:CLA:H92 | 21:B:831:CLA:H43 | 1.90 | 0.54 |
| 24:A:854:BCR:C35 | 24:K:205:BCR:C32 | 2.80 | 0.54 |
| 24:K:205:BCR:H391 | 21:9:611:CLA:H43 | 1.89 | 0.54 |
| 21:7:401:CLA:HMB1 | 21:7:402:CLA:H3A | 1.89 | 0.54 |
| 21:b:303:CLA:HBC1 | 23:b:319:LHG:H291 | 1.88 | 0.54 |
| 1:A:31:HIS:NE2 | 21:A:812:CLA:O1A | 2.41 | 0.54 |
| 21:A:819:CLA:HAB | 21:A:819:CLA:H8 | 1.89 | 0.54 |
| 15:5:158:GLU:HB2 | 15:5:164:ARG:HD3 | 1.89 | 0.54 |
| 19:9:265:ASP:HB3 | 19:9:268:ILE:HG12 | 1.88 | 0.54 |
| 19:9:300:SER:HB2 | 19:9:301:PRO:HD3 | 1.90 | 0.54 |
| 2:B:721:TYR:HB2 | 21:B:801:CLA:HED2 | 1.89 | 0.54 |
| 28:6:615:LMG:HC3 | 19:9:147:LYS:HE2 | 1.90 | 0.54 |
| 18:8:224:LYS:HA | 18:8:227:ARG:HD2 | 1.90 | 0.54 |
| 20:c:143:LEU:HD21 | 21:c:604:CLA:HAA2 | 1.90 | 0.54 |
| 2:B:273:MET:HE3 | 21:B:817:CLA:HMA3 | 1.89 | 0.54 |
| 1:A:532:LEU:O | 1:A:536:ILE:HG12 | 2.08 | 0.53 |
| 17:7:212:GLU:CG | 21:7:407:CLA:C2B | 2.86 | 0.53 |
| 1:A:530:ASP:HA | 1:A:533:VAL:HG12 | 1.90 | 0.53 |
| 17:7:121:PHE:N | 21:7:401:CLA:OBD | 2.41 | 0.53 |
| 19:9:168:TRP:CE2 | 29:9:608:CHL:HED2 | 2.43 | 0.53 |
| 1:A:534:HIS:HD2 | 21:A:837:CLA:C1B | 2.21 | 0.53 |
| 21:A:825:CLA:HBA1 | 21:A:829:CLA:H203 | 1.90 | 0.53 |
| 2:B:516:ASP:OD1 | 2:B:593:TYR:OH | 2.21 | 0.53 |
| 21:5:605:CLA:HBC3 | 29:5:606:CHL:HBC2 | 1.89 | 0.53 |
| 21:7:402:CLA:HBC1 | 21:7:407:CLA:CAC | 2.37 | 0.53 |
| 18:8:138:TRP:CH2 | 18:8:247:PRO:HD3 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:180:SER:HB3 | 21:B:819:CLA:HAC2 | 1.90 | 0.53 |
| 14:O:92:PHE:HE1 | 14:O:116:TRP:HD1 | 1.55 | 0.53 |
| 23:4:618:LHG:O4 | 23:4:618:LHG:O2 | 2.23 | 0.53 |
| 2:B:455:ILE:HD12 | 24:J:104:BCR:C32 | 2.37 | 0.53 |
| 21:O:203:CLA:H3A | 21:O:203:CLA:H11 | 1.89 | 0.53 |
| 29:4:614:CHL:HHC | 29:4:614:CHL:HBB1 | 1.90 | 0.53 |
| 20:b:229:VAL:HG21 | 21:b:314:CLA:HAC2 | 1.90 | 0.53 |
| 16:6:167:ARG:HH11 | 16:6:178:VAL:HB | 1.74 | 0.53 |
| 26:A:856:LMU:O4' | 26:3:420:LMU:O6' | 2.27 | 0.53 |
| 7:G:149:ASN:ND2 | 21:G:202:CLA:OBD | 2.41 | 0.53 |
| 21:2:604:CLA:C1C | 24:2:618:BCR:H272 | 2.38 | 0.53 |
| 15:5:72:LEU:HD22 | 21:5:602:CLA:H42 | 1.90 | 0.53 |
| 17:7:155:GLY:HA2 | 31:7:416:XAT:H181 | 1.91 | 0.53 |
| 17:7:209:GLY:O | 17:7:213:HIS:ND1 | 2.41 | 0.53 |
| 21:b:311:CLA:HBA1 | 30:b:316:LUT:H382 | 1.90 | 0.53 |
| 21:1:312:CLA:HHC | 21:1:312:CLA:HBB1 | 1.91 | 0.53 |
| 15:5:111:TRP:CH2 | 15:5:203:PHE:HB3 | 2.44 | 0.53 |
| 19:9:179:PRO:HA | 19:9:182:ILE:HG12 | 1.90 | 0.53 |
| 2:B:414:HIS:CD2 | 21:B:829:CLA:NA | 2.77 | 0.52 |
| 3:C:24:ASP:OD2 | 3:C:44:ARG:NH2 | 2.36 | 0.52 |
| 3:C:60:THR:O | 3:C:61:ASP:C | 2.51 | 0.52 |
| 15:1:149:ALA:HA | 21:1:309:CLA:HAB | 1.90 | 0.52 |
| 21:7:402:CLA:HBC2 | 21:7:407:CLA:HAC1 | 1.90 | 0.52 |
| 29:9:607:CHL:HHC | 29:9:607:CHL:HBB1 | 1.91 | 0.52 |
| 21:F:302:CLA:O1D | 21:F:302:CLA:H2A | 2.09 | 0.52 |
| 21:K:201:CLA:HED1 | 24:K:205:BCR:H383 | 1.92 | 0.52 |
| 16:2:165:GLU:HG3 | 21:2:608:CLA:NB | 2.24 | 0.52 |
| 29:2:614:CHL:HHC | 29:2:614:CHL:HBB1 | 1.90 | 0.52 |
| 15:5:228:HIS:NE2 | 18:8:147:PHE:O | 2.41 | 0.52 |
| 1:A:293:HIS:HE1 | 21:A:817:CLA:ND | 2.05 | 0.52 |
| 2:B:65:LEU:CD1 | 24:B:843:BCR:C40 | 2.88 | 0.52 |
| 2:B:707:LEU:HD22 | 27:B:847:DGD:HB22 | 1.91 | 0.52 |
| 15:5:98:PRO:HA | 15:5:101:LEU:HG | 1.90 | 0.52 |
| 16:6:116:LEU:HB3 | 21:6:604:CLA:HBB2 | 1.91 | 0.52 |
| 29:c:608:CHL:HHC | 29:c:608:CHL:HBB1 | 1.91 | 0.52 |
| 2:B:26:ALA:HA | 21:B:828:CLA:H43 | 1.92 | 0.52 |
| 2:B:58:PHE:HD1 | 2:B:142:LEU:HD22 | 1.75 | 0.52 |
| 2:B:142:LEU:CG | 24:B:843:BCR:H403 | 2.39 | 0.52 |
| 2:B:351:HIS:CD2 | 21:B:825:CLA:NC | 2.77 | 0.52 |
| 1:A:54:HIS:HE1 | 21:A:805:CLA:NC | 2.05 | 0.52 |
| 1:A:91:HIS:HE1 | 21:A:808:CLA:C1A | 2.23 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:2:609:CLA:C1B | 21:2:609:CLA:H12 | 2.40 | 0.52 |
| 18:8:224:LYS:HD3 | 21:8:609:CLA:CMD | 2.39 | 0.52 |
| 29:c:607:CHL:HHC | 29:c:607:CHL:HBB1 | 1.92 | 0.52 |
| 26:O:206:LMU:H62 | 26:b:301:LMU:H41 | 1.91 | 0.52 |
| 17:7:269:LYS:HD3 | 21:7:410:CLA:HAA2 | 1.92 | 0.52 |
| 20:b:222:PHE:CE2 | 21:b:314:CLA:HAB | 2.43 | 0.52 |
| 24:G:201:BCR:H362 | 24:G:205:BCR:H312 | 1.91 | 0.52 |
| 10:J:12:PRO:HB2 | 24:J:101:BCR:H391 | 1.92 | 0.52 |
| 16:6:197:PRO:HB3 | 29:6:607:CHL:HBC2 | 1.92 | 0.52 |
| 20:b:152:VAL:HG23 | 20:b:153:HIS:H | 1.74 | 0.52 |
| 21:B:816:CLA:HMD3 | 21:B:817:CLA:H141 | 1.92 | 0.52 |
| 15:5:231:ILE:HG22 | 15:5:235:LEU:HG | 1.91 | 0.52 |
| 19:9:243:VAL:HG12 | 19:9:245:GLU:H | 1.73 | 0.52 |
| 20:a:135:ALA:HA | 20:a:138:PHE:HB2 | 1.91 | 0.52 |
| 1:A:179:HIS:HE1 | 21:A:812:CLA:NA | 2.08 | 0.52 |
| 16:2:197:PRO:HD2 | 21:2:609:CLA:OBD | 2.10 | 0.52 |
| 21:2:604:CLA:NC | 24:2:618:BCR:H272 | 2.24 | 0.52 |
| 20:b:58:LEU:HB2 | 20:b:62:SER:HA | 1.92 | 0.52 |
| 17:3:112:ASP:OD1 | 17:3:113:GLY:N | 2.43 | 0.52 |
| 19:9:215:PHE:O | 19:9:217:ASN:N | 2.43 | 0.52 |
| 21:A:841:CLA:HBA1 | 21:A:841:CLA:HBD | 1.93 | 0.51 |
| 18:4:167:ARG:HD3 | 29:4:607:CHL:HBB1 | 1.92 | 0.51 |
| 15:5:102:ILE:HD12 | 21:5:604:CLA:HAC2 | 1.93 | 0.51 |
| 19:9:287:MET:HG3 | 30:9:615:LUT:H12 | 1.92 | 0.51 |
| 1:A:118:ILE:HD13 | 24:J:101:BCR:H313 | 1.93 | 0.51 |
| 9:I:29:TYR:HH | 13:M:31:TYR:HH | 1.56 | 0.51 |
| 2:B:69:ALA:HB2 | 2:B:135:LEU:HB2 | 1.92 | 0.51 |
| 16:6:104:VAL:HA | 16:6:107:GLU:HG2 | 1.92 | 0.51 |
| 29:8:605:CHL:H3A | 24:8:616:BCR:C21 | 2.41 | 0.51 |
| 21:b:312:CLA:C3C | 23:b:319:LHG:HC61 | 2.40 | 0.51 |
| 15:1:97:ILE:HD11 | 30:1:317:LUT:H15 | 1.92 | 0.51 |
| 18:8:138:TRP:HH2 | 18:8:247:PRO:HD3 | 1.75 | 0.51 |
| 18:8:215:LEU:HD13 | 18:8:219:ARG:HE | 1.76 | 0.51 |
| 20:b:66:PRO:HB2 | 20:b:69:LEU:HD13 | 1.92 | 0.51 |
| 21:B:814:CLA:H121 | 24:G:201:BCR:H21C | 1.93 | 0.51 |
| 29:b:306:CHL:HHD | 29:b:307:CHL:OBD | 2.09 | 0.51 |
| 29:1:307:CHL:HHC | 29:1:307:CHL:HBB1 | 1.92 | 0.51 |
| 21:a:602:CLA:H52 | 30:a:616:LUT:H28 | 1.92 | 0.51 |
| 20:c:168:MET:HA | 20:c:171:VAL:HG22 | 1.91 | 0.51 |
| 20:c:233:VAL:HG11 | 21:c:613:CLA:HMD2 | 1.93 | 0.51 |
| 2:B:436:LEU:CD1 | 24:J:104:BCR:H311 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:515:GLY:O | 2:B:519:VAL:HG23 | 2.10 | 0.51 |
| 11:K:116:HIS:CD2 | 21:K:203:CLA:NC | 2.78 | 0.51 |
| 19:9:232:MET:HE1 | 32:9:617:NEX:H30 | 1.91 | 0.51 |
| 20:b:129:VAL:HB | 20:b:132:LYS:HB2 | 1.93 | 0.51 |
| 20:b:229:VAL:HG21 | 21:b:314:CLA:CAC | 2.41 | 0.51 |
| 21:3:404:CLA:C4B | 24:3:418:BCR:H281 | 2.30 | 0.51 |
| 17:7:266:LEU:O | 17:7:270:GLU:HG2 | 2.11 | 0.51 |
| 20:a:104:TRP:CE2 | 29:a:608:CHL:HED2 | 2.46 | 0.51 |
| 15:1:208:VAL:HG23 | 21:1:315:CLA:HBC3 | 1.92 | 0.51 |
| 16:6:122:PHE:CE2 | 30:6:616:LUT:H28 | 2.46 | 0.51 |
| 17:7:212:GLU:CD | 21:7:407:CLA:C1B | 2.84 | 0.51 |
| 24:J:103:BCR:H12C | 24:J:103:BCR:H341 | 1.91 | 0.51 |
| 15:5:80:GLU:HA | 15:5:83:LYS:HE3 | 1.92 | 0.51 |
| 1:A:503:THR:HG21 | 21:A:827:CLA:HAB | 1.92 | 0.50 |
| 19:9:259:PRO:HD2 | 30:9:614:LUT:H23 | 1.91 | 0.50 |
| 20:a:162:ALA:O | 20:a:165:VAL:HG22 | 2.10 | 0.50 |
| 29:a:609:CHL:HMB3 | 29:b:302:CHL:HHB | 1.92 | 0.50 |
| 1:A:582:CYS:HB2 | 2:B:667:TRP:HB3 | 1.94 | 0.50 |
| 8:H:93:THR:O | 12:L:193:ALA:HB1 | 2.11 | 0.50 |
| 21:3:404:CLA:C4A | 24:3:418:BCR:H271 | 2.41 | 0.50 |
| 16:6:201:TRP:CE2 | 29:6:614:CHL:ND | 2.79 | 0.50 |
| 18:8:108:LEU:HD21 | 18:8:196:TYR:CZ | 2.47 | 0.50 |
| 23:8:617:LHG:H302 | 23:8:617:LHG:H141 | 1.93 | 0.50 |
| 19:9:307:ASP:OD2 | 19:9:308:TRP:N | 2.44 | 0.50 |
| 20:a:66:PRO:HB2 | 20:a:69:LEU:HB2 | 1.92 | 0.50 |
| 20:a:102:ALA:HB1 | 20:a:217:GLY:HA3 | 1.92 | 0.50 |
| 20:b:245:HIS:CD2 | 21:b:315:CLA:NC | 2.78 | 0.50 |
| 2:B:257:PHE:HD1 | 21:B:816:CLA:HMB3 | 1.77 | 0.50 |
| 20:a:91:PHE:O | 20:a:95:ARG:HG3 | 2.12 | 0.50 |
| 1:A:448:HIS:HE1 | 21:A:833:CLA:C1A | 2.25 | 0.50 |
| 21:B:824:CLA:HMA1 | 24:B:845:BCR:H14C | 1.94 | 0.50 |
| 4:D:161:PHE:CE2 | 4:D:174:HIS:HB2 | 2.46 | 0.50 |
| 15:5:95:LEU:HB3 | 21:5:604:CLA:HBB2 | 1.93 | 0.50 |
| 16:6:255:HIS:CD2 | 21:6:613:CLA:NC | 2.79 | 0.50 |
| 29:9:605:CHL:HHC | 29:9:605:CHL:HBB1 | 1.94 | 0.50 |
| 2:B:142:LEU:HD11 | 24:B:843:BCR:H402 | 1.94 | 0.50 |
| 16:6:227:GLY:O | 16:6:231:MET:HG3 | 2.12 | 0.50 |
| 21:6:604:CLA:HBA2 | 24:6:618:BCR:H292 | 1.93 | 0.50 |
| 20:c:195:ASP:OD1 | 20:c:195:ASP:N | 2.44 | 0.50 |
| 2:B:436:LEU:HD11 | 24:J:104:BCR:H311 | 1.93 | 0.50 |
| 26:O:206:LMU:H122 | 26:b:301:LMU:H123 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:4:113:TRP:CE2 | 29:4:607:CHL:HED2 | 2.47 | 0.50 |
| 16:6:110:HIS:CE1 | 21:6:603:CLA:NA | 2.80 | 0.50 |
| 29:a:609:CHL:HHC | 29:a:609:CHL:HBB1 | 1.92 | 0.50 |
| 1:A:534:HIS:HD2 | 21:A:837:CLA:NB | 2.05 | 0.50 |
| 1:A:559:ARG:O | 4:D:140:ARG:NH1 | 2.45 | 0.50 |
| 2:B:92:TRP:CZ3 | 2:B:94:PRO:HG3 | 2.47 | 0.50 |
| 2:B:667:TRP:O | 2:B:671:TRP:HD1 | 1.95 | 0.50 |
| 21:B:827:CLA:H161 | 24:B:843:BCR:H361 | 1.93 | 0.50 |
| 29:9:601:CHL:HED1 | 30:9:615:LUT:H362 | 1.92 | 0.50 |
| 24:L:305:BCR:H403 | 24:L:305:BCR:H23C | 1.93 | 0.50 |
| 21:3:404:CLA:NA | 24:3:418:BCR:H271 | 2.27 | 0.50 |
| 18:4:198:GLY:HA2 | 21:4:609:CLA:CED | 2.42 | 0.50 |
| 19:9:209:TYR:CD1 | 19:9:210:LEU:HD23 | 2.47 | 0.50 |
| 5:E:76:GLY:HA2 | 5:E:94:LYS:HZ3 | 1.75 | 0.49 |
| 15:1:75:VAL:HB | 15:1:78:ASN:HB2 | 1.94 | 0.49 |
| 21:3:402:CLA:HAB | 31:3:417:XAT:H32 | 1.92 | 0.49 |
| 16:6:162:ALA:HA | 21:6:608:CLA:HBB1 | 1.94 | 0.49 |
| 29:6:606:CHL:HHC | 29:6:606:CHL:HBB1 | 1.94 | 0.49 |
| 29:a:601:CHL:HMA3 | 23:a:617:LHG:H112 | 1.92 | 0.49 |
| 20:b:102:ALA:HB1 | 20:b:217:GLY:HA3 | 1.94 | 0.49 |
| 21:c:602:CLA:HBA1 | 30:c:616:LUT:H382 | 1.93 | 0.49 |
| 26:A:856:LMU:H3B | 26:3:420:LMU:H4' | 1.94 | 0.49 |
| 2:B:273:MET:HE3 | 21:B:817:CLA:H2A | 1.93 | 0.49 |
| 2:B:319:HIS:CD2 | 21:B:822:CLA:ND | 2.80 | 0.49 |
| 5:E:82:LEU:HD11 | 5:E:131:GLU:HG3 | 1.94 | 0.49 |
| 12:L:62:GLU:N | 14:O:140:ASP:O | 2.45 | 0.49 |
| 20:a:162:ALA:HA | 20:a:165:VAL:HG22 | 1.94 | 0.49 |
| 29:c:609:CHL:HHC | 29:c:609:CHL:HBB1 | 1.94 | 0.49 |
| 1:A:582:CYS:HB3 | 2:B:667:TRP:HE3 | 1.77 | 0.49 |
| 15:1:149:ALA:CB | 21:1:309:CLA:HAB | 2.43 | 0.49 |
| 29:2:606:CHL:HHC | 29:2:606:CHL:HBB1 | 1.93 | 0.49 |
| 19:9:135:GLY:O | 19:9:136:GLU:HG2 | 2.11 | 0.49 |
| 29:a:609:CHL:O1A | 20:b:79:TRP:NE1 | 2.38 | 0.49 |
| 30:a:615:LUT:H392 | 30:a:615:LUT:C24 | 2.42 | 0.49 |
| 2:B:528:HIS:CD2 | 21:B:837:CLA:NB | 2.79 | 0.49 |
| 21:B:827:CLA:H142 | 24:B:843:BCR:C37 | 2.42 | 0.49 |
| 17:7:230:PHE:HD2 | 17:7:233:LEU:HB2 | 1.77 | 0.49 |
| 21:B:813:CLA:HBA1 | 24:B:843:BCR:C39 | 2.41 | 0.49 |
| 1:A:264:LEU:HD21 | 11:K:120:VAL:HG22 | 1.94 | 0.49 |
| 21:B:836:CLA:H142 | 21:B:836:CLA:HMC2 | 1.94 | 0.49 |
| 21:4:602:CLA:CHB | 21:4:602:CLA:H11 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:a:209:LEU:HG | 21:a:610:CLA:HHB | 1.95 | 0.49 |
| 15:1:222:HIS:CD2 | 21:1:314:CLA:NC | 2.80 | 0.49 |
| 16:6:113:TRP:CE2 | 29:6:607:CHL:HED2 | 2.47 | 0.49 |
| 16:6:163:TRP:HE1 | 16:6:167:ARG:HH21 | 1.61 | 0.49 |
| 20:a:228:PHE:O | 20:a:232:ILE:HG12 | 2.12 | 0.49 |
| 20:c:143:LEU:O | 20:c:152:VAL:HG13 | 2.12 | 0.49 |
| 29:6:614:CHL:HHC | 29:6:614:CHL:HBB1 | 1.95 | 0.49 |
| 20:c:97:LEU:HD11 | 21:c:603:CLA:HBD | 1.94 | 0.49 |
| 21:A:840:CLA:HAB | 21:A:840:CLA:H93 | 1.94 | 0.49 |
| 4:D:140:ARG:NH2 | 4:D:142:GLU:OE1 | 2.46 | 0.49 |
| 21:9:611:CLA:H41 | 21:9:611:CLA:H61 | 1.55 | 0.49 |
| 20:a:212:LYS:HD3 | 20:a:215:LYS:HD2 | 1.94 | 0.49 |
| 1:A:559:ARG:NH2 | 4:D:94:THR:O | 2.45 | 0.49 |
| 16:2:272:GLY:HA2 | 17:3:186:PRO:HG2 | 1.93 | 0.49 |
| 29:6:605:CHL:HHC | 29:6:605:CHL:HBB1 | 1.95 | 0.49 |
| 1:A:317:HIS:HE1 | 21:A:822:CLA:C4A | 2.25 | 0.48 |
| 24:A:854:BCR:C13 | 24:K:205:BCR:C32 | 2.89 | 0.48 |
| 21:4:601:CLA:HBB1 | 23:4:618:LHG:H262 | 1.94 | 0.48 |
| 16:6:122:PHE:CZ | 30:6:616:LUT:H28 | 2.48 | 0.48 |
| 23:6:619:LHG:HC81 | 24:7:417:BCR:H333 | 1.94 | 0.48 |
| 20:b:253:ASN:ND2 | 20:b:255:TRP:HD1 | 2.11 | 0.48 |
| 17:7:172:PRO:O | 17:7:175:THR:OG1 | 2.31 | 0.48 |
| 21:A:826:CLA:HAA2 | 21:A:827:CLA:OBD | 2.13 | 0.48 |
| 18:4:254:HIS:CD2 | 21:4:613:CLA:NC | 2.81 | 0.48 |
| 16:6:187:ASN:HB3 | 29:6:614:CHL:C2D | 2.43 | 0.48 |
| 21:6:604:CLA:C1C | 24:6:618:BCR:H272 | 2.43 | 0.48 |
| 18:8:225:ASN:OD1 | 30:8:614:LUT:H201 | 2.14 | 0.48 |
| 20:a:151:LEU:C | 20:a:152:VAL:HG22 | 2.39 | 0.48 |
| 21:b:311:CLA:H2 | 30:b:316:LUT:H28 | 1.94 | 0.48 |
| 1:A:216:HIS:HE1 | 21:A:816:CLA:C4D | 2.27 | 0.48 |
| 1:A:262:PHE:HA | 21:K:203:CLA:HBC3 | 1.94 | 0.48 |
| 24:A:854:BCR:H23C | 11:K:114:LEU:HD13 | 1.95 | 0.48 |
| 21:B:831:CLA:HBC3 | 21:B:831:CLA:HHD | 1.95 | 0.48 |
| 16:6:212:ASP:OD1 | 16:6:216:LEU:N | 2.46 | 0.48 |
| 17:7:132:ALA:HA | 17:7:136:ILE:HD12 | 1.95 | 0.48 |
| 18:8:215:LEU:HB2 | 18:8:219:ARG:HE | 1.78 | 0.48 |
| 20:a:151:LEU:O | 20:a:152:VAL:CG2 | 2.61 | 0.48 |
| 21:a:611:CLA:H2A | 21:a:611:CLA:CED | 2.43 | 0.48 |
| 20:b:160:ILE:HG12 | 29:b:306:CHL:HAC1 | 1.95 | 0.48 |
| 20:c:171:VAL:HB | 20:c:175:ARG:NH1 | 2.28 | 0.48 |
| 21:4:602:CLA:HBC1 | 23:4:618:LHG:H252 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:5:136:ASN:O | 15:5:140:ILE:HG12 | 2.13 | 0.48 |
| 16:6:112:ARG:HB3 | 29:6:607:CHL:HED1 | 1.95 | 0.48 |
| 17:7:260:GLU:O | 17:7:264:GLN:HG2 | 2.13 | 0.48 |
| 17:7:281:VAL:HG12 | 17:7:285:PHE:CE2 | 2.46 | 0.48 |
| 20:c:247:ALA:O | 20:c:252:ASN:ND2 | 2.47 | 0.48 |
| 20:b:106:MET:HE3 | 21:b:311:CLA:HMC2 | 1.96 | 0.48 |
| 1:A:450:PHE:HD2 | 21:B:802:CLA:H61 | 1.79 | 0.48 |
| 1:A:657:ILE:HD12 | 2:B:621:ARG:HG3 | 1.94 | 0.48 |
| 2:B:29:HIS:HE1 | 21:B:803:CLA:C4B | 2.27 | 0.48 |
| 24:J:104:BCR:HC8 | 24:J:104:BCR:H331 | 1.95 | 0.48 |
| 18:8:94:ALA:HB2 | 21:8:602:CLA:HBA1 | 1.95 | 0.48 |
| 18:8:149:ASP:HB3 | 18:8:152:THR:HG23 | 1.96 | 0.48 |
| 20:c:137:ILE:HD11 | 20:c:161:TRP:HZ2 | 1.79 | 0.48 |
| 2:B:441:ASP:OD1 | 2:B:615:TYR:HB2 | 2.14 | 0.48 |
| 21:2:609:CLA:CBC | 21:2:609:CLA:CHD | 2.78 | 0.48 |
| 18:4:69:LEU:HD13 | 21:4:601:CLA:HMA3 | 1.96 | 0.48 |
| 20:c:164:GLN:HB2 | 29:c:606:CHL:HMA3 | 1.95 | 0.48 |
| 1:A:118:ILE:HG13 | 1:A:119:VAL:HG13 | 1.94 | 0.48 |
| 2:B:173:SER:O | 2:B:177:HIS:HD2 | 1.97 | 0.48 |
| 2:B:323:TYR:CE1 | 21:B:823:CLA:HBC1 | 2.49 | 0.48 |
| 20:a:209:LEU:HD23 | 21:a:610:CLA:H3A | 1.96 | 0.48 |
| 21:a:604:CLA:H2 | 29:a:606:CHL:HAA1 | 1.96 | 0.48 |
| 20:b:50:TYR:CZ | 20:b:207:ALA:HB1 | 2.49 | 0.48 |
| 21:B:836:CLA:HMC2 | 21:B:836:CLA:H112 | 1.95 | 0.48 |
| 29:2:602:CHL:HBB1 | 29:2:602:CHL:HHC | 1.96 | 0.48 |
| 21:5:602:CLA:HAB | 31:5:616:XAT:C32 | 2.44 | 0.48 |
| 17:7:245:TYR:OH | 21:7:408:CLA:H2A | 2.13 | 0.48 |
| 17:7:313:THR:HG22 | 20:b:250:VAL:HG21 | 1.96 | 0.48 |
| 19:9:297:THR:HG22 | 19:9:298:GLY:N | 2.29 | 0.48 |
| 21:A:805:CLA:HMC3 | 21:A:807:CLA:HED3 | 1.95 | 0.47 |
| 21:A:818:CLA:H62 | 21:A:818:CLA:H41 | 1.62 | 0.47 |
| 21:B:839:CLA:H192 | 12:L:157:ILE:HD13 | 1.96 | 0.47 |
| 5:E:101:ALA:HB3 | 5:E:104:VAL:HG23 | 1.95 | 0.47 |
| 21:2:609:CLA:C4B | 21:2:609:CLA:H42 | 2.44 | 0.47 |
| 18:4:202:PHE:HB3 | 21:4:609:CLA:HMD1 | 1.94 | 0.47 |
| 21:A:840:CLA:H92 | 21:B:831:CLA:H11 | 1.95 | 0.47 |
| 2:B:276:HIS:HB2 | 21:B:816:CLA:C1B | 2.44 | 0.47 |
| 21:3:408:CLA:HBB1 | 21:3:408:CLA:HHC | 1.96 | 0.47 |
| 19:9:118:LEU:HB3 | 19:9:124:THR:HG21 | 1.96 | 0.47 |
| 1:A:511:ASP:OD1 | 1:A:511:ASP:N | 2.47 | 0.47 |
| 16:2:156:ILE:HG12 | 21:4:613:CLA:HAA2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:7:117:GLY:HA2 | 17:7:268:VAL:HG23 | 1.95 | 0.47 |
| 2:B:192:GLY:O | 2:B:196:HIS:HB2 | 2.13 | 0.47 |
| 3:C:61:ASP:HB2 | 5:E:123:ASN:ND2 | 2.29 | 0.47 |
| 17:3:302:HIS:CD2 | 21:3:413:CLA:NC | 2.81 | 0.47 |
| 20:a:215:LYS:NZ | 21:a:611:CLA:O1D | 2.47 | 0.47 |
| 21:B:809:CLA:HBA1 | 21:B:809:CLA:H3A | 1.68 | 0.47 |
| 21:3:404:CLA:CHC | 24:3:418:BCR:H393 | 2.45 | 0.47 |
| 17:7:143:TYR:O | 17:7:147:ILE:HG12 | 2.14 | 0.47 |
| 18:8:224:LYS:CD | 21:8:609:CLA:C2D | 2.93 | 0.47 |
| 20:a:172:GLU:OE1 | 20:a:175:ARG:NE | 2.46 | 0.47 |
| 20:c:102:ALA:HB2 | 20:c:221:MET:HE2 | 1.96 | 0.47 |
| 11:K:59:MET:HE1 | 11:K:116:HIS:HA | 1.97 | 0.47 |
| 15:5:162:GLU:HG2 | 15:5:165:LYS:HZ1 | 1.78 | 0.47 |
| 16:6:183:VAL:HG22 | 21:8:609:CLA:HBB1 | 1.94 | 0.47 |
| 1:A:50:HIS:CE1 | 21:A:804:CLA:C4D | 2.97 | 0.47 |
| 1:A:133:GLN:OE1 | 6:F:113:ARG:NH2 | 2.48 | 0.47 |
| 2:B:287:ALA:HB2 | 21:B:818:CLA:HBC2 | 1.97 | 0.47 |
| 21:B:807:CLA:H11 | 21:B:826:CLA:HBA2 | 1.96 | 0.47 |
| 21:B:813:CLA:H3A | 24:B:843:BCR:H393 | 1.96 | 0.47 |
| 14:O:135:PHE:C | 14:O:137:GLY:H | 2.23 | 0.47 |
| 15:1:110:ASN:C | 15:1:112:VAL:H | 2.23 | 0.47 |
| 21:4:609:CLA:H12 | 21:4:609:CLA:CHB | 2.45 | 0.47 |
| 18:8:80:GLY:HA2 | 18:8:85:ASP:HB3 | 1.95 | 0.47 |
| 31:9:616:XAT:H11 | 31:9:616:XAT:H191 | 1.76 | 0.47 |
| 20:c:152:VAL:HG13 | 20:c:153:HIS:N | 2.28 | 0.47 |
| 21:A:820:CLA:HBB1 | 24:A:854:BCR:H14C | 1.97 | 0.47 |
| 20:a:130:TRP:H | 20:a:130:TRP:CD1 | 2.33 | 0.47 |
| 20:c:148:ASN:HB3 | 20:c:151:LEU:HD12 | 1.97 | 0.47 |
| 2:B:662:MET:HB2 | 21:B:802:CLA:C1C | 2.45 | 0.47 |
| 16:6:117:GLY:HA3 | 31:6:617:XAT:H10 | 1.96 | 0.47 |
| 18:8:197:PRO:HB3 | 29:8:607:CHL:HBC2 | 1.97 | 0.47 |
| 30:8:614:LUT:H30 | 21:8:618:CLA:CAB | 2.41 | 0.47 |
| 20:a:61:PHE:HD1 | 20:c:177:ALA:HB3 | 1.80 | 0.47 |
| 20:a:184:ILE:HD11 | 20:a:187:PRO:HA | 1.97 | 0.47 |
| 20:b:175:ARG:NH2 | 29:b:310:CHL:O1D | 2.40 | 0.47 |
| 1:A:25:LYS:HB2 | 21:A:812:CLA:HAA2 | 1.97 | 0.47 |
| 21:A:801:CLA:C1A | 21:B:801:CLA:HAB | 2.45 | 0.47 |
| 2:B:498:LEU:HA | 2:B:501:ILE:HG22 | 1.96 | 0.47 |
| 21:B:804:CLA:H3A | 21:B:804:CLA:HBA1 | 1.31 | 0.47 |
| 29:2:614:CHL:HBB2 | 24:2:618:BCR:H321 | 1.96 | 0.47 |
| 15:5:154:GLN:HE22 | 21:5:607:CLA:C4C | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:7:284:TYR:HE1 | 30:7:415:LUT:H21 | 1.78 | 0.47 |
| 18:8:99:ARG:O | 18:8:103:MET:HG2 | 2.14 | 0.47 |
| 1:A:294:HIS:CD2 | 1:A:298:ILE:HG12 | 2.50 | 0.46 |
| 21:A:825:CLA:H143 | 21:A:825:CLA:H161 | 1.76 | 0.46 |
| 2:B:657:TRP:CD2 | 21:B:801:CLA:HMA2 | 2.50 | 0.46 |
| 29:2:602:CHL:H3A | 29:2:602:CHL:HBA2 | 1.60 | 0.46 |
| 29:4:606:CHL:HHC | 29:4:606:CHL:HBB1 | 1.97 | 0.46 |
| 29:a:607:CHL:HAA1 | 31:a:618:XAT:H42 | 1.96 | 0.46 |
| 21:A:842:CLA:HMD3 | 24:B:846:BCR:C38 | 2.43 | 0.46 |
| 24:A:854:BCR:H402 | 11:K:114:LEU:HD22 | 1.97 | 0.46 |
| 21:B:809:CLA:H92 | 12:L:143:ALA:HA | 1.97 | 0.46 |
| 28:G:206:LMG:H122 | 29:1:307:CHL:H12 | 1.97 | 0.46 |
| 11:K:72:PHE:O | 11:K:74:LEU:N | 2.45 | 0.46 |
| 21:6:609:CLA:HBB1 | 21:6:611:CLA:H3A | 1.96 | 0.46 |
| 17:7:194:TRP:CD1 | 17:7:194:TRP:H | 2.32 | 0.46 |
| 17:7:214:ARG:HH11 | 17:7:225:MET:HE3 | 1.80 | 0.46 |
| 18:8:224:LYS:HE2 | 21:8:609:CLA:C2D | 2.45 | 0.46 |
| 18:8:254:HIS:CD2 | 21:8:612:CLA:NC | 2.82 | 0.46 |
| 20:a:186:ASP:N | 20:a:186:ASP:OD1 | 2.47 | 0.46 |
| 16:2:263:THR:HG23 | 16:2:265:PHE:H | 1.80 | 0.46 |
| 17:3:269:LYS:HD3 | 21:3:411:CLA:HAA2 | 1.97 | 0.46 |
| 21:3:412:CLA:H2 | 21:3:412:CLA:H61 | 1.67 | 0.46 |
| 18:8:201:TRP:CE2 | 29:8:613:CHL:ND | 2.83 | 0.46 |
| 29:9:606:CHL:HBB1 | 30:9:615:LUT:H161 | 1.96 | 0.46 |
| 23:9:618:LHG:HC62 | 23:9:618:LHG:H242 | 1.62 | 0.46 |
| 1:A:287:TRP:HB2 | 1:A:290:ASP:OD2 | 2.15 | 0.46 |
| 21:A:821:CLA:H52 | 21:A:824:CLA:H2 | 1.96 | 0.46 |
| 15:1:128:LEU:O | 15:1:128:LEU:HD23 | 2.15 | 0.46 |
| 15:1:141:LEU:HD13 | 29:1:307:CHL:HBC1 | 1.96 | 0.46 |
| 29:2:607:CHL:HHC | 29:2:607:CHL:HBB1 | 1.96 | 0.46 |
| 21:4:609:CLA:H41 | 21:4:609:CLA:H62 | 1.45 | 0.46 |
| 29:6:601:CHL:OBD | 17:7:214:ARG:NH1 | 2.48 | 0.46 |
| 17:7:240:SER:OG | 17:7:246:PRO:O | 2.32 | 0.46 |
| 20:c:164:GLN:OE1 | 29:c:606:CHL:NA | 2.48 | 0.46 |
| 1:A:498:ASN:HB2 | 21:A:836:CLA:HED2 | 1.98 | 0.46 |
| 2:B:89:HIS:CD2 | 21:B:807:CLA:NA | 2.83 | 0.46 |
| 2:B:209:TRP:CH2 | 24:B:843:BCR:H351 | 2.51 | 0.46 |
| 17:3:256:PHE:CB | 21:3:409:CLA:HBA1 | 2.44 | 0.46 |
| 29:7:406:CHL:HMA1 | 24:7:417:BCR:H361 | 1.97 | 0.46 |
| 29:b:308:CHL:H62 | 29:b:308:CHL:H41 | 1.56 | 0.46 |
| 1:A:360:LEU:O | 1:A:364:VAL:HG23 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:A:840:CLA:HED2 | 2:B:420:SER:HB3 | 1.97 | 0.46 |
| 21:A:842:CLA:HMD2 | 24:B:846:BCR:H383 | 1.95 | 0.46 |
| 3:C:32:ASP:OD1 | 3:C:32:ASP:N | 2.48 | 0.46 |
| 6:F:158:VAL:HG12 | 6:F:168:PHE:HB2 | 1.97 | 0.46 |
| 14:O:96:ILE:HG22 | 14:O:104:PRO:HG2 | 1.96 | 0.46 |
| 17:3:247:GLY:HA2 | 21:3:409:CLA:HED3 | 1.97 | 0.46 |
| 18:8:224:LYS:CE | 21:8:609:CLA:C2D | 2.93 | 0.46 |
| 20:a:161:TRP:HB2 | 29:a:607:CHL:HBC1 | 1.98 | 0.46 |
| 1:A:197:HIS:HE1 | 21:A:813:CLA:NA | 2.12 | 0.46 |
| 21:B:806:CLA:HBB1 | 21:B:806:CLA:HMB3 | 1.97 | 0.46 |
| 16:2:113:TRP:CE2 | 29:2:607:CHL:HED2 | 2.51 | 0.46 |
| 1:A:328:GLY:N | 23:A:845:LHG:HC32 | 2.31 | 0.46 |
| 15:1:148:ILE:HG21 | 21:1:309:CLA:CMC | 2.45 | 0.46 |
| 18:4:196:TYR:HB3 | 21:4:609:CLA:O1D | 2.15 | 0.46 |
| 21:6:609:CLA:O1D | 21:6:609:CLA:H2A | 2.16 | 0.46 |
| 20:c:229:VAL:O | 20:c:233:VAL:HG12 | 2.15 | 0.46 |
| 1:A:291:THR:HG23 | 21:A:819:CLA:HMA3 | 1.97 | 0.46 |
| 1:A:578:ARG:HG2 | 3:C:78:GLY:HA3 | 1.98 | 0.46 |
| 21:A:840:CLA:HAA2 | 21:B:830:CLA:HMB1 | 1.98 | 0.46 |
| 2:B:47:PHE:CE2 | 2:B:51:PHE:HE2 | 2.34 | 0.46 |
| 21:B:814:CLA:H91 | 21:B:814:CLA:H112 | 1.72 | 0.46 |
| 21:5:607:CLA:HBA2 | 21:5:607:CLA:H3A | 1.52 | 0.46 |
| 17:7:311:VAL:HG13 | 17:7:312:LEU:N | 2.26 | 0.46 |
| 21:9:610:CLA:H2 | 30:9:614:LUT:H28 | 1.96 | 0.46 |
| 20:b:207:ALA:O | 20:b:211:VAL:HG23 | 2.16 | 0.46 |
| 1:A:432:ASP:OD1 | 4:D:94:THR:OG1 | 2.30 | 0.46 |
| 2:B:95:HIS:HE1 | 21:B:809:CLA:NB | 2.05 | 0.46 |
| 24:K:205:BCR:H361 | 24:K:205:BCR:H20C | 1.75 | 0.46 |
| 18:4:115:MET:SD | 21:4:609:CLA:HAB | 2.56 | 0.46 |
| 21:4:609:CLA:HMB3 | 21:4:609:CLA:HBB1 | 1.97 | 0.46 |
| 15:5:183:GLU:OE1 | 15:5:183:GLU:N | 2.49 | 0.46 |
| 17:7:312:LEU:HG | 17:7:314:ASN:H | 1.81 | 0.46 |
| 18:8:254:HIS:HB2 | 21:8:611:CLA:HAA2 | 1.98 | 0.46 |
| 29:8:607:CHL:HHC | 29:8:607:CHL:HBB1 | 1.97 | 0.46 |
| 20:a:116:GLU:HB3 | 20:a:239:LEU:HD22 | 1.97 | 0.46 |
| 20:a:224:MET:HE2 | 30:a:616:LUT:H12 | 1.98 | 0.46 |
| 20:c:167:LEU:O | 20:c:171:VAL:HG13 | 2.16 | 0.46 |
| 21:c:602:CLA:H92 | 21:c:603:CLA:HMA3 | 1.97 | 0.46 |
| 1:A:366:HIS:HA | 1:A:369:TYR:CE1 | 2.51 | 0.45 |
| 2:B:33:SER:HB3 | 27:B:847:DGD:HE62 | 1.98 | 0.45 |
| 2:B:142:LEU:HD21 | 24:B:843:BCR:H23C | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:149:ASN:OD1 | 7:G:150:GLY:N | 2.50 | 0.45 |
| 16:2:112:ARG:HB3 | 21:2:609:CLA:HAC2 | 1.98 | 0.45 |
| 18:4:154:PHE:O | 18:4:157:GLU:HG2 | 2.16 | 0.45 |
| 16:6:255:HIS:CE1 | 16:6:259:PRO:HB3 | 2.51 | 0.45 |
| 19:9:224:VAL:O | 19:9:228:GLN:HG2 | 2.16 | 0.45 |
| 20:b:79:TRP:CE3 | 30:b:317:LUT:H383 | 2.51 | 0.45 |
| 2:B:624:LEU:HD22 | 21:B:801:CLA:CMD | 2.43 | 0.45 |
| 21:B:817:CLA:H112 | 21:B:817:CLA:H72 | 1.53 | 0.45 |
| 15:5:67:PHE:HB3 | 21:5:602:CLA:CAD | 2.46 | 0.45 |
| 15:5:111:TRP:HZ3 | 15:5:215:PRO:HD3 | 1.81 | 0.45 |
| 1:A:729:HIS:HE1 | 21:A:841:CLA:C4D | 2.29 | 0.45 |
| 2:B:191:THR:HG21 | 2:B:278:LEU:HB2 | 1.96 | 0.45 |
| 12:L:97:PRO:O | 12:L:108:ARG:HD2 | 2.17 | 0.45 |
| 29:2:602:CHL:HBB1 | 31:2:617:XAT:H32 | 1.97 | 0.45 |
| 17:3:108:LEU:HB3 | 17:3:110:TYR:CE2 | 2.51 | 0.45 |
| 17:7:140:TRP:CZ3 | 21:7:402:CLA:HBA1 | 2.48 | 0.45 |
| 17:7:302:HIS:CG | 21:7:411:CLA:HAA2 | 2.51 | 0.45 |
| 21:8:611:CLA:H51 | 21:8:611:CLA:H8 | 1.53 | 0.45 |
| 19:9:308:TRP:NE1 | 21:9:613:CLA:HBA1 | 2.31 | 0.45 |
| 20:a:99:VAL:HG21 | 20:a:188:ILE:HG13 | 1.98 | 0.45 |
| 20:a:245:HIS:CD2 | 21:a:614:CLA:NC | 2.84 | 0.45 |
| 1:A:275:PHE:HE2 | 1:A:499:ALA:HB2 | 1.81 | 0.45 |
| 1:A:356:MET:HE3 | 21:A:821:CLA:H93 | 1.98 | 0.45 |
| 1:A:393:TRP:CD1 | 21:A:828:CLA:HAB | 2.51 | 0.45 |
| 2:B:156:HIS:HE1 | 21:B:810:CLA:C1A | 2.29 | 0.45 |
| 21:B:827:CLA:H142 | 21:B:827:CLA:H112 | 1.80 | 0.45 |
| 7:G:149:ASN:CG | 7:G:151:TYR:H | 2.23 | 0.45 |
| 16:2:218:GLU:OE2 | 16:2:222:LYS:NZ | 2.34 | 0.45 |
| 17:3:208:MET:HB2 | 21:3:408:CLA:HBB1 | 1.98 | 0.45 |
| 17:7:201:PHE:O | 17:7:204:GLU:HG3 | 2.16 | 0.45 |
| 21:A:810:CLA:HAB | 21:B:832:CLA:HMD2 | 1.99 | 0.45 |
| 21:A:838:CLA:HBB1 | 21:A:838:CLA:HMB3 | 1.98 | 0.45 |
| 6:F:227:GLY:C | 18:4:99:ARG:HH21 | 2.23 | 0.45 |
| 21:G:202:CLA:CGA | 21:G:202:CLA:H3A | 2.42 | 0.45 |
| 9:I:19:PRO:HA | 9:I:22:THR:HG22 | 1.98 | 0.45 |
| 29:1:302:CHL:HBA1 | 29:1:302:CHL:H3A | 1.78 | 0.45 |
| 21:5:602:CLA:O1A | 31:5:616:XAT:H241 | 2.16 | 0.45 |
| 20:a:73:PHE:HZ | 20:a:95:ARG:HG2 | 1.81 | 0.45 |
| 21:A:809:CLA:CHC | 21:A:810:CLA:HMD2 | 2.47 | 0.45 |
| 3:C:47:ASP:OD2 | 4:D:141:LYS:NZ | 2.44 | 0.45 |
| 21:K:201:CLA:NA | 24:K:205:BCR:H402 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:6:239:VAL:HG11 | 21:6:612:CLA:HAC2 | 1.98 | 0.45 |
| 18:8:113:TRP:CZ2 | 29:8:607:CHL:HED2 | 2.51 | 0.45 |
| 20:b:169:GLY:HA2 | 29:b:310:CHL:HAB | 1.99 | 0.45 |
| 1:A:642:ASN:HB2 | 2:B:651:LEU:HD11 | 1.99 | 0.45 |
| 21:A:830:CLA:HMD2 | 23:A:844:LHG:H271 | 1.99 | 0.45 |
| 23:A:855:LHG:HC61 | 23:A:855:LHG:H241 | 1.58 | 0.45 |
| 15:5:148:ILE:HA | 15:5:151:VAL:HG22 | 1.99 | 0.45 |
| 18:8:146:TYR:CE1 | 21:8:604:CLA:HAA2 | 2.52 | 0.45 |
| 29:8:605:CHL:C1B | 24:8:616:BCR:H383 | 2.47 | 0.45 |
| 19:9:236:GLU:HG3 | 29:9:609:CHL:C4B | 2.47 | 0.45 |
| 20:b:152:VAL:HG23 | 20:b:153:HIS:N | 2.30 | 0.45 |
| 21:B:814:CLA:H112 | 24:G:201:BCR:H23C | 1.99 | 0.45 |
| 21:B:840:CLA:HBB1 | 21:B:840:CLA:HMB3 | 1.99 | 0.45 |
| 18:4:137:SER:HB3 | 18:4:140:LYS:HG2 | 1.99 | 0.45 |
| 29:5:601:CHL:OBD | 18:8:167:ARG:NH1 | 2.50 | 0.45 |
| 30:7:415:LUT:H15 | 30:7:415:LUT:H201 | 1.80 | 0.45 |
| 19:9:273:LYS:O | 19:9:277:ILE:HG12 | 2.17 | 0.45 |
| 31:9:616:XAT:H391 | 31:9:616:XAT:H31 | 1.66 | 0.45 |
| 20:c:245:HIS:HB2 | 21:c:613:CLA:HAA2 | 1.97 | 0.45 |
| 21:B:801:CLA:HBA2 | 21:B:801:CLA:H3A | 1.66 | 0.45 |
| 24:J:103:BCR:H341 | 24:J:103:BCR:C12 | 2.46 | 0.45 |
| 18:4:181:ASP:HB3 | 18:4:184:PHE:O | 2.17 | 0.45 |
| 17:7:230:PHE:CD2 | 17:7:233:LEU:HB2 | 2.52 | 0.45 |
| 20:b:222:PHE:HE2 | 21:b:314:CLA:HAB | 1.80 | 0.45 |
| 1:A:294:HIS:HD2 | 1:A:294:HIS:O | 2.00 | 0.45 |
| 21:1:306:CLA:HED2 | 21:1:306:CLA:HBD | 1.82 | 0.45 |
| 29:a:607:CHL:HBC2 | 20:b:255:TRP:CH2 | 2.51 | 0.45 |
| 20:b:104:TRP:CE2 | 29:b:309:CHL:HED2 | 2.52 | 0.45 |
| 1:A:713:GLN:NE2 | 5:E:114:LYS:HB2 | 2.32 | 0.44 |
| 4:D:161:PHE:CZ | 4:D:174:HIS:HB2 | 2.52 | 0.44 |
| 24:7:418:BCR:H361 | 24:7:418:BCR:H20C | 1.85 | 0.44 |
| 20:c:101:HIS:HE1 | 21:c:603:CLA:ND | 2.10 | 0.44 |
| 20:c:160:ILE:HG13 | 20:c:161:TRP:CD1 | 2.48 | 0.44 |
| 2:B:180:SER:OG | 2:B:288:GLY:HA3 | 2.18 | 0.44 |
| 15:1:184:GLU:HG2 | 15:1:188:LYS:HE3 | 1.98 | 0.44 |
| 21:1:304:CLA:H51 | 21:1:304:CLA:H11 | 1.72 | 0.44 |
| 15:5:151:VAL:O | 15:5:154:GLN:HG3 | 2.17 | 0.44 |
| 21:7:402:CLA:HMD3 | 21:7:407:CLA:ND | 2.32 | 0.44 |
| 18:8:167:ARG:HH21 | 18:8:178:VAL:HB | 1.83 | 0.44 |
| 19:9:260:LEU:HD21 | 20:b:197:LEU:HD22 | 1.99 | 0.44 |
| 20:a:76:ASP:OD1 | 20:a:76:ASP:N | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:a:612:CLA:HBA1 | 21:a:612:CLA:H3A | 1.81 | 0.44 |
| 21:A:826:CLA:HAB | 24:A:849:BCR:H311 | 2.00 | 0.44 |
| 15:5:120:THR:OG1 | 15:5:121:PRO:HD3 | 2.17 | 0.44 |
| 16:6:234:VAL:HG23 | 16:6:235:LEU:HD12 | 2.00 | 0.44 |
| 21:8:609:CLA:C1B | 23:8:617:LHG:HC32 | 2.47 | 0.44 |
| 21:A:830:CLA:CAD | 23:A:844:LHG:H252 | 2.48 | 0.44 |
| 21:B:827:CLA:H161 | 24:B:843:BCR:C36 | 2.47 | 0.44 |
| 21:B:836:CLA:H143 | 21:B:836:CLA:H161 | 1.81 | 0.44 |
| 6:F:146:LEU:HD21 | 10:J:38:VAL:HG11 | 1.99 | 0.44 |
| 12:L:165:GLU:N | 12:L:165:GLU:OE1 | 2.50 | 0.44 |
| 21:3:409:CLA:H3A | 21:3:409:CLA:HBA2 | 1.42 | 0.44 |
| 18:4:231:LEU:HD23 | 18:4:231:LEU:HA | 1.87 | 0.44 |
| 20:c:168:MET:HE1 | 29:c:609:CHL:HHC | 2.00 | 0.44 |
| 20:c:184:ILE:HG13 | 20:c:184:ILE:O | 2.18 | 0.44 |
| 21:A:802:CLA:CGA | 21:A:802:CLA:H3A | 2.48 | 0.44 |
| 21:A:832:CLA:HBB1 | 21:A:842:CLA:HAA2 | 1.98 | 0.44 |
| 21:A:842:CLA:H152 | 21:A:842:CLA:H112 | 1.75 | 0.44 |
| 24:I:101:BCR:H11C | 24:I:101:BCR:H341 | 1.86 | 0.44 |
| 21:4:602:CLA:O1A | 31:4:616:XAT:H241 | 2.17 | 0.44 |
| 15:5:73:GLY:HA3 | 15:5:79:LEU:HD13 | 2.00 | 0.44 |
| 17:7:165:LEU:HD23 | 17:7:165:LEU:HA | 1.87 | 0.44 |
| 19:9:237:TYR:CE1 | 19:9:241:LYS:HG3 | 2.53 | 0.44 |
| 29:9:601:CHL:HHC | 29:9:601:CHL:HBB1 | 2.00 | 0.44 |
| 20:b:50:TYR:CE1 | 20:b:207:ALA:HB1 | 2.53 | 0.44 |
| 2:B:593:TYR:CZ | 21:B:835:CLA:HBC3 | 2.53 | 0.44 |
| 21:B:823:CLA:H111 | 21:B:823:CLA:H91 | 1.62 | 0.44 |
| 16:2:111:CYS:SG | 16:2:231:MET:HE2 | 2.57 | 0.44 |
| 21:3:409:CLA:H41 | 30:3:416:LUT:C29 | 2.48 | 0.44 |
| 21:4:609:CLA:H43 | 30:4:615:LUT:H26 | 1.99 | 0.44 |
| 16:6:111:CYS:HB2 | 16:6:227:GLY:HA3 | 2.00 | 0.44 |
| 17:7:208:MET:HB3 | 21:7:407:CLA:HAB | 2.00 | 0.44 |
| 21:8:603:CLA:HMC1 | 31:8:615:XAT:H203 | 1.99 | 0.44 |
| 7:G:83:PHE:O | 7:G:87:ASN:ND2 | 2.25 | 0.44 |
| 31:1:318:XAT:H35 | 31:1:318:XAT:H401 | 1.89 | 0.44 |
| 21:3:401:CLA:HBB1 | 21:3:401:CLA:HMB3 | 1.98 | 0.44 |
| 15:5:169:GLY:O | 15:5:170:PRO:C | 2.61 | 0.44 |
| 30:7:415:LUT:H191 | 30:7:415:LUT:H12 | 2.00 | 0.44 |
| 18:8:161:MET:HG2 | 21:8:608:CLA:HMC3 | 2.00 | 0.44 |
| 19:9:91:ALA:C | 19:9:93:TRP:H | 2.26 | 0.44 |
| 20:b:248:ASP:O | 20:b:252:ASN:ND2 | 2.32 | 0.44 |
| 16:2:201:TRP:HH2 | 29:2:614:CHL:NB | 2.14 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:4:615:LUT:H11 | 30:4:615:LUT:H191 | 1.87 | 0.44 |
| 29:6:607:CHL:HMA1 | 24:6:618:BCR:H362 | 1.99 | 0.44 |
| 17:7:121:PHE:HB3 | 21:7:401:CLA:HMD2 | 1.99 | 0.44 |
| 1:A:480:PHE:HB3 | 21:A:837:CLA:H12 | 2.00 | 0.44 |
| 2:B:359:ALA:O | 2:B:360:PHE:HB2 | 2.18 | 0.44 |
| 2:B:395:ILE:HD12 | 2:B:555:TYR:HD1 | 1.83 | 0.44 |
| 2:B:519:VAL:HG11 | 2:B:593:TYR:CG | 2.52 | 0.44 |
| 21:B:817:CLA:H143 | 21:B:817:CLA:H161 | 1.80 | 0.44 |
| 11:K:88:LEU:HD12 | 21:K:204:CLA:HED3 | 2.00 | 0.44 |
| 21:1:306:CLA:HBB2 | 29:1:307:CHL:CBB | 2.48 | 0.44 |
| 19:9:92:GLU:HA | 19:9:95:LYS:HB3 | 1.99 | 0.44 |
| 1:A:195:LEU:HD12 | 1:A:319:MET:HE1 | 1.99 | 0.43 |
| 1:A:302:PHE:CE1 | 21:A:821:CLA:HAB | 2.52 | 0.43 |
| 21:B:807:CLA:H8 | 21:B:807:CLA:HBB1 | 2.01 | 0.43 |
| 7:G:69:THR:HA | 7:G:136:GLY:HA3 | 2.00 | 0.43 |
| 15:1:151:VAL:HG13 | 21:1:308:CLA:C1B | 2.48 | 0.43 |
| 16:2:198:GLY:HA2 | 21:2:609:CLA:CED | 2.48 | 0.43 |
| 16:2:223:GLU:HG3 | 21:2:609:CLA:C4B | 2.48 | 0.43 |
| 16:6:230:ALA:O | 16:6:234:VAL:HG22 | 2.18 | 0.43 |
| 21:7:401:CLA:HBB2 | 31:7:416:XAT:H34 | 1.98 | 0.43 |
| 29:9:605:CHL:HBA1 | 29:9:605:CHL:H3A | 1.80 | 0.43 |
| 20:a:69:LEU:HD23 | 20:a:69:LEU:HA | 1.85 | 0.43 |
| 31:c:617:XAT:H31 | 31:c:617:XAT:H391 | 1.87 | 0.43 |
| 2:B:62:SER:HB2 | 2:B:142:LEU:HB2 | 2.01 | 0.43 |
| 21:B:806:CLA:H93 | 21:B:806:CLA:H61 | 1.70 | 0.43 |
| 24:L:306:BCR:H20C | 24:L:306:BCR:H361 | 1.86 | 0.43 |
| 15:1:199:ALA:HA | 21:1:313:CLA:HBB1 | 2.00 | 0.43 |
| 16:2:187:ASN:HB3 | 29:2:614:CHL:C2D | 2.47 | 0.43 |
| 16:2:255:HIS:CD2 | 21:2:613:CLA:NC | 2.86 | 0.43 |
| 17:3:216:ALA:HB2 | 21:3:408:CLA:HMA1 | 1.99 | 0.43 |
| 21:3:408:CLA:H62 | 21:3:408:CLA:H41 | 1.53 | 0.43 |
| 24:3:418:BCR:H11C | 24:3:418:BCR:H341 | 1.88 | 0.43 |
| 29:5:606:CHL:HBB1 | 29:5:606:CHL:HHC | 2.00 | 0.43 |
| 21:8:611:CLA:HED2 | 21:8:611:CLA:HBD | 1.81 | 0.43 |
| 20:c:41:VAL:O | 20:c:42:LYS:HG3 | 2.18 | 0.43 |
| 32:c:618:NEX:H15 | 32:c:618:NEX:H201 | 1.90 | 0.43 |
| 1:A:305:ALA:HB2 | 21:A:821:CLA:HBC2 | 1.99 | 0.43 |
| 24:A:849:BCR:H15C | 24:A:849:BCR:H351 | 1.90 | 0.43 |
| 2:B:196:HIS:HE1 | 21:B:814:CLA:C1A | 2.30 | 0.43 |
| 21:B:839:CLA:HBA1 | 21:B:839:CLA:HBD | 2.01 | 0.43 |
| 8:H:102:LEU:HD11 | 12:L:152:THR:HG22 | 1.98 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:1:304:CLA:HED2 | 21:1:304:CLA:H43 | 2.00 | 0.43 |
| 18:4:167:ARG:NE | 29:4:607:CHL:OMC | 2.39 | 0.43 |
| 15:5:142:ALA:O | 15:5:146:ILE:HG12 | 2.18 | 0.43 |
| 29:6:607:CHL:HHC | 29:6:607:CHL:HBB1 | 2.00 | 0.43 |
| 21:7:410:CLA:HAB | 30:7:415:LUT:C14 | 2.48 | 0.43 |
| 2:B:388:ALA:O | 2:B:392:ILE:HG13 | 2.19 | 0.43 |
| 21:B:805:CLA:H151 | 21:B:827:CLA:HBB2 | 2.00 | 0.43 |
| 17:3:245:TYR:CD1 | 21:3:409:CLA:O1D | 2.71 | 0.43 |
| 29:7:406:CHL:HHC | 29:7:406:CHL:HBB1 | 2.01 | 0.43 |
| 18:8:193:ASP:OD1 | 18:8:193:ASP:N | 2.52 | 0.43 |
| 20:c:114:THR:HG21 | 21:c:604:CLA:HAC2 | 2.00 | 0.43 |
| 32:c:618:NEX:H35 | 32:c:618:NEX:H401 | 1.85 | 0.43 |
| 1:A:175:TRP:HB2 | 21:A:812:CLA:HMC3 | 2.00 | 0.43 |
| 4:D:130:ARG:NH2 | 8:H:51:SER:OG | 2.52 | 0.43 |
| 16:2:114:ALA:CB | 16:2:231:MET:HG2 | 2.49 | 0.43 |
| 15:5:194:ARG:O | 15:5:198:VAL:HG22 | 2.18 | 0.43 |
| 16:6:234:VAL:CG2 | 31:6:617:XAT:H14 | 2.49 | 0.43 |
| 19:9:187:THR:HB | 19:9:190:PHE:HB2 | 2.00 | 0.43 |
| 20:b:101:HIS:HB3 | 20:b:221:MET:HE3 | 1.99 | 0.43 |
| 32:b:318:NEX:H15 | 32:b:318:NEX:H201 | 1.90 | 0.43 |
| 1:A:367:HIS:ND1 | 21:A:818:CLA:OBD | 2.49 | 0.43 |
| 2:B:142:LEU:HG | 24:B:843:BCR:H403 | 2.00 | 0.43 |
| 4:D:120:GLU:O | 4:D:150:ARG:NH1 | 2.51 | 0.43 |
| 7:G:121:PRO:HG2 | 21:G:204:CLA:HBC2 | 2.00 | 0.43 |
| 9:I:5:TYR:O | 9:I:8:SER:OG | 2.32 | 0.43 |
| 24:L:301:BCR:H352 | 21:L:303:CLA:HAB | 2.00 | 0.43 |
| 15:5:72:LEU:HB3 | 15:5:82:PHE:HE2 | 1.84 | 0.43 |
| 16:6:129:LYS:HE2 | 16:6:253:LEU:HD11 | 2.01 | 0.43 |
| 16:6:136:PRO:HD2 | 21:6:604:CLA:HED2 | 2.01 | 0.43 |
| 20:a:49:TRP:CZ2 | 21:a:611:CLA:HED2 | 2.53 | 0.43 |
| 21:A:821:CLA:H101 | 24:A:849:BCR:H10C | 2.00 | 0.43 |
| 21:B:808:CLA:H13 | 27:B:847:DGD:HAW2 | 2.01 | 0.43 |
| 21:B:811:CLA:H3A | 21:B:811:CLA:HBA2 | 1.63 | 0.43 |
| 21:B:830:CLA:H3A | 21:B:830:CLA:HBA2 | 1.58 | 0.43 |
| 24:M:101:BCR:H15C | 24:M:101:BCR:H351 | 1.86 | 0.43 |
| 15:1:124:GLN:HB3 | 15:1:135:GLY:C | 2.44 | 0.43 |
| 24:2:618:BCR:H15C | 24:2:618:BCR:H351 | 1.89 | 0.43 |
| 16:6:67:LEU:O | 17:7:229:TYR:OH | 2.25 | 0.43 |
| 17:7:146:ILE:HD11 | 17:7:244:ALA:HB1 | 2.01 | 0.43 |
| 19:9:236:GLU:HG3 | 29:9:609:CHL:NB | 2.33 | 0.43 |
| 21:a:613:CLA:H61 | 21:a:613:CLA:H2 | 1.70 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:b:206:PHE:CZ | 20:b:210:LYS:HE3 | 2.54 | 0.43 |
| 1:A:588:ASP:HA | 1:A:591:PHE:HB3 | 2.01 | 0.43 |
| 1:A:672:LEU:HD11 | 2:B:617:MET:HB2 | 2.00 | 0.43 |
| 21:A:833:CLA:H143 | 22:B:841:PQN:H191 | 2.00 | 0.43 |
| 4:D:113:SER:OG | 4:D:115:LYS:O | 2.37 | 0.43 |
| 6:F:175:PHE:HB2 | 24:F:301:BCR:H321 | 2.00 | 0.43 |
| 20:b:215:LYS:HE3 | 23:b:319:LHG:O10 | 2.18 | 0.43 |
| 20:c:181:LEU:HD23 | 20:c:181:LEU:HA | 1.86 | 0.43 |
| 1:A:669:LEU:HD22 | 21:A:852:CLA:C7 | 2.49 | 0.43 |
| 21:B:839:CLA:O1D | 21:B:839:CLA:H2A | 2.19 | 0.43 |
| 15:1:84:GLU:O | 15:1:88:ILE:HG12 | 2.19 | 0.43 |
| 16:6:108:LEU:O | 16:6:112:ARG:HD3 | 2.19 | 0.43 |
| 16:2:112:ARG:HA | 16:2:115:MET:HE3 | 2.01 | 0.43 |
| 16:2:116:LEU:HD23 | 16:2:116:LEU:HA | 1.89 | 0.43 |
| 17:7:275:ARG:HG2 | 21:7:401:CLA:C4C | 2.49 | 0.43 |
| 18:8:239:GLN:HA | 18:8:242:VAL:HG12 | 2.01 | 0.43 |
| 19:9:281:ARG:O | 19:9:285:MET:HG2 | 2.19 | 0.43 |
| 21:A:838:CLA:H61 | 21:A:838:CLA:H41 | 1.82 | 0.42 |
| 12:L:218:ASN:O | 12:L:224:LYS:NZ | 2.48 | 0.42 |
| 16:2:256:LEU:HD23 | 16:2:256:LEU:HA | 1.89 | 0.42 |
| 18:4:224:LYS:HD2 | 23:4:618:LHG:HC61 | 2.01 | 0.42 |
| 17:7:108:LEU:HB2 | 17:7:110:TYR:CD1 | 2.54 | 0.42 |
| 18:8:79:ASP:OD1 | 18:8:79:ASP:N | 2.52 | 0.42 |
| 30:9:615:LUT:H31 | 30:9:615:LUT:H391 | 1.91 | 0.42 |
| 20:b:132:LYS:HA | 29:b:308:CHL:HED2 | 2.01 | 0.42 |
| 20:b:225:PHE:O | 20:b:229:VAL:HG22 | 2.19 | 0.42 |
| 21:b:312:CLA:NA | 23:b:319:LHG:O4 | 2.52 | 0.42 |
| 1:A:535:HIS:HE1 | 21:A:838:CLA:ND | 2.18 | 0.42 |
| 21:A:817:CLA:H62 | 21:A:817:CLA:H41 | 1.37 | 0.42 |
| 2:B:707:LEU:HD23 | 27:B:847:DGD:HA21 | 2.01 | 0.42 |
| 21:B:805:CLA:H172 | 21:B:827:CLA:HBB2 | 2.01 | 0.42 |
| 30:7:415:LUT:H30 | 30:7:415:LUT:H27 | 1.79 | 0.42 |
| 23:8:617:LHG:H241 | 23:8:617:LHG:HC62 | 1.61 | 0.42 |
| 19:9:157:ARG:HG2 | 19:9:161:GLN:HE22 | 1.84 | 0.42 |
| 21:A:819:CLA:H3A | 21:A:819:CLA:HBA2 | 1.47 | 0.42 |
| 2:B:432:HIS:HE1 | 21:B:831:CLA:C4D | 2.32 | 0.42 |
| 6:F:228:GLU:HG2 | 6:F:233:LYS:HZ1 | 1.83 | 0.42 |
| 21:4:609:CLA:H43 | 30:4:615:LUT:H28 | 1.91 | 0.42 |
| 15:5:111:TRP:CZ2 | 15:5:203:PHE:HB3 | 2.54 | 0.42 |
| 16:6:168:ARG:O | 16:6:172:ILE:HG12 | 2.19 | 0.42 |
| 23:A:855:LHG:H141 | 10:J:4:VAL:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:K:201:CLA:HED1 | 24:K:205:BCR:H381 | 2.01 | 0.42 |
| 21:K:203:CLA:HMC2 | 24:K:205:BCR:H311 | 1.90 | 0.42 |
| 15:5:53:ARG:HH22 | 15:5:65:PHE:HA | 1.84 | 0.42 |
| 16:6:168:ARG:HA | 16:6:171:ASP:OD2 | 2.19 | 0.42 |
| 16:6:219:LEU:HB3 | 21:6:609:CLA:HMA2 | 2.01 | 0.42 |
| 24:6:618:BCR:H24C | 24:6:618:BCR:H371 | 1.88 | 0.42 |
| 24:7:417:BCR:H351 | 24:7:417:BCR:H15C | 1.87 | 0.42 |
| 18:8:262:THR:OG1 | 18:8:263:ILE:N | 2.53 | 0.42 |
| 31:c:617:XAT:H11 | 31:c:617:XAT:H191 | 1.89 | 0.42 |
| 21:A:827:CLA:C4D | 21:A:835:CLA:HMB1 | 2.49 | 0.42 |
| 21:A:833:CLA:HAA2 | 24:L:301:BCR:C14 | 2.49 | 0.42 |
| 2:B:365:PHE:HB3 | 2:B:602:TRP:CZ3 | 2.54 | 0.42 |
| 2:B:494:LEU:HD23 | 2:B:494:LEU:HA | 1.86 | 0.42 |
| 24:G:201:BCR:H15C | 24:G:201:BCR:H351 | 1.91 | 0.42 |
| 14:O:102:HIS:O | 14:O:104:PRO:HD3 | 2.19 | 0.42 |
| 31:1:318:XAT:H31 | 31:1:318:XAT:H391 | 1.90 | 0.42 |
| 15:5:178:LYS:H | 15:5:178:LYS:HG2 | 1.67 | 0.42 |
| 16:6:263:THR:OG1 | 16:6:264:ILE:N | 2.51 | 0.42 |
| 29:6:601:CHL:C1C | 23:6:619:LHG:HC82 | 2.50 | 0.42 |
| 17:7:133:GLY:H | 17:7:136:ILE:HB | 1.84 | 0.42 |
| 1:A:356:MET:HG3 | 21:A:825:CLA:HHB | 2.02 | 0.42 |
| 21:A:803:CLA:H2 | 2:B:655:LEU:HD22 | 2.02 | 0.42 |
| 21:A:819:CLA:H161 | 21:A:819:CLA:H122 | 1.42 | 0.42 |
| 23:A:855:LHG:HC82 | 16:2:95:SER:OG | 2.19 | 0.42 |
| 17:3:167:ARG:HD2 | 17:3:167:ARG:HA | 1.76 | 0.42 |
| 21:8:602:CLA:H43 | 31:8:615:XAT:O24 | 2.20 | 0.42 |
| 29:a:606:CHL:HHC | 29:a:606:CHL:HBB1 | 2.02 | 0.42 |
| 30:a:615:LUT:H31 | 30:a:615:LUT:H391 | 1.89 | 0.42 |
| 23:b:319:LHG:H242 | 23:b:319:LHG:HC62 | 1.75 | 0.42 |
| 20:c:46:ASP:N | 20:c:46:ASP:OD1 | 2.52 | 0.42 |
| 21:B:824:CLA:HBA2 | 21:B:824:CLA:H3A | 1.72 | 0.42 |
| 21:B:835:CLA:HMB1 | 21:B:835:CLA:HBB1 | 2.01 | 0.42 |
| 24:O:205:BCR:H11C | 24:O:205:BCR:H341 | 1.85 | 0.42 |
| 16:2:177:CYS:SG | 16:2:178:VAL:HG13 | 2.59 | 0.42 |
| 21:2:609:CLA:HBA2 | 21:2:609:CLA:H3A | 1.45 | 0.42 |
| 30:2:616:LUT:H15 | 30:2:616:LUT:H201 | 1.81 | 0.42 |
| 21:4:602:CLA:HBA2 | 21:4:602:CLA:H3A | 1.25 | 0.42 |
| 16:6:104:VAL:O | 16:6:108:LEU:HG | 2.19 | 0.42 |
| 17:7:149:GLY:O | 17:7:153:MET:HG2 | 2.19 | 0.42 |
| 21:8:604:CLA:HMB1 | 21:8:604:CLA:HBB1 | 2.00 | 0.42 |
| 19:9:234:LEU:HD23 | 32:9:617:NEX:H203 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:c:619:LHG:HC62 | 23:c:619:LHG:H242 | 1.64 | 0.42 |
| 1:A:317:HIS:HE1 | 21:A:822:CLA:NA | 2.08 | 0.42 |
| 1:A:405:HIS:HA | 1:A:408:ILE:HD12 | 2.02 | 0.42 |
| 9:I:1:MET:HB3 | 9:I:4:SER:HB3 | 2.02 | 0.42 |
| 21:L:302:CLA:HBA1 | 24:L:306:BCR:H363 | 2.02 | 0.42 |
| 15:1:110:ASN:O | 15:1:111:TRP:CD1 | 2.73 | 0.42 |
| 17:3:106:GLN:HG2 | 17:3:107:SER:N | 2.35 | 0.42 |
| 15:5:230:THR:HA | 21:5:612:CLA:HAA1 | 2.01 | 0.42 |
| 21:8:609:CLA:CHA | 21:8:609:CLA:HBA1 | 2.37 | 0.42 |
| 20:a:96:GLU:O | 20:a:100:ILE:HG12 | 2.20 | 0.42 |
| 20:c:204:ASP:OD1 | 20:c:205:THR:N | 2.49 | 0.42 |
| 30:c:616:LUT:H35 | 30:c:616:LUT:H401 | 1.91 | 0.42 |
| 32:c:618:NEX:H11 | 32:c:618:NEX:H191 | 1.91 | 0.42 |
| 1:A:235:PRO:HG2 | 1:A:240:PHE:CZ | 2.55 | 0.42 |
| 2:B:583:MET:HE3 | 2:B:583:MET:HB3 | 1.97 | 0.42 |
| 8:H:46:LYS:HB2 | 8:H:61:ASN:HB3 | 2.02 | 0.42 |
| 24:6:618:BCR:H15C | 24:6:618:BCR:H351 | 1.88 | 0.42 |
| 19:9:280:GLY:O | 19:9:284:MET:HG3 | 2.20 | 0.42 |
| 20:a:91:PHE:HD2 | 20:a:95:ARG:HH21 | 1.68 | 0.42 |
| 20:c:125:PHE:HB3 | 21:c:604:CLA:HED1 | 2.01 | 0.42 |
| 2:B:273:MET:CE | 21:B:817:CLA:H2A | 2.50 | 0.42 |
| 24:F:301:BCR:H11C | 24:F:301:BCR:H341 | 1.95 | 0.42 |
| 13:M:6:ASP:O | 13:M:10:ILE:HG12 | 2.20 | 0.42 |
| 16:2:225:LYS:HB2 | 16:2:225:LYS:HE2 | 1.73 | 0.42 |
| 30:2:616:LUT:H191 | 30:2:616:LUT:H11 | 1.79 | 0.42 |
| 21:3:408:CLA:H12 | 21:3:415:CLA:HBB2 | 2.01 | 0.42 |
| 17:7:212:GLU:OE1 | 21:7:407:CLA:C4A | 2.68 | 0.42 |
| 18:8:234:LEU:HB2 | 31:8:615:XAT:H35 | 2.01 | 0.42 |
| 21:8:611:CLA:H92 | 21:8:611:CLA:HMC1 | 2.01 | 0.42 |
| 19:9:260:LEU:HD13 | 30:9:614:LUT:H221 | 2.01 | 0.42 |
| 20:a:73:PHE:CE2 | 21:a:602:CLA:HED3 | 2.54 | 0.42 |
| 20:a:108:GLY:HA2 | 30:a:616:LUT:H181 | 2.02 | 0.42 |
| 20:b:179:GLY:H | 29:b:309:CHL:HMC | 1.84 | 0.42 |
| 21:b:312:CLA:C4C | 23:b:319:LHG:HC61 | 2.49 | 0.42 |
| 20:c:181:LEU:HD12 | 29:c:608:CHL:C3B | 2.50 | 0.42 |
| 21:B:830:CLA:H41 | 21:B:830:CLA:H62 | 1.45 | 0.41 |
| 21:B:836:CLA:H93 | 21:B:837:CLA:HBC1 | 2.01 | 0.41 |
| 24:B:846:BCR:H15C | 24:B:846:BCR:H351 | 1.85 | 0.41 |
| 14:O:78:SER:O | 14:O:85:GLY:HA3 | 2.19 | 0.41 |
| 18:8:102:TRP:CZ2 | 21:8:608:CLA:HAA2 | 2.55 | 0.41 |
| 18:8:235:GLY:O | 18:8:239:GLN:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:423:LEU:HD13 | 21:A:824:CLA:C1C | 2.50 | 0.41 |
| 1:A:676:PHE:CD2 | 24:A:850:BCR:H363 | 2.56 | 0.41 |
| 21:A:834:CLA:H51 | 24:L:301:BCR:H363 | 2.02 | 0.41 |
| 2:B:95:HIS:HE1 | 21:B:809:CLA:C4B | 2.32 | 0.41 |
| 2:B:270:LEU:HD23 | 2:B:270:LEU:HA | 1.89 | 0.41 |
| 2:B:357:PRO:HG3 | 21:B:817:CLA:HBA1 | 2.02 | 0.41 |
| 21:B:807:CLA:H202 | 21:B:807:CLA:H161 | 1.83 | 0.41 |
| 21:B:817:CLA:H3A | 21:B:817:CLA:HBA2 | 1.40 | 0.41 |
| 14:O:141:GLY:C | 14:O:143:TRP:H | 2.28 | 0.41 |
| 15:1:149:ALA:HA | 21:1:309:CLA:CAB | 2.50 | 0.41 |
| 18:4:212:GLU:O | 18:4:213:ASP:HB2 | 2.21 | 0.41 |
| 18:4:234:LEU:HG | 21:4:612:CLA:HBC2 | 2.02 | 0.41 |
| 15:5:86:GLU:HB2 | 21:5:602:CLA:C1B | 2.50 | 0.41 |
| 30:8:614:LUT:H31 | 30:8:614:LUT:H391 | 1.95 | 0.41 |
| 30:a:616:LUT:H15 | 30:a:616:LUT:H201 | 1.90 | 0.41 |
| 1:A:311:THR:HG22 | 1:A:312:ASN:N | 2.19 | 0.41 |
| 2:B:389:HIS:HE1 | 21:B:828:CLA:C4A | 2.33 | 0.41 |
| 24:B:844:BCR:H15C | 24:B:844:BCR:H351 | 1.89 | 0.41 |
| 21:3:409:CLA:HED2 | 21:3:409:CLA:HBD | 1.91 | 0.41 |
| 31:3:417:XAT:H31 | 31:3:417:XAT:H391 | 1.94 | 0.41 |
| 21:7:402:CLA:CMD | 21:7:407:CLA:ND | 2.83 | 0.41 |
| 31:a:618:XAT:H11 | 31:a:618:XAT:H191 | 1.92 | 0.41 |
| 21:B:805:CLA:H92 | 21:B:805:CLA:H61 | 1.78 | 0.41 |
| 21:1:303:CLA:H3A | 21:1:303:CLA:HBA2 | 1.27 | 0.41 |
| 24:3:419:BCR:H11C | 24:3:419:BCR:H341 | 1.81 | 0.41 |
| 15:5:48:LEU:HD12 | 15:5:48:LEU:HA | 1.84 | 0.41 |
| 15:5:90:ALA:O | 15:5:94:MET:HG3 | 2.19 | 0.41 |
| 15:5:214:GLY:O | 15:5:217:GLU:HG3 | 2.19 | 0.41 |
| 21:5:602:CLA:H93 | 21:5:602:CLA:H61 | 1.77 | 0.41 |
| 24:7:418:BCR:H341 | 24:7:418:BCR:H11C | 1.84 | 0.41 |
| 18:8:154:PHE:HD1 | 29:8:606:CHL:HMC | 1.85 | 0.41 |
| 24:8:616:BCR:H20C | 24:8:616:BCR:H361 | 1.97 | 0.41 |
| 20:a:195:ASP:CG | 21:a:610:CLA:HBA2 | 2.46 | 0.41 |
| 20:a:212:LYS:HA | 20:a:215:LYS:HG2 | 2.01 | 0.41 |
| 21:b:311:CLA:H52 | 30:b:316:LUT:H30 | 2.01 | 0.41 |
| 1:A:72:SER:OG | 1:A:178:TYR:HB2 | 2.20 | 0.41 |
| 21:A:821:CLA:HBB1 | 21:A:821:CLA:HMB3 | 2.02 | 0.41 |
| 2:B:576:PHE:O | 2:B:580:VAL:HG23 | 2.21 | 0.41 |
| 4:D:177:ASP:OD1 | 4:D:177:ASP:N | 2.48 | 0.41 |
| 24:M:101:BCR:H20C | 24:M:101:BCR:H361 | 1.89 | 0.41 |
| 16:2:201:TRP:CE2 | 29:2:614:CHL:ND | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4:609:CLA:ND | 30:4:615:LUT:H382 | 2.36 | 0.41 |
| 16:6:122:PHE:CE2 | 30:6:616:LUT:H30 | 2.55 | 0.41 |
| 17:7:275:ARG:HG2 | 21:7:401:CLA:C3C | 2.50 | 0.41 |
| 17:7:293:VAL:HG21 | 17:7:297:GLN:OE1 | 2.21 | 0.41 |
| 20:a:217:GLY:O | 20:a:221:MET:HG2 | 2.20 | 0.41 |
| 29:b:310:CHL:HHC | 29:b:310:CHL:HBB1 | 2.01 | 0.41 |
| 8:H:81:GLN:HG2 | 21:H:201:CLA:NC | 2.34 | 0.41 |
| 15:1:124:GLN:HG2 | 15:1:136:ASN:HA | 2.03 | 0.41 |
| 21:2:603:CLA:HED2 | 21:2:603:CLA:HBD | 1.75 | 0.41 |
| 17:3:235:LYS:NZ | 15:5:77:GLU:HG3 | 2.36 | 0.41 |
| 15:5:235:LEU:HD12 | 18:8:155:ILE:HD11 | 2.03 | 0.41 |
| 16:6:198:GLY:HA2 | 16:6:203:ASP:OD2 | 2.20 | 0.41 |
| 21:6:604:CLA:CHB | 24:6:618:BCR:H392 | 2.51 | 0.41 |
| 17:7:148:ASN:CG | 21:7:407:CLA:HMD1 | 2.45 | 0.41 |
| 21:7:404:CLA:H3A | 24:7:417:BCR:C21 | 2.50 | 0.41 |
| 18:8:112:ARG:O | 18:8:115:MET:HG2 | 2.20 | 0.41 |
| 18:8:189:LEU:HD11 | 29:8:613:CHL:HBC1 | 2.03 | 0.41 |
| 20:a:255:TRP:CE2 | 20:c:161:TRP:HZ3 | 2.39 | 0.41 |
| 20:c:157:ILE:HG23 | 20:c:161:TRP:CE2 | 2.56 | 0.41 |
| 1:A:294:HIS:CD2 | 1:A:294:HIS:O | 2.74 | 0.41 |
| 1:A:597:MET:HE3 | 1:A:597:MET:HB3 | 2.00 | 0.41 |
| 21:A:827:CLA:H152 | 21:A:827:CLA:H111 | 1.61 | 0.41 |
| 21:A:831:CLA:H2A | 21:A:831:CLA:O2D | 2.20 | 0.41 |
| 2:B:308:HIS:HE1 | 21:B:821:CLA:NC | 2.19 | 0.41 |
| 2:B:395:ILE:HD13 | 2:B:555:TYR:HA | 2.03 | 0.41 |
| 2:B:421:HIS:CD2 | 21:B:830:CLA:NC | 2.89 | 0.41 |
| 24:B:845:BCR:H11C | 24:B:845:BCR:H341 | 1.90 | 0.41 |
| 15:1:113:SER:HA | 15:1:116:LYS:HB2 | 2.02 | 0.41 |
| 21:8:604:CLA:HBA2 | 21:8:604:CLA:H3A | 1.55 | 0.41 |
| 20:b:225:PHE:HD1 | 21:b:304:CLA:HBB2 | 1.85 | 0.41 |
| 21:A:827:CLA:O1D | 21:A:835:CLA:HAB | 2.21 | 0.41 |
| 21:A:834:CLA:H141 | 21:A:834:CLA:H161 | 1.78 | 0.41 |
| 21:A:841:CLA:H142 | 21:A:841:CLA:H112 | 1.69 | 0.41 |
| 2:B:53:GLN:HE21 | 21:B:804:CLA:HMB3 | 1.86 | 0.41 |
| 2:B:275:HIS:HB3 | 21:B:816:CLA:HMB2 | 2.02 | 0.41 |
| 21:B:803:CLA:HHC | 21:B:805:CLA:OBD | 2.21 | 0.41 |
| 21:B:808:CLA:H111 | 27:B:847:DGD:HAH2 | 2.03 | 0.41 |
| 24:B:842:BCR:H15C | 24:B:842:BCR:H351 | 1.92 | 0.41 |
| 27:B:847:DGD:HB72 | 27:B:847:DGD:HB41 | 1.83 | 0.41 |
| 29:6:602:CHL:HBB1 | 31:6:617:XAT:H30 | 2.02 | 0.41 |
| 17:7:309:ASN:OD1 | 17:7:310:ASN:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:9:119:TRP:H | 19:9:119:TRP:CD1 | 2.39 | 0.41 |
| 19:9:284:MET:HE1 | 21:9:602:CLA:CAB | 2.50 | 0.41 |
| 20:b:74:ALA:HB2 | 20:b:210:LYS:HB3 | 2.03 | 0.41 |
| 1:A:116:TRP:CD2 | 21:A:810:CLA:HED3 | 2.56 | 0.41 |
| 1:A:669:LEU:HD21 | 2:B:445:ALA:HB2 | 2.03 | 0.41 |
| 21:A:806:CLA:H111 | 21:A:806:CLA:H91 | 1.71 | 0.41 |
| 21:A:852:CLA:H41 | 21:A:852:CLA:H61 | 1.70 | 0.41 |
| 2:B:15:ASP:OD2 | 2:B:17:THR:OG1 | 2.36 | 0.41 |
| 2:B:432:HIS:CD2 | 24:J:104:BCR:H333 | 2.56 | 0.41 |
| 2:B:649:MET:HE2 | 24:B:846:BCR:H322 | 2.02 | 0.41 |
| 2:B:667:TRP:O | 2:B:671:TRP:CD1 | 2.73 | 0.41 |
| 3:C:29:VAL:HG22 | 4:D:188:ARG:HB3 | 2.03 | 0.41 |
| 3:C:35:LYS:HE3 | 3:C:35:LYS:HB2 | 1.89 | 0.41 |
| 7:G:149:ASN:ND2 | 7:G:151:TYR:H | 2.18 | 0.41 |
| 24:J:104:BCR:H24C | 24:J:104:BCR:H21C | 1.82 | 0.41 |
| 24:M:101:BCR:H11C | 24:M:101:BCR:H341 | 1.84 | 0.41 |
| 16:2:115:MET:HG3 | 16:2:227:GLY:HA2 | 2.03 | 0.41 |
| 16:2:156:ILE:O | 16:2:160:LEU:HG | 2.21 | 0.41 |
| 21:3:409:CLA:H43 | 30:3:416:LUT:H26 | 2.03 | 0.41 |
| 31:4:616:XAT:H15 | 31:4:616:XAT:H201 | 1.93 | 0.41 |
| 15:5:105:ALA:HA | 15:5:216:LEU:HD22 | 2.03 | 0.41 |
| 15:5:145:PHE:HA | 15:5:148:ILE:HG22 | 2.03 | 0.41 |
| 16:6:69:PHE:CD1 | 29:6:601:CHL:HMA3 | 2.56 | 0.41 |
| 16:6:197:PRO:HG2 | 16:6:202:PHE:CD2 | 2.45 | 0.41 |
| 21:7:408:CLA:C1B | 30:7:415:LUT:H373 | 2.50 | 0.41 |
| 21:9:611:CLA:H91 | 21:9:611:CLA:H111 | 1.63 | 0.41 |
| 30:a:616:LUT:H11 | 30:a:616:LUT:H191 | 1.88 | 0.41 |
| 31:c:617:XAT:H15 | 31:c:617:XAT:H201 | 1.86 | 0.41 |
| 2:B:519:VAL:HG11 | 2:B:593:TYR:HB2 | 2.03 | 0.41 |
| 6:F:103:GLU:O | 6:F:107:ILE:HG12 | 2.20 | 0.41 |
| 24:8:616:BCR:H11C | 24:8:616:BCR:H341 | 1.87 | 0.41 |
| 20:a:84:LEU:HD22 | 21:a:602:CLA:H11 | 2.03 | 0.41 |
| 31:a:618:XAT:H201 | 31:a:618:XAT:H15 | 1.83 | 0.41 |
| 31:a:618:XAT:O3 | 20:b:258:ALA:HA | 2.20 | 0.41 |
| 21:b:303:CLA:H93 | 21:b:304:CLA:HMB1 | 2.02 | 0.41 |
| 30:b:317:LUT:H35 | 30:b:317:LUT:H401 | 1.90 | 0.41 |
| 21:c:613:CLA:H91 | 21:c:613:CLA:H112 | 1.84 | 0.41 |
| 1:A:294:HIS:HD2 | 1:A:298:ILE:HG12 | 1.85 | 0.40 |
| 1:A:448:HIS:HE1 | 21:A:833:CLA:C4D | 2.34 | 0.40 |
| 1:A:521:LEU:HD23 | 1:A:521:LEU:HA | 1.96 | 0.40 |
| 1:A:570:ARG:NH1 | 23:A:844:LHG:O10 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:A:847:BCR:H11C | 24:A:847:BCR:H341 | 1.91 | 0.40 |
| 21:5:602:CLA:H111 | 21:5:602:CLA:H91 | 1.79 | 0.40 |
| 21:5:614:CLA:H3A | 21:5:614:CLA:HBA1 | 1.84 | 0.40 |
| 16:6:240:GLN:HG2 | 21:6:612:CLA:C1D | 2.51 | 0.40 |
| 32:9:617:NEX:H35 | 32:9:617:NEX:H401 | 1.91 | 0.40 |
| 21:b:304:CLA:HBA1 | 21:b:304:CLA:H3A | 1.80 | 0.40 |
| 30:b:317:LUT:H31 | 30:b:317:LUT:H391 | 1.94 | 0.40 |
| 1:A:275:PHE:HD1 | 21:A:818:CLA:HMB3 | 1.86 | 0.40 |
| 1:A:380:ASP:OD2 | 1:A:383:THR:OG1 | 2.32 | 0.40 |
| 21:B:816:CLA:HBA2 | 21:B:825:CLA:HBB2 | 2.02 | 0.40 |
| 3:C:73:THR:H | 3:C:76:SER:HB2 | 1.86 | 0.40 |
| 8:H:73:ASP:HB3 | 12:L:100:ARG:HH22 | 1.86 | 0.40 |
| 24:J:101:BCR:H24C | 24:J:101:BCR:H371 | 1.98 | 0.40 |
| 29:4:607:CHL:HBB1 | 29:4:607:CHL:HHC | 2.02 | 0.40 |
| 30:6:616:LUT:H15 | 30:6:616:LUT:H201 | 1.82 | 0.40 |
| 31:7:416:XAT:H35 | 31:7:416:XAT:H401 | 1.90 | 0.40 |
| 18:8:154:PHE:CD1 | 29:8:606:CHL:HAC2 | 2.57 | 0.40 |
| 19:9:232:MET:O | 19:9:236:GLU:HG2 | 2.22 | 0.40 |
| 20:a:92:ALA:O | 20:a:96:GLU:OE1 | 2.38 | 0.40 |
| 20:b:79:TRP:CD1 | 20:b:81:THR:HG23 | 2.57 | 0.40 |
| 29:b:309:CHL:HHC | 29:b:309:CHL:HBB1 | 2.02 | 0.40 |
| 1:A:448:HIS:HE1 | 21:A:833:CLA:CHA | 2.34 | 0.40 |
| 21:A:807:CLA:HED2 | 21:A:807:CLA:HBD | 1.92 | 0.40 |
| 21:A:842:CLA:HHD | 24:B:846:BCR:C38 | 2.52 | 0.40 |
| 2:B:418:ILE:HG23 | 21:B:837:CLA:HBB2 | 2.03 | 0.40 |
| 2:B:697:PRO:O | 3:C:81:TYR:OH | 2.30 | 0.40 |
| 21:B:838:CLA:HBB2 | 22:B:841:PQN:H141 | 2.04 | 0.40 |
| 24:G:205:BCR:H15C | 24:G:205:BCR:H351 | 1.93 | 0.40 |
| 21:2:610:CLA:CAB | 24:3:418:BCR:H312 | 2.51 | 0.40 |
| 18:4:154:PHE:O | 18:4:158:LEU:HG | 2.21 | 0.40 |
| 16:6:165:GLU:CD | 21:6:608:CLA:NB | 2.79 | 0.40 |
| 21:9:611:CLA:H62 | 21:9:611:CLA:H92 | 1.79 | 0.40 |
| 29:a:605:CHL:HBB1 | 29:a:605:CHL:HHC | 2.04 | 0.40 |
| 21:b:311:CLA:C2 | 30:b:316:LUT:H28 | 2.52 | 0.40 |
| 20:c:101:HIS:HE1 | 21:c:603:CLA:C4D | 2.35 | 0.40 |
| 1:A:294:HIS:HB2 | 21:A:818:CLA:C2B | 2.51 | 0.40 |
| 24:A:854:BCR:H20C | 24:A:854:BCR:H361 | 1.89 | 0.40 |
| 21:B:827:CLA:H142 | 24:B:843:BCR:H372 | 2.04 | 0.40 |
| 14:O:74:TRP:CD1 | 14:O:124:LEU:HB2 | 2.56 | 0.40 |
| 15:1:225:ASP:OD1 | 15:1:228:HIS:ND1 | 2.55 | 0.40 |
| 16:2:236:GLY:O | 16:2:240:GLN:HG3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:4:616:XAT:H31 | 31:4:616:XAT:H391 | 1.91 | 0.40 |
| 30:7:415:LUT:H35 | 30:7:415:LUT:H401 | 1.94 | 0.40 |
| 31:7:416:XAT:H15 | 31:7:416:XAT:H201 | 1.93 | 0.40 |
| 29:8:613:CHL:HHC | 29:8:613:CHL:HBB1 | 2.04 | 0.40 |
| 31:8:615:XAT:H191 | 31:8:615:XAT:H11 | 1.88 | 0.40 |
| 20:a:54:ARG:NH1 | 20:a:71:GLY:H | 2.20 | 0.40 |
| 20:a:152:VAL:CG2 | 20:a:153:HIS:N | 2.56 | 0.40 |
| 20:c:212:LYS:HD3 | 21:c:612:CLA:HAA2 | 2.04 | 0.40 |
| 30:c:615:LUT:H11 | 30:c:615:LUT:H191 | 1.93 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 740/742 (100%) | 715 (97%) | 25 (3%) | 0 | 100 | 100 |
| 2 | B | 731/733 (100%) | 701 (96%) | 30 (4%) | 0 | 100 | 100 |
| 3 | C | 78/80 (98%) | 72 (92%) | 6 (8%) | 0 | 100 | 100 |
| 4 | D | 139/141 (99%) | 132 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | E | 60/62 (97%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 7 | G | 96/98 (98%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 8 | H | 93/95 (98%) | 90 (97%) | 3 (3%) | 0 | 100 | 100 |
| 9 | I | 32/34 (94%) | 29 (91%) | 3 (9%) | 0 | 100 | 100 |
| 10 | J | 39/41 (95%) | 39 (100%) | 0 | 0 | 100 | 100 |
| 11 | K | 79/81 (98%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 12 | L | 161/163 (99%) | 153 (95%) | 8 (5%) | 0 | 100 | 100 |
| 13 | M | 30/32 (94%) | 29 (97%) | 0 | 1 (3%) | 3 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 14 | O | 87/89 (98%) | 79 (91%) | 8 (9%) | 0 | 100 | 100 |
| 15 | 1 | 190/192 (99%) | 183 (96%) | 7 (4%) | 0 | 100 | 100 |
| 15 | 5 | 190/192 (99%) | 176 (93%) | 12 (6%) | 2 (1%) | 11 | 26 |
| 16 | 2 | 209/211 (99%) | 201 (96%) | 8 (4%) | 0 | 100 | 100 |
| 16 | 6 | 203/211 (96%) | 199 (98%) | 4 (2%) | 0 | 100 | 100 |
| 17 | 3 | 214/216 (99%) | 203 (95%) | 11 (5%) | 0 | 100 | 100 |
| 17 | 7 | 211/216 (98%) | 198 (94%) | 12 (6%) | 1 (0%) | 24 | 45 |
| 18 | 4 | 203/205 (99%) | 193 (95%) | 10 (5%) | 0 | 100 | 100 |
| 18 | 8 | 202/205 (98%) | 192 (95%) | 10 (5%) | 0 | 100 | 100 |
| 19 | 9 | 223/225 (99%) | 201 (90%) | 22 (10%) | 0 | 100 | 100 |
| 20 | a | 216/227 (95%) | 208 (96%) | 7 (3%) | 1 (0%) | 24 | 45 |
| 20 | b | 216/227 (95%) | 208 (96%) | 7 (3%) | 1 (0%) | 24 | 45 |
| 20 | c | 224/227 (99%) | 215 (96%) | 8 (4%) | 1 (0%) | 30 | 51 |
| All | All | 5023/5104 (98%) | 4800 (96%) | 216 (4%) | 7 (0%) | 49 | 71 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 5 | 170 | PRO |
| 20 | b | 152 | VAL |
| 20 | c | 152 | VAL |
| 20 | a | 152 | VAL |
| 13 | M | 4 | ILE |
| 15 | 5 | 168 | GLY |
| 17 | 7 | 311 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 603/603 (100%) | 602 (100%) | 1 (0%) | 87 | 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | B | 595/595 (100%) | 595 (100%) | 0 | 100 100 |
| 3 | C | 67/67 (100%) | 67 (100%) | 0 | 100 100 |
| 4 | D | 115/115 (100%) | 115 (100%) | 0 | 100 100 |
| 5 | E | 52/52 (100%) | 52 (100%) | 0 | 100 100 |
| 6 | F | 129/129 (100%) | 129 (100%) | 0 | 100 100 |
| 7 | G | 78/78 (100%) | 78 (100%) | 0 | 100 100 |
| 8 | H | 77/77 (100%) | 77 (100%) | 0 | 100 100 |
| 9 | I | 30/30 (100%) | 30 (100%) | 0 | 100 100 |
| 10 | J | 35/35 (100%) | 35 (100%) | 0 | 100 100 |
| 11 | K | 58/58 (100%) | 58 (100%) | 0 | 100 100 |
| 12 | L | 126/126 (100%) | 126 (100%) | 0 | 100 100 |
| 13 | M | 27/27 (100%) | 27 (100%) | 0 | 100 100 |
| 14 | O | 73/73 (100%) | 73 (100%) | 0 | 100 100 |
| 15 | 1 | 151/151 (100%) | 151 (100%) | 0 | 100 100 |
| 15 | 5 | 150/151 (99%) | 149 (99%) | 1 (1%) | 76 89 |
| 16 | 2 | 168/168 (100%) | 168 (100%) | 0 | 100 100 |
| 16 | 6 | 163/168 (97%) | 163 (100%) | 0 | 100 100 |
| 17 | 3 | 169/169 (100%) | 169 (100%) | 0 | 100 100 |
| 17 | 7 | 166/169 (98%) | 165 (99%) | 1 (1%) | 78 90 |
| 18 | 4 | 164/164 (100%) | 164 (100%) | 0 | 100 100 |
| 18 | 8 | 163/164 (99%) | 162 (99%) | 1 (1%) | 78 90 |
| 19 | 9 | 179/179 (100%) | 179 (100%) | 0 | 100 100 |
| 20 | a | 165/173 (95%) | 165 (100%) | 0 | 100 100 |
| 20 | b | 165/173 (95%) | 164 (99%) | 1 (1%) | 78 90 |
| 20 | c | 173/173 (100%) | 173 (100%) | 0 | 100 100 |
| All | All | 4041/4067 (99%) | 4036 (100%) | 5 (0%) | 87 96 |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 585 | SER |
| 15 | 5 | 115 | GLN |
| 17 | 7 | 302 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | 8 | 165 | GLU |
| 20 | b | 68 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 121 | GLN |
| 1 | A | 222 | ASN |
| 1 | A | 265 | ASN |
| 1 | A | 294 | HIS |
| 1 | A | 623 | GLN |
| 2 | B | 53 | GLN |
| 2 | B | 114 | ASN |
| 2 | B | 177 | HIS |
| 2 | B | 308 | HIS |
| 2 | B | 452 | GLN |
| 2 | B | 461 | GLN |
| 2 | B | 641 | ASN |
| 2 | B | 704 | GLN |
| 4 | D | 158 | GLN |
| 4 | D | 185 | ASN |
| 7 | G | 119 | ASN |
| 8 | H | 130 | GLN |
| 12 | L | 116 | HIS |
| 12 | L | 180 | GLN |
| 14 | O | 86 | ASN |
| 15 | 1 | 130 | ASN |
| 15 | 1 | 192 | ASN |
| 16 | 2 | 63 | ASN |
| 17 | 3 | 273 | ASN |
| 18 | 4 | 110 | HIS |
| 15 | 5 | 110 | ASN |
| 15 | 5 | 154 | GLN |
| 15 | 5 | 206 | GLN |
| 16 | 6 | 187 | ASN |
| 16 | 6 | 240 | GLN |
| 16 | 6 | 242 | ASN |
| 16 | 6 | 251 | ASN |
| 16 | 6 | 261 | HIS |
| 17 | 7 | 264 | GLN |
| 17 | 7 | 308 | HIS |
| 19 | 9 | 105 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | 9 | 310 | HIS |
| 20 | b | 153 | HIS |
| 20 | b | 155 | GLN |
| 20 | b | 216 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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 | TPO | c | 40 | 20 | 8,10,11 | 1.64 | 1 (12%) | 10,14,16 | 1.96 | 1 (10%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | TPO | c | 40 | 20 | - | 2/9/11/13 | - |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | c | 40 | TPO | P-O1P | 3.50 | 1.61 | 1.50 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | c | 40 | TPO | P-OG1-CB | -5.48 | 108.44 | 123.33 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | c | 40 | TPO | CB-OG1-P-O2P |
| 20 | c | 40 | TPO | O-C-CA-CB |

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)

364 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 | $\#\|Z\| > 2$ |
| 21 | CLA | A | 835 | - | 54,58,73 | 1.28 | 7 (12%) | 64,95,113 | 1.40 | 6 (9%) |
| 24 | BCR | I | 101 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.40 | 10 (17%) |
| 21 | CLA | G | 203 | - | 54,58,73 | 1.32 | 8 (14%) | 64,95,113 | 1.37 | 6 (9%) |
| 21 | CLA | 9 | 604 | - | 49,53,73 | 1.38 | 9 (18%) | 58,89,113 | 1.46 | 5 (8%) |
| 21 | CLA | A | 841 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.32 | 5 (6%) |
| 29 | CHL | c | 605 | - | 36,51,74 | 4.36 | 17 (47%) | 29,86,114 | 3.73 | 11 (37%) |
| 26 | LMU | O | 206 | - | 36,36,36 | 0.41 | 0 | 47,47,47 | 0.69 | 0 |
| 21 | CLA | b | 312 | 23 | 49,53,73 | 1.39 | 6 (12%) | 58,89,113 | 1.38 | 4 (6%) |
| 24 | BCR | B | 844 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 2.10 | 21 (37%) |
| 29 | CHL | 6 | 601 | 16 | 38,52,74 | 3.92 | 18 (47%) | 35,88,114 | 4.04 | 14 (40%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 7 | 403 | - | 45,50,73 | 1.55 | 9 (20%) | 55,86,113 | 1.46 | 6 (10%) |
| 29 | CHL | 2 | 606 | - | 40,54,74 | 4.06 | 19 (47%) | 34,90,114 | 3.79 | 16 (47%) |
| 21 | CLA | G | 202 | - | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.49 | 4 (6%) |
| 29 | CHL | 4 | 607 | - | 45,59,74 | 3.80 | 18 (40%) | 40,96,114 | 3.58 | 19 (47%) |
| 21 | CLA | 1 | 310 | 15 | 46,51,73 | 1.41 | 8 (17%) | 54,87,113 | 1.42 | 6 (11%) |
| 24 | BCR | B | 843 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 2.56 | 24 (42%) |
| 21 | CLA | b | 304 | - | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.46 | 4 (6%) |
| 21 | CLA | 1 | 306 | - | 44,48,73 | 1.43 | 8 (18%) | 51,82,113 | 1.51 | 5 (9%) |
| 29 | CHL | 3 | 407 | - | 33,48,74 | 3.89 | 16 (48%) | 30,83,114 | 3.20 | 16 (53%) |
| 23 | LHG | 1 | 319 | 21 | 27,27,48 | 0.35 | 0 | 30,33,54 | 0.47 | 0 |
| 29 | CHL | c | 609 | 20 | 38,52,74 | 3.92 | 18 (47%) | 34,88,114 | 3.58 | 14 (41%) |
| 21 | CLA | B | 810 | - | 58,62,73 | 1.35 | 9 (15%) | 71,100,113 | 1.36 | 8 (11%) |
| 28 | LMG | J | 105 | - | 30,30,55 | 0.25 | 0 | 38,38,63 | 0.35 | 0 |
| 21 | CLA | A | 821 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.29 | 7 (8%) |
| 24 | BCR | A | 849 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.63 | 12 (21%) |
| 21 | CLA | 7 | 409 | - | 43,48,73 | 1.46 | 8 (18%) | 51,83,113 | 1.48 | 5 (9%) |
| 29 | CHL | b | 309 | - | 43,57,74 | 3.93 | 19 (44%) | 37,93,114 | 3.58 | 17 (45%) |
| 22 | PQN | A | 843 | - | 34,34,34 | 0.41 | 0 | 43,45,45 | 0.58 | 1 (2%) |
| 21 | CLA | B | 819 | - | 47,51,73 | 1.37 | 9 (19%) | 55,86,113 | 1.43 | 4 (7%) |
| 21 | CLA | 8 | 611 | - | 58,62,73 | 1.28 | 8 (13%) | 68,99,113 | 1.31 | 5 (7%) |
| 29 | CHL | 6 | 606 | - | 40,54,74 | 4.14 | 18 (45%) | 34,90,114 | 3.75 | 15 (44%) |
| 31 | XAT | 2 | 617 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 1.54 | 12 (22%) |
| 29 | CHL | 8 | 606 | - | 40,54,74 | 4.19 | 18 (45%) | 34,90,114 | 3.89 | 16 (47%) |
| 29 | CHL | 9 | 608 | - | 40,54,74 | 4.07 | 18 (45%) | 34,90,114 | 3.69 | 16 (47%) |
| 24 | BCR | G | 205 | - | 41,41,41 | 1.38 | 8 (19%) | 56,56,56 | 1.47 | 9 (16%) |
| 21 | CLA | A | 840 | - | 69,73,73 | 1.14 | 9 (13%) | 82,113,113 | 1.27 | 6 (7%) |
| 21 | CLA | b | 311 | 20 | 58,62,73 | 1.26 | 8 (13%) | 68,99,113 | 1.34 | 8 (11%) |
| 29 | CHL | a | 607 | - | 37,51,74 | 4.23 | 17 (45%) | 30,86,114 | 3.94 | 13 (43%) |
| 21 | CLA | J | 102 | 10 | 46,50,73 | 1.39 | 9 (19%) | 53,85,113 | 1.42 | 4 (7%) |
| 30 | LUT | a | 616 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.49 | 9 (17%) |
| 23 | LHG | c | 619 | 21 | 48,48,48 | 0.27 | 0 | 51,54,54 | 0.31 | 0 |
| 24 | BCR | B | 846 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.96 | 18 (32%) |
| 31 | XAT | 3 | 417 | - | 41,47,47 | 1.29 | 8 (19%) | 54,74,74 | 1.54 | 9 (16%) |
| 24 | BCR | L | 306 | - | 41,41,41 | 1.37 | 8 (19%) | 56,56,56 | 1.68 | 11 (19%) |
| 21 | CLA | K | 202 | - | 54,58,73 | 1.30 | 8 (14%) | 64,95,113 | 1.52 | 9 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | A | 825 | - | 69,73,73 | 1.16 | 8 (11%) | 82,113,113 | 1.28 | 7 (8%) |
| 21 | CLA | 1 | 308 | - | 47,52,73 | 1.41 | 9 (19%) | 55,88,113 | 1.43 | 4 (7%) |
| 21 | CLA | F | 304 | - | 49,53,73 | 1.38 | 7 (14%) | 58,89,113 | 1.40 | 4 (6%) |
| 21 | CLA | 8 | 602 | 18 | 61,66,73 | 1.24 | 7 (11%) | 71,104,113 | 1.28 | 7 (9%) |
| 21 | CLA | A | 811 | - | 49,53,73 | 1.35 | 8 (16%) | 58,89,113 | 1.45 | 4 (6%) |
| 21 | CLA | B | 831 | - | 60,64,73 | 1.24 | 8 (13%) | 71,102,113 | 1.31 | 7 (9%) |
| 23 | LHG | b | 319 | 21 | 48,48,48 | 0.27 | 0 | 51,54,54 | 0.32 | 0 |
| 21 | CLA | 3 | 410 | - | 43,48,73 | 1.44 | 8 (18%) | 51,83,113 | 1.43 | 5 (9%) |
| 29 | CHL | 6 | 614 | - | 40,54,74 | 4.19 | 18 (45%) | 34,90,114 | 3.73 | 16 (47%) |
| 24 | BCR | G | 201 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.44 | 9 (16%) |
| 21 | CLA | 4 | 608 | 18 | 46,51,73 | 1.52 | 9 (19%) | 53,86,113 | 1.37 | 4 (7%) |
| 21 | CLA | 5 | 607 | - | 47,52,73 | 1.41 | 7 (14%) | 55,88,113 | 1.40 | 5 (9%) |
| 21 | CLA | 2 | 612 | 16 | 49,53,73 | 1.37 | 7 (14%) | 58,89,113 | 1.43 | 6 (10%) |
| 29 | CHL | 2 | 607 | - | 45,59,74 | 3.81 | 18 (40%) | 40,96,114 | 3.55 | 19 (47%) |
| 21 | CLA | 2 | 611 | - | 45,49,73 | 1.39 | 8 (17%) | 54,84,113 | 1.49 | 7 (12%) |
| 21 | CLA | A | 804 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.32 | 6 (7%) |
| 29 | CHL | a | 601 | 20 | 40,54,74 | 4.21 | 18 (45%) | 34,90,114 | 4.01 | 16 (47%) |
| 23 | LHG | 2 | 619 | 21 | 34,34,48 | 0.33 | 0 | 37,40,54 | 0.42 | 0 |
| 21 | CLA | B | 826 | - | 56,60,73 | 1.28 | 8 (14%) | 65,97,113 | 1.36 | 8 (12%) |
| 21 | CLA | c | 612 | 20 | 47,52,73 | 1.40 | 9 (19%) | 55,87,113 | 1.39 | 4 (7%) |
| 24 | BCR | A | 854 | - | 41,41,41 | 1.40 | 8 (19%) | 56,56,56 | 1.34 | 9 (16%) |
| 29 | CHL | 6 | 605 | - | 40,54,74 | 4.15 | 18 (45%) | 34,90,114 | 3.69 | 14 (41%) |
| 30 | LUT | 9 | 615 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.50 | 11 (21%) |
| 31 | XAT | 6 | 617 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 1.71 | 12 (22%) |
| 21 | CLA | O | 203 | - | 52,58,73 | 1.30 | 9 (17%) | 65,94,113 | 1.37 | 6 (9%) |
| 21 | CLA | B | 830 | - | 60,64,73 | 1.24 | 8 (13%) | 71,102,113 | 1.28 | 5 (7%) |
| 21 | CLA | 6 | 609 | - | 46,50,73 | 1.40 | 8 (17%) | 53,85,113 | 1.51 | 6 (11%) |
| 29 | CHL | 2 | 602 | 16 | 47,61,74 | 3.77 | 18 (38%) | 41,98,114 | 3.50 | 19 (46%) |
| 21 | CLA | 7 | 413 | - | 40,44,73 | 1.51 | 8 (20%) | 49,77,113 | 1.43 | 6 (12%) |
| 23 | LHG | 9 | 618 | 21 | 48,48,48 | 0.27 | 0 | 51,54,54 | 0.33 | 0 |
| 21 | CLA | 4 | 603 | - | 47,52,73 | 1.41 | 9 (19%) | 55,88,113 | 1.39 | 4 (7%) |
| 21 | CLA | A | 838 | - | 69,73,73 | 1.15 | 8 (11%) | 82,113,113 | 1.30 | 7 (8%) |
| 29 | CHL | 2 | 614 | - | 40,54,74 | 4.10 | 18 (45%) | 34,90,114 | 3.68 | 15 (44%) |
| 21 | CLA | A | 833 | - | 69,73,73 | 1.17 | 9 (13%) | 82,113,113 | 1.26 | 5 (6%) |
| 29 | CHL | a | 609 | - | 40,54,74 | 4.22 | 18 (45%) | 34,90,114 | 3.96 | 14 (41%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | b | 314 | - | 57,61,73 | 1.29 | 9 (15%) | 67,98,113 | 1.36 | 6 (8%) |
| 21 | CLA | 2 | 608 | 16 | 59,63,73 | 1.24 | 9 (15%) | 70,101,113 | 1.29 | 6 (8%) |
| 21 | CLA | 8 | 604 | - | 46,51,73 | 1.42 | 8 (17%) | 54,86,113 | 1.44 | 6 (11%) |
| 21 | CLA | A | 827 | - | 67,72,73 | 1.17 | 9 (13%) | 79,112,113 | 1.28 | 7 (8%) |
| 24 | BCR | 7 | 417 | - | 41,41,41 | 1.37 | 8 (19%) | 56,56,56 | 1.41 | 8 (14%) |
| 31 | XAT | 4 | 616 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 1.57 | 12 (22%) |
| 32 | NEX | 9 | 617 | - | 40,46,46 | 1.20 | 6 (15%) | 50,70,70 | 1.50 | 8 (16%) |
| 21 | CLA | a | 603 | - | 45,49,73 | 1.42 | 7 (15%) | 54,84,113 | 1.46 | 6 (11%) |
| 31 | XAT | 1 | 318 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 1.57 | 12 (22%) |
| 21 | CLA | 5 | 611 | 15 | 49,53,73 | 1.39 | 8 (16%) | 58,89,113 | 1.43 | 5 (8%) |
| 21 | CLA | a | 602 | - | 64,68,73 | 1.21 | 8 (12%) | 76,107,113 | 1.29 | 6 (7%) |
| 23 | LHG | 4 | 619 | - | 48,48,48 | 0.28 | 0 | 51,54,54 | 0.63 | 1 (1%) |
| 21 | CLA | A | 802 | - | 56,60,73 | 1.30 | 8 (14%) | 65,97,113 | 1.36 | 7 (10%) |
| 21 | CLA | L | 302 | 12 | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.47 | 5 (8%) |
| 21 | CLA | A | 832 | - | 49,53,73 | 1.36 | 9 (18%) | 58,89,113 | 1.41 | 6 (10%) |
| 26 | LMU | b | 301 | - | 36,36,36 | 0.37 | 0 | 47,47,47 | 0.77 | 1 (2%) |
| 21 | CLA | 3 | 409 | 17 | 56,60,73 | 1.57 | 10 (17%) | 65,97,113 | 2.09 | 17 (26%) |
| 21 | CLA | A | 813 | - | 58,62,73 | 1.25 | 9 (15%) | 68,99,113 | 1.42 | 6 (8%) |
| 21 | CLA | c | 603 | - | 59,63,73 | 1.26 | 9 (15%) | 70,101,113 | 1.27 | 6 (8%) |
| 21 | CLA | 7 | 405 | 17 | 43,48,73 | 1.55 | 9 (20%) | 51,83,113 | 1.48 | 6 (11%) |
| 21 | CLA | 6 | 603 | - | 49,53,73 | 1.41 | 6 (12%) | 58,89,113 | 1.42 | 3 (5%) |
| 29 | CHL | 6 | 602 | - | 47,61,74 | 3.77 | 18 (38%) | 41,98,114 | 3.56 | 19 (46%) |
| 29 | CHL | b | 306 | 20 | 40,54,74 | 4.13 | 18 (45%) | 34,90,114 | 3.74 | 16 (47%) |
| 24 | BCR | J | 101 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.82 | 10 (17%) |
| 21 | CLA | A | 822 | - | 48,52,73 | 1.39 | 9 (18%) | 57,88,113 | 1.48 | 4 (7%) |
| 21 | CLA | 5 | 604 | - | 53,57,73 | 1.33 | 8 (15%) | 61,93,113 | 1.39 | 4 (6%) |
| 31 | XAT | 7 | 416 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 1.66 | 13 (24%) |
| 21 | CLA | A | 816 | - | 46,50,73 | 1.37 | 9 (19%) | 53,85,113 | 1.45 | 6 (11%) |
| 21 | CLA | 6 | 608 | 16 | 49,53,73 | 1.40 | 8 (16%) | 58,89,113 | 1.38 | 4 (6%) |
| 21 | CLA | A | 809 | 1 | 63,67,73 | 1.20 | 8 (12%) | 74,105,113 | 1.34 | 7 (9%) |
| 21 | CLA | O | 204 | - | 43,48,73 | 1.46 | 6 (13%) | 49,83,113 | 1.38 | 4 (8%) |
| 24 | BCR | J | 104 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 2.33 | 23 (41%) |
| 21 | CLA | A | 842 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.27 | 5 (6%) |
| 21 | CLA | O | 201 | 23 | 46,50,73 | 1.38 | 9 (19%) | 53,85,113 | 1.47 | 5 (9%) |
| 24 | BCR | A | 848 | - | 41,41,41 | 1.40 | 8 (19%) | 56,56,56 | 1.25 | 8 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 28 | LMG | 6 | 615 | - | 13,13,55 | 0.20 | 0 | 18,18,63 | 0.49 | 0 |
| 21 | CLA | A | 803 | - | 56,60,73 | 1.28 | 8 (14%) | 65,97,113 | 1.33 | 8 (12%) |
| 25 | SF4 | C | 102 | 3 | 0,12,12 | - | - | - | | |
| 31 | XAT | 5 | 616 | - | 41,47,47 | 1.27 | 8 (19%) | 54,74,74 | 1.48 | 9 (16%) |
| 21 | CLA | 1 | 305 | - | 53,57,73 | 1.31 | 8 (15%) | 61,93,113 | 1.40 | 5 (8%) |
| 21 | CLA | 4 | 602 | 18 | 61,66,73 | 1.23 | 8 (13%) | 71,104,113 | 1.32 | 7 (9%) |
| 21 | CLA | 3 | 412 | - | 57,62,73 | 1.28 | 9 (15%) | 67,100,113 | 1.28 | 5 (7%) |
| 21 | CLA | 9 | 610 | 19 | 58,62,73 | 1.26 | 9 (15%) | 68,99,113 | 1.34 | 8 (11%) |
| 21 | CLA | B | 832 | - | 60,64,73 | 1.24 | 9 (15%) | 71,102,113 | 1.40 | 9 (12%) |
| 21 | CLA | c | 613 | - | 69,73,73 | 1.17 | 9 (13%) | 82,113,113 | 1.28 | 5 (6%) |
| 24 | BCR | 8 | 616 | - | 41,41,41 | 1.38 | 8 (19%) | 56,56,56 | 1.40 | 9 (16%) |
| 21 | CLA | 6 | 613 | - | 46,50,73 | 1.42 | 8 (17%) | 53,85,113 | 1.41 | 4 (7%) |
| 30 | LUT | c | 615 | - | 42,43,43 | 1.29 | 8 (19%) | 51,60,60 | 1.42 | 10 (19%) |
| 21 | CLA | 2 | 613 | - | 46,50,73 | 1.39 | 8 (17%) | 53,85,113 | 1.42 | 4 (7%) |
| 21 | CLA | B | 805 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.29 | 5 (6%) |
| 29 | CHL | 1 | 307 | - | 45,59,74 | 3.85 | 18 (40%) | 40,96,114 | 3.56 | 19 (47%) |
| 29 | CHL | 7 | 406 | - | 33,48,74 | 4.06 | 16 (48%) | 30,83,114 | 3.62 | 14 (46%) |
| 29 | CHL | 2 | 601 | 16 | 47,61,74 | 3.73 | 18 (38%) | 41,98,114 | 3.49 | 17 (41%) |
| 21 | CLA | B | 837 | - | 67,72,73 | 1.17 | 8 (11%) | 79,112,113 | 1.26 | 5 (6%) |
| 25 | SF4 | A | 851 | 2,1 | 0,12,12 | - | - | - | | |
| 29 | CHL | c | 606 | 20 | 40,54,74 | 4.16 | 18 (45%) | 34,90,114 | 3.84 | 16 (47%) |
| 29 | CHL | c | 607 | - | 40,54,74 | 4.19 | 18 (45%) | 34,90,114 | 3.81 | 16 (47%) |
| 21 | CLA | 3 | 411 | 17 | 47,51,73 | 1.38 | 9 (19%) | 55,86,113 | 1.41 | 4 (7%) |
| 29 | CHL | a | 608 | - | 40,54,74 | 4.11 | 18 (45%) | 34,90,114 | 3.70 | 15 (44%) |
| 21 | CLA | B | 816 | - | 56,60,73 | 1.29 | 9 (16%) | 65,97,113 | 1.42 | 5 (7%) |
| 21 | CLA | 7 | 401 | 17 | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.45 | 5 (8%) |
| 21 | CLA | 8 | 612 | - | 47,51,73 | 1.40 | 7 (14%) | 55,86,113 | 1.38 | 4 (7%) |
| 29 | CHL | 8 | 607 | - | 45,59,74 | 3.86 | 18 (40%) | 40,96,114 | 3.49 | 19 (47%) |
| 21 | CLA | B | 834 | - | 49,53,73 | 1.36 | 9 (18%) | 58,89,113 | 1.46 | 6 (10%) |
| 29 | CHL | 8 | 613 | - | 36,50,74 | 4.32 | 17 (47%) | 29,85,114 | 3.90 | 15 (51%) |
| 30 | LUT | a | 615 | - | 42,43,43 | 1.27 | 7 (16%) | 51,60,60 | 1.73 | 11 (21%) |
| 21 | CLA | 5 | 614 | 15 | 47,51,73 | 1.52 | 9 (19%) | 58,87,113 | 1.46 | 6 (10%) |
| 30 | LUT | 3 | 416 | - | 42,43,43 | 1.28 | 7 (16%) | 51,60,60 | 1.62 | 11 (21%) |
| 21 | CLA | a | 611 | - | 51,55,73 | 1.36 | 7 (13%) | 60,91,113 | 1.38 | 4 (6%) |
| 21 | CLA | 8 | 601 | 18 | 49,53,73 | 1.40 | 7 (14%) | 58,89,113 | 1.40 | 4 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 5 | 603 | - | 49,53,73 | 1.41 | 8 (16%) | 58,89,113 | 1.36 | 3 (5%) |
| 21 | CLA | A | 815 | - | 49,53,73 | 1.36 | 9 (18%) | 58,89,113 | 1.44 | 5 (8%) |
| 21 | CLA | 4 | 604 | - | 46,51,73 | 1.40 | 8 (17%) | 54,86,113 | 1.41 | 4 (7%) |
| 24 | BCR | F | 303 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.42 | 11 (19%) |
| 23 | LHG | 1 | 301 | 21 | 22,22,48 | 0.34 | 0 | 25,28,54 | 0.68 | 1 (4%) |
| 21 | CLA | 5 | 602 | 15 | 65,69,73 | 1.21 | 8 (12%) | 77,108,113 | 1.27 | 6 (7%) |
| 21 | CLA | 4 | 611 | 18 | 48,52,73 | 1.40 | 9 (18%) | 57,88,113 | 1.45 | 5 (8%) |
| 21 | CLA | B | 839 | - | 69,73,73 | 1.16 | 8 (11%) | 82,113,113 | 1.27 | 6 (7%) |
| 32 | NEX | b | 318 | - | 40,46,46 | 1.20 | 6 (15%) | 50,70,70 | 1.50 | 8 (16%) |
| 28 | LMG | G | 206 | - | 55,55,55 | 0.21 | 0 | 63,63,63 | 0.27 | 0 |
| 21 | CLA | 6 | 611 | - | 45,49,73 | 1.42 | 8 (17%) | 54,84,113 | 1.49 | 5 (9%) |
| 21 | CLA | B | 817 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.27 | 6 (7%) |
| 21 | CLA | 3 | 402 | 17 | 64,68,73 | 1.20 | 8 (12%) | 76,107,113 | 1.30 | 6 (7%) |
| 30 | LUT | c | 616 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.49 | 11 (21%) |
| 21 | CLA | 3 | 415 | - | 43,48,73 | 1.43 | 8 (18%) | 51,83,113 | 1.40 | 5 (9%) |
| 23 | LHG | A | 845 | 21 | 26,26,48 | 0.33 | 0 | 29,32,54 | 0.45 | 0 |
| 21 | CLA | 2 | 610 | 23 | 44,50,73 | 1.42 | 8 (18%) | 56,85,113 | 1.44 | 4 (7%) |
| 24 | BCR | L | 301 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.33 | 9 (16%) |
| 21 | CLA | A | 852 | - | 56,60,73 | 1.29 | 9 (16%) | 65,97,113 | 1.32 | 8 (12%) |
| 29 | CHL | 2 | 605 | - | 40,54,74 | 4.08 | 18 (45%) | 34,90,114 | 3.87 | 15 (44%) |
| 23 | LHG | 8 | 617 | 21 | 36,36,48 | 0.31 | 0 | 39,42,54 | 0.36 | 0 |
| 21 | CLA | A | 814 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.32 | 7 (8%) |
| 24 | BCR | O | 205 | - | 41,41,41 | 1.37 | 8 (19%) | 56,56,56 | 1.57 | 11 (19%) |
| 21 | CLA | 3 | 406 | 17 | 43,48,73 | 1.54 | 9 (20%) | 51,83,113 | 1.48 | 6 (11%) |
| 21 | CLA | A | 830 | - | 56,60,73 | 1.46 | 8 (14%) | 65,97,113 | 1.94 | 11 (16%) |
| 21 | CLA | B | 806 | - | 67,71,73 | 1.16 | 9 (13%) | 79,110,113 | 1.28 | 8 (10%) |
| 21 | CLA | b | 315 | - | 49,53,73 | 1.39 | 8 (16%) | 58,89,113 | 1.35 | 4 (6%) |
| 21 | CLA | 2 | 604 | - | 49,53,73 | 1.39 | 8 (16%) | 58,89,113 | 1.43 | 5 (8%) |
| 21 | CLA | a | 612 | - | 49,53,73 | 1.41 | 8 (16%) | 58,89,113 | 1.41 | 4 (6%) |
| 21 | CLA | 9 | 603 | 19 | 49,53,73 | 1.39 | 7 (14%) | 58,89,113 | 1.45 | 4 (6%) |
| 21 | CLA | a | 613 | - | 61,65,73 | 1.25 | 9 (14%) | 72,103,113 | 1.33 | 6 (8%) |
| 21 | CLA | B | 815 | - | 57,62,73 | 1.28 | 9 (15%) | 67,100,113 | 1.32 | 6 (8%) |
| 21 | CLA | 7 | 412 | - | 43,48,73 | 1.50 | 7 (16%) | 51,83,113 | 1.44 | 5 (9%) |
| 26 | LMU | 3 | 420 | - | 36,36,36 | 0.40 | 0 | 47,47,47 | 0.73 | 1 (2%) |
| 30 | LUT | 4 | 615 | - | 42,43,43 | 1.29 | 8 (19%) | 51,60,60 | 1.65 | 10 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 29 | CHL | 4 | 614 | 18 | 36,50,74 | 4.23 | 17 (47%) | 29,85,114 | 3.73 | 15 (51%) |
| 21 | CLA | a | 604 | - | 50,55,73 | 1.36 | 7 (14%) | 58,91,113 | 1.38 | 5 (8%) |
| 21 | CLA | 1 | 304 | - | 59,63,73 | 1.26 | 8 (13%) | 70,101,113 | 1.34 | 7 (10%) |
| 21 | CLA | b | 305 | - | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.41 | 4 (6%) |
| 30 | LUT | b | 317 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.44 | 10 (19%) |
| 23 | LHG | 4 | 618 | 21 | 36,36,48 | 0.32 | 0 | 39,42,54 | 0.40 | 0 |
| 29 | CHL | 5 | 601 | 15 | 40,54,74 | 4.12 | 19 (47%) | 34,90,114 | 3.77 | 14 (41%) |
| 21 | CLA | 1 | 311 | 23 | 41,46,73 | 1.57 | 10 (24%) | 51,81,113 | 1.52 | 8 (15%) |
| 21 | CLA | A | 828 | - | 64,68,73 | 1.19 | 9 (14%) | 76,107,113 | 1.23 | 7 (9%) |
| 21 | CLA | B | 827 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.21 | 6 (7%) |
| 30 | LUT | b | 316 | - | 42,43,43 | 1.27 | 8 (19%) | 51,60,60 | 1.49 | 9 (17%) |
| 21 | CLA | 5 | 612 | - | 49,53,73 | 1.41 | 8 (16%) | 58,89,113 | 1.42 | 4 (6%) |
| 21 | CLA | 4 | 613 | - | 47,51,73 | 1.38 | 8 (17%) | 55,86,113 | 1.40 | 4 (7%) |
| 21 | CLA | B | 801 | - | 69,73,73 | 2.04 | 20 (28%) | 82,113,113 | 2.69 | 32 (39%) |
| 21 | CLA | B | 821 | - | 59,63,73 | 1.23 | 7 (11%) | 70,101,113 | 1.37 | 7 (10%) |
| 29 | CHL | 8 | 605 | 18 | 36,49,74 | 3.84 | 16 (44%) | 32,84,114 | 3.85 | 14 (43%) |
| 21 | CLA | 7 | 408 | - | 45,49,73 | 1.42 | 7 (15%) | 54,84,113 | 1.43 | 5 (9%) |
| 24 | BCR | A | 846 | - | 41,41,41 | 1.38 | 8 (19%) | 56,56,56 | 1.54 | 8 (14%) |
| 26 | LMU | A | 853 | - | 36,36,36 | 0.39 | 0 | 47,47,47 | 0.81 | 1 (2%) |
| 21 | CLA | 6 | 610 | - | 44,50,73 | 1.45 | 8 (18%) | 56,85,113 | 1.41 | 4 (7%) |
| 21 | CLA | 8 | 610 | - | 48,52,73 | 1.42 | 8 (16%) | 57,88,113 | 1.42 | 4 (7%) |
| 29 | CHL | 9 | 601 | 19 | 37,51,74 | 4.28 | 17 (45%) | 30,86,114 | 4.06 | 15 (50%) |
| 21 | CLA | B | 812 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.29 | 6 (7%) |
| 21 | CLA | A | 817 | - | 69,73,73 | 1.14 | 9 (13%) | 82,113,113 | 1.29 | 5 (6%) |
| 21 | CLA | B | 808 | 2 | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.28 | 7 (8%) |
| 32 | NEX | c | 618 | - | 40,46,46 | 1.18 | 6 (15%) | 50,70,70 | 1.52 | 9 (18%) |
| 21 | CLA | 1 | 315 | - | 49,53,73 | 1.40 | 8 (16%) | 58,89,113 | 1.42 | 5 (8%) |
| 21 | CLA | B | 802 | - | 69,73,73 | 1.16 | 8 (11%) | 82,113,113 | 1.29 | 6 (7%) |
| 21 | CLA | B | 804 | - | 69,73,73 | 1.16 | 8 (11%) | 82,113,113 | 1.30 | 6 (7%) |
| 21 | CLA | 5 | 605 | - | 44,48,73 | 1.45 | 8 (18%) | 51,82,113 | 1.46 | 6 (11%) |
| 29 | CHL | b | 308 | - | 47,61,74 | 3.78 | 18 (38%) | 41,98,114 | 3.55 | 20 (48%) |
| 21 | CLA | A | 818 | - | 56,60,73 | 1.33 | 9 (16%) | 65,97,113 | 1.40 | 8 (12%) |
| 21 | CLA | 3 | 403 | - | 59,63,73 | 1.27 | 9 (15%) | 70,101,113 | 1.31 | 4 (5%) |
| 28 | LMG | 2 | 615 | - | 13,13,55 | 0.18 | 0 | 18,18,63 | 0.34 | 0 |
| 21 | CLA | A | 829 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.20 | 5 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 2 | 603 | - | 49,53,73 | 1.39 | 9 (18%) | 58,89,113 | 1.36 | 4 (6%) |
| 21 | CLA | A | 806 | - | 69,73,73 | 1.14 | 9 (13%) | 82,113,113 | 1.29 | 5 (6%) |
| 21 | CLA | B | 835 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.27 | 8 (9%) |
| 21 | CLA | B | 818 | - | 62,66,73 | 1.22 | 9 (14%) | 73,104,113 | 1.31 | 4 (5%) |
| 21 | CLA | 5 | 610 | - | 41,46,73 | 1.59 | 9 (21%) | 51,81,113 | 1.54 | 7 (13%) |
| 24 | BCR | F | 301 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.48 | 8 (14%) |
| 27 | DGD | B | 847 | - | 67,67,67 | 0.84 | 2 (2%) | 81,81,81 | 0.99 | 3 (3%) |
| 21 | CLA | L | 303 | - | 49,53,73 | 1.36 | 9 (18%) | 58,89,113 | 1.45 | 5 (8%) |
| 21 | CLA | H | 201 | 8 | 49,53,73 | 1.39 | 9 (18%) | 58,89,113 | 1.43 | 4 (6%) |
| 24 | BCR | B | 845 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.39 | 8 (14%) |
| 21 | CLA | 1 | 314 | - | 41,46,73 | 1.58 | 9 (21%) | 51,81,113 | 1.45 | 8 (15%) |
| 23 | LHG | A | 855 | - | 48,48,48 | 0.28 | 0 | 51,54,54 | 0.37 | 0 |
| 29 | CHL | 9 | 606 | 19 | 40,54,74 | 4.11 | 18 (45%) | 34,90,114 | 3.77 | 15 (44%) |
| 21 | CLA | c | 604 | - | 49,53,73 | 1.39 | 9 (18%) | 58,89,113 | 1.45 | 4 (6%) |
| 21 | CLA | 7 | 410 | - | 47,51,73 | 1.40 | 7 (14%) | 55,86,113 | 1.41 | 4 (7%) |
| 24 | BCR | 3 | 418 | - | 41,41,41 | 1.36 | 8 (19%) | 56,56,56 | 1.38 | 8 (14%) |
| 24 | BCR | L | 305 | - | 41,41,41 | 1.40 | 8 (19%) | 56,56,56 | 1.38 | 9 (16%) |
| 21 | CLA | A | 826 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.30 | 8 (9%) |
| 21 | CLA | F | 302 | - | 65,69,73 | 1.20 | 8 (12%) | 77,108,113 | 1.33 | 7 (9%) |
| 21 | CLA | 3 | 408 | 17 | 63,67,73 | 1.23 | 9 (14%) | 74,105,113 | 1.31 | 6 (8%) |
| 30 | LUT | 9 | 614 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.47 | 11 (21%) |
| 21 | CLA | B | 840 | 23 | 69,73,73 | 1.14 | 9 (13%) | 82,113,113 | 1.30 | 7 (8%) |
| 21 | CLA | 7 | 414 | - | 43,48,73 | 1.46 | 7 (16%) | 51,83,113 | 1.48 | 6 (11%) |
| 21 | CLA | B | 809 | - | 65,70,73 | 1.20 | 9 (13%) | 76,109,113 | 1.24 | 5 (6%) |
| 21 | CLA | b | 313 | 20 | 49,53,73 | 1.40 | 9 (18%) | 58,89,113 | 1.37 | 4 (6%) |
| 21 | CLA | c | 610 | 20 | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.42 | 5 (8%) |
| 21 | CLA | K | 204 | 11 | 49,53,73 | 1.38 | 9 (18%) | 58,89,113 | 1.43 | 4 (6%) |
| 21 | CLA | 8 | 618 | - | 45,49,73 | 1.41 | 7 (15%) | 54,84,113 | 1.45 | 6 (11%) |
| 21 | CLA | B | 825 | - | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.29 | 8 (9%) |
| 21 | CLA | A | 819 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.25 | 7 (8%) |
| 21 | CLA | 5 | 609 | - | 46,51,73 | 1.43 | 8 (17%) | 54,87,113 | 1.40 | 4 (7%) |
| 23 | LHG | A | 844 | - | 48,48,48 | 0.28 | 0 | 51,54,54 | 0.35 | 0 |
| 21 | CLA | 1 | 312 | 15 | 49,53,73 | 1.39 | 9 (18%) | 58,89,113 | 1.39 | 4 (6%) |
| 21 | CLA | A | 824 | - | 59,63,73 | 1.25 | 9 (15%) | 70,101,113 | 1.33 | 5 (7%) |
| 21 | CLA | A | 807 | 1 | 69,73,73 | 1.16 | 9 (13%) | 82,113,113 | 1.29 | 5 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 29 | CHL | c | 601 | 20 | 43,57,74 | 3.90 | 18 (41%) | 37,93,114 | 3.56 | 17 (45%) |
| 21 | CLA | B | 807 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.27 | 6 (7%) |
| 29 | CHL | 5 | 606 | - | 40,54,74 | 4.18 | 18 (45%) | 34,90,114 | 3.84 | 14 (41%) |
| 21 | CLA | B | 803 | - | 59,63,73 | 1.25 | 9 (15%) | 70,101,113 | 1.34 | 5 (7%) |
| 24 | BCR | 3 | 419 | - | 41,41,41 | 1.38 | 8 (19%) | 56,56,56 | 1.82 | 13 (23%) |
| 21 | CLA | 1 | 313 | 15 | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.42 | 4 (6%) |
| 22 | PQN | B | 841 | - | 34,34,34 | 0.41 | 0 | 43,45,45 | 0.52 | 1 (2%) |
| 30 | LUT | 6 | 616 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.59 | 13 (25%) |
| 21 | CLA | 9 | 612 | 19 | 49,53,73 | 1.38 | 7 (14%) | 58,89,113 | 1.39 | 4 (6%) |
| 29 | CHL | 9 | 607 | - | 40,54,74 | 4.11 | 18 (45%) | 34,90,114 | 3.74 | 16 (47%) |
| 21 | CLA | L | 304 | - | 46,50,73 | 1.38 | 8 (17%) | 53,85,113 | 1.44 | 5 (9%) |
| 24 | BCR | A | 850 | - | 41,41,41 | 1.40 | 8 (19%) | 56,56,56 | 1.70 | 9 (16%) |
| 21 | CLA | c | 614 | - | 49,53,73 | 1.39 | 9 (18%) | 58,89,113 | 1.33 | 4 (6%) |
| 21 | CLA | 4 | 610 | 23 | 49,53,73 | 1.37 | 8 (16%) | 58,89,113 | 1.44 | 4 (6%) |
| 21 | CLA | 6 | 612 | - | 49,53,73 | 1.41 | 7 (14%) | 58,89,113 | 1.45 | 4 (6%) |
| 21 | CLA | 7 | 407 | 17 | 47,52,73 | 2.26 | 14 (29%) | 55,88,113 | 3.73 | 20 (36%) |
| 23 | LHG | 5 | 617 | - | 27,27,48 | 0.35 | 0 | 30,33,54 | 0.45 | 0 |
| 31 | XAT | c | 617 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 1.59 | 10 (18%) |
| 21 | CLA | 4 | 601 | 18 | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.44 | 4 (6%) |
| 21 | CLA | A | 820 | - | 48,52,73 | 1.41 | 9 (18%) | 57,88,113 | 1.45 | 4 (7%) |
| 21 | CLA | A | 805 | - | 59,63,73 | 1.25 | 9 (15%) | 70,101,113 | 1.31 | 7 (10%) |
| 24 | BCR | 7 | 418 | - | 41,41,41 | 1.37 | 8 (19%) | 56,56,56 | 1.89 | 13 (23%) |
| 29 | CHL | 4 | 606 | - | 40,54,74 | 4.08 | 18 (45%) | 34,90,114 | 3.68 | 14 (41%) |
| 21 | CLA | B | 838 | - | 69,73,73 | 1.15 | 8 (11%) | 82,113,113 | 1.24 | 5 (6%) |
| 21 | CLA | 9 | 611 | 23 | 61,65,73 | 1.24 | 8 (13%) | 72,103,113 | 1.32 | 6 (8%) |
| 21 | CLA | B | 833 | - | 49,53,73 | 1.37 | 8 (16%) | 58,89,113 | 1.42 | 4 (6%) |
| 21 | CLA | 4 | 612 | - | 59,63,73 | 1.26 | 7 (11%) | 70,101,113 | 1.32 | 5 (7%) |
| 21 | CLA | 1 | 309 | 15 | 45,49,73 | 1.62 | 10 (22%) | 54,84,113 | 2.14 | 16 (29%) |
| 21 | CLA | O | 202 | - | 41,46,73 | 1.50 | 8 (19%) | 47,80,113 | 1.49 | 5 (10%) |
| 21 | CLA | 5 | 608 | 15 | 44,48,73 | 1.52 | 9 (20%) | 55,83,113 | 1.51 | 7 (12%) |
| 29 | CHL | c | 608 | - | 40,54,74 | 4.15 | 18 (45%) | 34,90,114 | 3.79 | 15 (44%) |
| 21 | CLA | 8 | 608 | 18 | 46,51,73 | 1.55 | 9 (19%) | 53,86,113 | 1.35 | 3 (5%) |
| 24 | BCR | A | 847 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.29 | 9 (16%) |
| 21 | CLA | 8 | 609 | 23 | 49,53,73 | 1.59 | 8 (16%) | 58,89,113 | 1.89 | 7 (12%) |
| 29 | CHL | b | 310 | - | 46,60,74 | 3.79 | 18 (39%) | 40,97,114 | 3.26 | 17 (42%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 3 | 405 | - | 44,49,73 | 1.41 | 9 (20%) | 50,84,113 | 1.47 | 4 (8%) |
| 21 | CLA | G | 204 | 7 | 47,52,73 | 1.42 | 8 (17%) | 55,88,113 | 1.41 | 4 (7%) |
| 21 | CLA | B | 823 | - | 69,73,73 | 1.16 | 8 (11%) | 82,113,113 | 1.38 | 7 (8%) |
| 21 | CLA | A | 837 | - | 55,59,73 | 1.32 | 8 (14%) | 64,96,113 | 1.29 | 6 (9%) |
| 21 | CLA | 4 | 609 | 18 | 56,60,73 | 1.65 | 11 (19%) | 65,97,113 | 2.16 | 16 (24%) |
| 24 | BCR | M | 101 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.74 | 12 (21%) |
| 21 | CLA | A | 810 | - | 49,53,73 | 1.37 | 8 (16%) | 58,89,113 | 1.45 | 5 (8%) |
| 29 | CHL | b | 302 | 20 | 40,54,74 | 4.17 | 18 (45%) | 34,90,114 | 3.99 | 16 (47%) |
| 21 | CLA | 6 | 604 | - | 49,53,73 | 1.40 | 8 (16%) | 58,89,113 | 1.38 | 4 (6%) |
| 21 | CLA | B | 829 | - | 49,53,73 | 1.38 | 7 (14%) | 58,89,113 | 1.52 | 5 (8%) |
| 21 | CLA | a | 610 | 20 | 49,53,73 | 1.38 | 8 (16%) | 58,89,113 | 1.42 | 4 (6%) |
| 21 | CLA | A | 801 | - | 56,60,73 | 1.71 | 9 (16%) | 65,97,113 | 2.08 | 18 (27%) |
| 21 | CLA | 5 | 613 | - | 41,46,73 | 1.59 | 8 (19%) | 51,81,113 | 1.50 | 7 (13%) |
| 21 | CLA | F | 305 | 6 | 45,49,73 | 1.39 | 9 (20%) | 54,84,113 | 1.46 | 5 (9%) |
| 21 | CLA | 8 | 603 | - | 47,52,73 | 1.43 | 8 (17%) | 55,88,113 | 1.39 | 4 (7%) |
| 21 | CLA | K | 201 | 11 | 50,54,73 | 1.35 | 8 (16%) | 59,90,113 | 1.42 | 4 (6%) |
| 30 | LUT | 7 | 415 | - | 42,43,43 | 1.31 | 8 (19%) | 51,60,60 | 1.78 | 14 (27%) |
| 29 | CHL | 1 | 302 | 15 | 45,59,74 | 3.84 | 18 (40%) | 40,96,114 | 3.67 | 19 (47%) |
| 21 | CLA | A | 812 | - | 69,73,73 | 1.14 | 8 (11%) | 82,113,113 | 1.21 | 5 (6%) |
| 21 | CLA | A | 831 | - | 59,63,73 | 1.25 | 9 (15%) | 70,101,113 | 1.38 | 6 (8%) |
| 21 | CLA | A | 808 | - | 49,53,73 | 1.37 | 9 (18%) | 58,89,113 | 1.46 | 6 (10%) |
| 21 | CLA | 3 | 404 | - | 45,50,73 | 1.53 | 9 (20%) | 55,86,113 | 1.48 | 6 (10%) |
| 21 | CLA | B | 828 | - | 56,60,73 | 1.28 | 9 (16%) | 65,97,113 | 1.35 | 6 (9%) |
| 21 | CLA | B | 820 | - | 50,54,73 | 1.35 | 7 (14%) | 59,90,113 | 1.39 | 4 (6%) |
| 29 | CHL | 4 | 605 | - | 36,49,74 | 3.83 | 16 (44%) | 32,84,114 | 3.87 | 14 (43%) |
| 21 | CLA | A | 823 | - | 60,64,73 | 1.25 | 9 (15%) | 71,102,113 | 1.30 | 5 (7%) |
| 24 | BCR | 2 | 618 | - | 41,41,41 | 1.37 | 8 (19%) | 56,56,56 | 1.45 | 10 (17%) |
| 29 | CHL | 6 | 607 | - | 45,59,74 | 3.92 | 18 (40%) | 40,96,114 | 3.52 | 17 (42%) |
| 21 | CLA | B | 814 | - | 64,68,73 | 1.20 | 9 (14%) | 76,107,113 | 1.34 | 6 (7%) |
| 21 | CLA | A | 834 | - | 69,73,73 | 1.16 | 8 (11%) | 82,113,113 | 1.26 | 6 (7%) |
| 23 | LHG | 6 | 619 | - | 34,34,48 | 0.31 | 0 | 37,40,54 | 0.37 | 0 |
| 21 | CLA | 2 | 609 | 16 | 55,59,73 | 1.37 | 7 (12%) | 63,95,113 | 1.89 | 11 (17%) |
| 21 | CLA | B | 811 | - | 49,53,73 | 1.41 | 8 (16%) | 58,89,113 | 1.51 | 4 (6%) |
| 21 | CLA | B | 822 | - | 49,53,73 | 1.38 | 9 (18%) | 58,89,113 | 1.44 | 4 (6%) |
| 21 | CLA | 7 | 402 | - | 49,53,73 | 1.40 | 7 (14%) | 58,89,113 | 1.40 | 5 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | a | 614 | - | 45,49,73 | 1.42 | 8 (17%) | 54,84,113 | 1.43 | 5 (9%) |
| 21 | CLA | A | 839 | - | 49,53,73 | 1.39 | 8 (16%) | 58,89,113 | 1.46 | 5 (8%) |
| 25 | SF4 | C | 101 | 3 | 0,12,12 | - | - | - | | |
| 21 | CLA | K | 203 | - | 48,52,73 | 1.47 | 10 (20%) | 59,88,113 | 1.49 | 6 (10%) |
| 26 | LMU | A | 856 | - | 36,36,36 | 0.39 | 0 | 47,47,47 | 0.75 | 1 (2%) |
| 31 | XAT | a | 618 | - | 41,47,47 | 1.27 | 8 (19%) | 54,74,74 | 1.68 | 10 (18%) |
| 31 | XAT | 9 | 616 | - | 41,47,47 | 1.28 | 8 (19%) | 54,74,74 | 2.24 | 15 (27%) |
| 29 | CHL | a | 606 | - | 40,54,74 | 4.16 | 18 (45%) | 34,90,114 | 3.99 | 16 (47%) |
| 21 | CLA | c | 611 | 23 | 62,66,73 | 1.22 | 8 (12%) | 73,104,113 | 1.31 | 5 (6%) |
| 21 | CLA | B | 824 | - | 69,73,73 | 1.15 | 8 (11%) | 82,113,113 | 1.29 | 6 (7%) |
| 21 | CLA | 7 | 404 | - | 44,49,73 | 1.44 | 7 (15%) | 50,84,113 | 1.43 | 4 (8%) |
| 30 | LUT | 8 | 614 | - | 42,43,43 | 1.30 | 8 (19%) | 51,60,60 | 1.58 | 9 (17%) |
| 31 | XAT | 8 | 615 | - | 41,47,47 | 1.27 | 8 (19%) | 54,74,74 | 1.59 | 9 (16%) |
| 21 | CLA | 7 | 411 | - | 57,62,73 | 1.30 | 8 (14%) | 67,100,113 | 1.28 | 6 (8%) |
| 29 | CHL | b | 307 | - | 40,54,74 | 4.07 | 18 (45%) | 34,90,114 | 3.85 | 15 (44%) |
| 21 | CLA | 9 | 613 | - | 57,61,73 | 1.28 | 8 (14%) | 67,98,113 | 1.39 | 6 (8%) |
| 29 | CHL | 9 | 605 | 19 | 40,54,74 | 4.15 | 18 (45%) | 34,90,114 | 3.78 | 16 (47%) |
| 29 | CHL | 9 | 609 | - | 40,54,74 | 4.12 | 18 (45%) | 34,90,114 | 3.66 | 16 (47%) |
| 30 | LUT | 5 | 615 | - | 42,43,43 | 1.29 | 8 (19%) | 51,60,60 | 1.62 | 11 (21%) |
| 21 | CLA | B | 836 | - | 69,73,73 | 1.15 | 9 (13%) | 82,113,113 | 1.34 | 7 (8%) |
| 21 | CLA | c | 602 | 20 | 64,68,73 | 1.21 | 9 (14%) | 76,107,113 | 1.27 | 6 (7%) |
| 23 | LHG | a | 617 | - | 48,48,48 | 0.27 | 0 | 51,54,54 | 0.36 | 0 |
| 29 | CHL | a | 605 | 20 | 39,53,74 | 4.26 | 18 (46%) | 33,89,114 | 3.77 | 16 (48%) |
| 24 | BCR | 6 | 618 | - | 41,41,41 | 1.37 | 8 (19%) | 56,56,56 | 1.56 | 10 (17%) |
| 24 | BCR | 4 | 617 | - | 41,41,41 | 1.38 | 8 (19%) | 56,56,56 | 1.38 | 10 (17%) |
| 21 | CLA | 9 | 602 | 19 | 57,61,73 | 1.28 | 9 (15%) | 67,98,113 | 1.37 | 6 (8%) |
| 21 | CLA | 1 | 303 | 15 | 65,69,73 | 1.19 | 9 (13%) | 77,108,113 | 1.31 | 5 (6%) |
| 30 | LUT | 1 | 317 | - | 42,43,43 | 1.30 | 8 (19%) | 51,60,60 | 1.61 | 10 (19%) |
| 30 | LUT | 2 | 616 | - | 42,43,43 | 1.28 | 8 (19%) | 51,60,60 | 1.66 | 12 (23%) |
| 21 | CLA | A | 836 | 1 | 49,53,73 | 1.38 | 9 (18%) | 58,89,113 | 1.39 | 4 (6%) |
| 21 | CLA | B | 813 | - | 47,52,73 | 1.39 | 7 (14%) | 55,88,113 | 1.43 | 5 (9%) |
| 24 | BCR | J | 103 | - | 41,41,41 | 1.39 | 8 (19%) | 56,56,56 | 1.51 | 10 (17%) |
| 21 | CLA | b | 303 | 20 | 63,67,73 | 1.23 | 9 (14%) | 74,105,113 | 1.29 | 6 (8%) |
| 21 | CLA | 1 | 316 | 15 | 47,51,73 | 1.52 | 10 (21%) | 58,87,113 | 1.48 | 6 (10%) |
| 21 | CLA | 3 | 413 | - | 43,48,73 | 1.44 | 9 (20%) | 51,83,113 | 1.43 | 5 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 3 | 414 | - | 40,44,73 | 1.48 | 9 (22%) | 49,77,113 | 1.46 | 4 (8%) |
| 24 | BCR | B | 842 | - | 41,41,41 | 1.38 | 8 (19%) | 56,56,56 | 1.36 | 8 (14%) |
| 21 | CLA | 3 | 401 | - | 43,48,73 | 1.42 | 8 (18%) | 51,83,113 | 1.55 | 6 (11%) |
| 24 | BCR | K | 205 | - | 41,41,41 | 0.73 | 1 (2%) | 56,56,56 | 2.14 | 19 (33%) |

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 |
|---|---|---|---|---|---|---|---|
| 21 | CLA | A | 835 | - | 1/1/12/20 | 1/21/97/115 | - |
| 24 | BCR | I | 101 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | G | 203 | - | 1/1/12/20 | 7/21/97/115 | - |
| 21 | CLA | 9 | 604 | - | 1/1/11/20 | 8/15/91/115 | - |
| 21 | CLA | A | 841 | - | 1/1/15/20 | 16/39/115/115 | - |
| 29 | CHL | c | 605 | - | 3/3/15/26 | 3/9/107/137 | - |
| 26 | LMU | O | 206 | - | - | 5/21/61/61 | 0/2/2/2 |
| 21 | CLA | b | 312 | 23 | 1/1/11/20 | 4/15/91/115 | - |
| 24 | BCR | B | 844 | - | - | 11/29/63/63 | 0/2/2/2 |
| 29 | CHL | 6 | 601 | 16 | 3/3/16/26 | 4/11/109/137 | - |
| 21 | CLA | 7 | 403 | - | 1/1/11/20 | 2/9/85/115 | - |
| 29 | CHL | 2 | 606 | - | 3/3/16/26 | 2/15/113/137 | - |
| 21 | CLA | G | 202 | - | 1/1/11/20 | 5/15/91/115 | - |
| 29 | CHL | 4 | 607 | - | 3/3/17/26 | 4/21/119/137 | - |
| 21 | CLA | 1 | 310 | 15 | 1/1/11/20 | 3/11/87/115 | - |
| 24 | BCR | B | 843 | - | - | 13/29/63/63 | 0/2/2/2 |
| 21 | CLA | b | 304 | - | 1/1/11/20 | 3/15/91/115 | - |
| 21 | CLA | 1 | 306 | - | 1/1/9/20 | 2/10/82/115 | - |
| 29 | CHL | 3 | 407 | - | 3/3/15/26 | 0/6/104/137 | - |
| 23 | LHG | 1 | 319 | 21 | - | 5/32/32/53 | - |
| 29 | CHL | c | 609 | 20 | 3/3/16/26 | 6/11/109/137 | - |
| 21 | CLA | B | 810 | - | 1/1/13/20 | 2/25/101/115 | - |
| 28 | LMG | J | 105 | - | - | 5/25/45/70 | 0/1/1/1 |
| 21 | CLA | A | 821 | - | 1/1/15/20 | 11/39/115/115 | - |
| 24 | BCR | A | 849 | - | - | 2/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 7 | 409 | - | 1/1/10/20 | 1/8/84/115 | - |
| 29 | CHL | b | 309 | - | 3/3/16/26 | 5/19/117/137 | - |
| 22 | PQN | A | 843 | - | - | 1/23/43/43 | 0/2/2/2 |
| 21 | CLA | B | 819 | - | 1/1/10/20 | 3/13/89/115 | - |
| 21 | CLA | 8 | 611 | - | 1/1/12/20 | 12/25/101/115 | - |
| 29 | CHL | 6 | 606 | - | 3/3/16/26 | 6/15/113/137 | - |
| 31 | XAT | 2 | 617 | - | - | 0/31/93/93 | 0/4/4/4 |
| 29 | CHL | 8 | 606 | - | 3/3/16/26 | 5/15/113/137 | - |
| 29 | CHL | 9 | 608 | - | 3/3/16/26 | 5/15/113/137 | - |
| 24 | BCR | G | 205 | - | - | 1/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 840 | - | 1/1/15/20 | 12/39/115/115 | - |
| 21 | CLA | b | 311 | 20 | 1/1/12/20 | 9/26/102/115 | - |
| 29 | CHL | a | 607 | - | 3/3/15/26 | 1/12/110/137 | - |
| 21 | CLA | J | 102 | 10 | 1/1/10/20 | 8/12/88/115 | - |
| 30 | LUT | a | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 23 | LHG | c | 619 | 21 | - | 3/53/53/53 | - |
| 24 | BCR | B | 846 | - | - | 3/29/63/63 | 0/2/2/2 |
| 31 | XAT | 3 | 417 | - | - | 0/31/93/93 | 0/4/4/4 |
| 24 | BCR | L | 306 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | K | 202 | - | 1/1/12/20 | 2/21/97/115 | - |
| 21 | CLA | A | 825 | - | 1/1/15/20 | 10/39/115/115 | - |
| 21 | CLA | 1 | 308 | - | 1/1/11/20 | 6/13/89/115 | - |
| 21 | CLA | F | 304 | - | 1/1/11/20 | 0/15/91/115 | - |
| 21 | CLA | 8 | 602 | 18 | 1/1/13/20 | 8/30/106/115 | - |
| 21 | CLA | A | 811 | - | 1/1/11/20 | 3/15/91/115 | - |
| 21 | CLA | B | 831 | - | 1/1/13/20 | 9/29/105/115 | - |
| 23 | LHG | b | 319 | 21 | - | 8/53/53/53 | - |
| 21 | CLA | 3 | 410 | - | 1/1/10/20 | 3/8/84/115 | - |
| 29 | CHL | 6 | 614 | - | 3/3/16/26 | 5/15/113/137 | - |
| 24 | BCR | G | 201 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | 4 | 608 | 18 | 1/1/10/20 | 0/9/87/115 | - |
| 21 | CLA | 5 | 607 | - | 1/1/11/20 | 4/13/89/115 | - |
| 21 | CLA | 2 | 612 | 16 | 1/1/11/20 | 7/15/91/115 | - |
| 29 | CHL | 2 | 607 | - | 3/3/17/26 | 6/21/119/137 | - |
| 21 | CLA | 2 | 611 | - | 1/1/10/20 | 0/10/86/115 | - |
| 21 | CLA | A | 804 | - | 1/1/15/20 | 10/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 29 | CHL | a | 601 | 20 | 3/3/16/26 | 2/15/113/137 | - |
| 23 | LHG | 2 | 619 | 21 | - | 6/39/39/53 | - |
| 21 | CLA | B | 826 | - | 1/1/12/20 | 8/24/100/115 | - |
| 21 | CLA | c | 612 | 20 | 1/1/10/20 | 4/14/90/115 | - |
| 29 | CHL | 6 | 605 | - | 3/3/16/26 | 5/15/113/137 | - |
| 24 | BCR | A | 854 | - | - | 0/29/63/63 | 0/2/2/2 |
| 30 | LUT | 9 | 615 | - | - | 2/29/67/67 | 0/2/2/2 |
| 31 | XAT | 6 | 617 | - | - | 7/31/93/93 | 0/4/4/4 |
| 21 | CLA | O | 203 | - | 1/1/11/20 | 4/19/95/115 | - |
| 21 | CLA | B | 830 | - | 1/1/13/20 | 11/29/105/115 | - |
| 21 | CLA | 6 | 609 | - | 1/1/10/20 | 4/12/88/115 | - |
| 29 | CHL | 2 | 602 | 16 | 3/3/17/26 | 9/24/122/137 | - |
| 21 | CLA | 7 | 413 | - | 1/1/8/20 | 0/2/74/115 | - |
| 23 | LHG | 9 | 618 | 21 | - | 9/53/53/53 | - |
| 21 | CLA | 4 | 603 | - | 1/1/11/20 | 6/13/89/115 | - |
| 21 | CLA | A | 838 | - | 1/1/15/20 | 10/39/115/115 | - |
| 29 | CHL | 2 | 614 | - | 3/3/16/26 | 3/15/113/137 | - |
| 21 | CLA | A | 833 | - | 1/1/15/20 | 8/39/115/115 | - |
| 29 | CHL | a | 609 | - | 3/3/16/26 | 7/15/113/137 | - |
| 21 | CLA | b | 314 | - | 1/1/12/20 | 7/25/101/115 | - |
| 21 | CLA | 2 | 608 | 16 | 1/1/13/20 | 8/27/103/115 | - |
| 21 | CLA | 8 | 604 | - | 1/1/10/20 | 6/12/88/115 | - |
| 21 | CLA | A | 827 | - | 1/1/15/20 | 17/37/113/115 | - |
| 24 | BCR | 7 | 417 | - | - | 2/29/63/63 | 0/2/2/2 |
| 31 | XAT | 4 | 616 | - | - | 0/31/93/93 | 0/4/4/4 |
| 32 | NEX | 9 | 617 | - | - | 2/27/83/83 | 0/3/3/3 |
| 21 | CLA | a | 603 | - | 1/1/10/20 | 2/10/86/115 | - |
| 31 | XAT | 1 | 318 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | 5 | 611 | 15 | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | a | 602 | - | 1/1/14/20 | 10/33/109/115 | - |
| 23 | LHG | 4 | 619 | - | - | 10/53/53/53 | - |
| 21 | CLA | A | 802 | - | 1/1/12/20 | 3/24/100/115 | - |
| 21 | CLA | L | 302 | 12 | 1/1/11/20 | 7/15/91/115 | - |
| 21 | CLA | A | 832 | - | 1/1/11/20 | 5/15/91/115 | - |
| 26 | LMU | b | 301 | - | - | 6/21/61/61 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 3 | 409 | 17 | 1/1/12/20 | 10/24/100/115 | - |
| 21 | CLA | A | 813 | - | 1/1/12/20 | 4/26/102/115 | - |
| 21 | CLA | c | 603 | - | 1/1/13/20 | 6/27/103/115 | - |
| 21 | CLA | 7 | 405 | 17 | 1/1/10/20 | 2/8/84/115 | - |
| 21 | CLA | 6 | 603 | - | 1/1/11/20 | 7/15/91/115 | - |
| 29 | CHL | 6 | 602 | - | 3/3/17/26 | 10/24/122/137 | - |
| 29 | CHL | b | 306 | 20 | 3/3/16/26 | 6/15/113/137 | - |
| 24 | BCR | J | 101 | - | - | 7/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 822 | - | 1/1/11/20 | 3/13/89/115 | - |
| 21 | CLA | 5 | 604 | - | 1/1/11/20 | 6/20/96/115 | - |
| 31 | XAT | 7 | 416 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | A | 816 | - | 1/1/10/20 | 2/12/88/115 | - |
| 21 | CLA | 6 | 608 | 16 | 1/1/11/20 | 7/15/91/115 | - |
| 21 | CLA | A | 809 | 1 | 1/1/13/20 | 5/32/108/115 | - |
| 21 | CLA | O | 204 | - | 1/1/10/20 | 2/8/84/115 | - |
| 24 | BCR | J | 104 | - | - | 9/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 842 | - | 1/1/15/20 | 14/39/115/115 | - |
| 21 | CLA | O | 201 | 23 | 1/1/10/20 | 2/12/88/115 | - |
| 24 | BCR | A | 848 | - | - | 1/29/63/63 | 0/2/2/2 |
| 28 | LMG | 6 | 615 | - | - | 3/4/24/70 | 0/1/1/1 |
| 21 | CLA | A | 803 | - | 1/1/12/20 | 6/24/100/115 | - |
| 25 | SF4 | C | 102 | 3 | - | - | 0/6/5/5 |
| 31 | XAT | 5 | 616 | - | - | 3/31/93/93 | 0/4/4/4 |
| 21 | CLA | 1 | 305 | - | 1/1/11/20 | 9/20/96/115 | - |
| 21 | CLA | 4 | 602 | 18 | 1/1/13/20 | 10/30/106/115 | - |
| 21 | CLA | 3 | 412 | - | 1/1/13/20 | 11/25/101/115 | - |
| 21 | CLA | 9 | 610 | 19 | 1/1/12/20 | 3/26/102/115 | - |
| 21 | CLA | B | 832 | - | 1/1/13/20 | 7/29/105/115 | - |
| 21 | CLA | c | 613 | - | 1/1/15/20 | 9/39/115/115 | - |
| 24 | BCR | 8 | 616 | - | - | 6/29/63/63 | 0/2/2/2 |
| 21 | CLA | 6 | 613 | - | 1/1/10/20 | 5/12/88/115 | - |
| 30 | LUT | c | 615 | - | - | 0/29/67/67 | 0/2/2/2 |
| 21 | CLA | 2 | 613 | - | 1/1/10/20 | 3/12/88/115 | - |
| 21 | CLA | B | 805 | - | 1/1/15/20 | 18/39/115/115 | - |
| 29 | CHL | 1 | 307 | - | 3/3/17/26 | 2/21/119/137 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 29 | CHL | 7 | 406 | - | 3/3/15/26 | 0/6/104/137 | - |
| 29 | CHL | 2 | 601 | 16 | 3/3/17/26 | 8/24/122/137 | - |
| 21 | CLA | B | 837 | - | 1/1/15/20 | 10/37/113/115 | - |
| 25 | SF4 | A | 851 | 2,1 | - | - | 0/6/5/5 |
| 29 | CHL | c | 606 | 20 | 3/3/16/26 | 4/15/113/137 | - |
| 29 | CHL | c | 607 | - | 3/3/16/26 | 3/15/113/137 | - |
| 21 | CLA | 3 | 411 | 17 | 1/1/10/20 | 2/13/89/115 | - |
| 29 | CHL | a | 608 | - | 3/3/16/26 | 7/15/113/137 | - |
| 21 | CLA | B | 816 | - | 1/1/12/20 | 5/24/100/115 | - |
| 21 | CLA | 7 | 401 | 17 | 1/1/11/20 | 8/15/91/115 | - |
| 21 | CLA | 8 | 612 | - | 1/1/10/20 | 3/13/89/115 | - |
| 29 | CHL | 8 | 607 | - | 3/3/17/26 | 7/21/119/137 | - |
| 21 | CLA | B | 834 | - | 1/1/11/20 | 5/15/91/115 | - |
| 29 | CHL | 8 | 613 | - | 3/3/15/26 | 2/10/108/137 | - |
| 30 | LUT | a | 615 | - | - | 4/29/67/67 | 0/2/2/2 |
| 21 | CLA | 5 | 614 | 15 | 1/1/11/20 | 5/11/87/115 | - |
| 30 | LUT | 3 | 416 | - | - | 5/29/67/67 | 0/2/2/2 |
| 21 | CLA | a | 611 | - | 1/1/11/20 | 6/18/94/115 | - |
| 21 | CLA | 8 | 601 | 18 | 1/1/11/20 | 9/15/91/115 | - |
| 21 | CLA | 5 | 603 | - | 1/1/11/20 | 6/15/91/115 | - |
| 21 | CLA | A | 815 | - | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | 4 | 604 | - | 1/1/10/20 | 2/12/88/115 | - |
| 24 | BCR | F | 303 | - | - | 0/29/63/63 | 0/2/2/2 |
| 23 | LHG | 1 | 301 | 21 | - | 7/26/26/53 | - |
| 21 | CLA | 5 | 602 | 15 | 1/1/14/20 | 15/35/111/115 | - |
| 21 | CLA | 4 | 611 | 18 | 1/1/11/20 | 4/13/89/115 | - |
| 21 | CLA | B | 839 | - | 1/1/15/20 | 10/39/115/115 | - |
| 32 | NEX | b | 318 | - | - | 2/27/83/83 | 0/3/3/3 |
| 28 | LMG | G | 206 | - | - | 9/50/70/70 | 0/1/1/1 |
| 21 | CLA | 6 | 611 | - | 1/1/10/20 | 6/10/86/115 | - |
| 21 | CLA | B | 817 | - | 1/1/15/20 | 20/39/115/115 | - |
| 21 | CLA | 3 | 402 | 17 | 1/1/14/20 | 5/33/109/115 | - |
| 30 | LUT | c | 616 | - | - | 0/29/67/67 | 0/2/2/2 |
| 21 | CLA | 3 | 415 | - | 1/1/10/20 | 0/8/84/115 | - |
| 23 | LHG | A | 845 | 21 | - | 5/31/31/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 2 | 610 | 23 | 1/1/10/20 | 2/9/85/115 | - |
| 24 | BCR | L | 301 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 852 | - | 1/1/12/20 | 6/24/100/115 | - |
| 29 | CHL | 2 | 605 | - | 3/3/16/26 | 3/15/113/137 | - |
| 23 | LHG | 8 | 617 | 21 | - | 9/41/41/53 | - |
| 21 | CLA | A | 814 | - | 1/1/15/20 | 8/39/115/115 | - |
| 24 | BCR | O | 205 | - | - | 6/29/63/63 | 0/2/2/2 |
| 21 | CLA | 3 | 406 | 17 | 1/1/10/20 | 0/8/84/115 | - |
| 21 | CLA | A | 830 | - | 1/1/12/20 | 4/24/100/115 | - |
| 21 | CLA | B | 806 | - | 1/1/14/20 | 7/37/113/115 | - |
| 21 | CLA | b | 315 | - | 1/1/11/20 | 11/15/91/115 | - |
| 21 | CLA | 2 | 604 | - | 1/1/11/20 | 2/15/91/115 | - |
| 21 | CLA | a | 612 | - | 1/1/11/20 | 6/15/91/115 | - |
| 21 | CLA | 9 | 603 | 19 | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | a | 613 | - | 1/1/13/20 | 5/30/106/115 | - |
| 21 | CLA | B | 815 | - | 1/1/13/20 | 5/25/101/115 | - |
| 21 | CLA | 7 | 412 | - | 1/1/10/20 | 2/8/84/115 | - |
| 26 | LMU | 3 | 420 | - | - | 3/21/61/61 | 0/2/2/2 |
| 30 | LUT | 4 | 615 | - | - | 4/29/67/67 | 0/2/2/2 |
| 29 | CHL | 4 | 614 | 18 | 3/3/15/26 | 2/10/108/137 | - |
| 21 | CLA | a | 604 | - | 1/1/11/20 | 9/17/93/115 | - |
| 21 | CLA | 1 | 304 | - | 1/1/13/20 | 6/27/103/115 | - |
| 21 | CLA | b | 305 | - | 1/1/11/20 | 5/15/91/115 | - |
| 30 | LUT | b | 317 | - | - | 2/29/67/67 | 0/2/2/2 |
| 29 | CHL | 5 | 601 | 15 | 3/3/16/26 | 5/15/113/137 | - |
| 23 | LHG | 4 | 618 | 21 | - | 9/41/41/53 | - |
| 21 | CLA | 1 | 311 | 23 | 1/1/10/20 | 2/4/80/115 | - |
| 21 | CLA | A | 828 | - | 1/1/14/20 | 14/33/109/115 | - |
| 21 | CLA | B | 827 | - | 1/1/15/20 | 10/39/115/115 | - |
| 30 | LUT | b | 316 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 5 | 612 | - | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | 4 | 613 | - | 1/1/10/20 | 2/13/89/115 | - |
| 21 | CLA | B | 801 | - | 1/1/15/20 | 14/39/115/115 | - |
| 21 | CLA | B | 821 | - | 1/1/13/20 | 4/27/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 29 | CHL | 8 | 605 | 18 | 3/3/15/26 | 2/10/106/137 | - |
| 21 | CLA | 7 | 408 | - | 1/1/10/20 | 4/10/86/115 | - |
| 24 | BCR | A | 846 | - | - | 4/29/63/63 | 0/2/2/2 |
| 26 | LMU | A | 853 | - | - | 0/21/61/61 | 0/2/2/2 |
| 21 | CLA | 6 | 610 | - | 1/1/10/20 | 1/9/85/115 | - |
| 21 | CLA | 8 | 610 | - | 1/1/11/20 | 7/13/89/115 | - |
| 29 | CHL | 9 | 601 | 19 | 3/3/15/26 | 2/12/110/137 | - |
| 21 | CLA | B | 812 | - | 1/1/15/20 | 18/39/115/115 | - |
| 21 | CLA | A | 817 | - | 1/1/15/20 | 17/39/115/115 | - |
| 21 | CLA | B | 808 | 2 | 1/1/15/20 | 7/39/115/115 | - |
| 32 | NEX | c | 618 | - | - | 2/27/83/83 | 0/3/3/3 |
| 21 | CLA | 1 | 315 | - | 1/1/11/20 | 6/15/91/115 | - |
| 21 | CLA | B | 802 | - | 1/1/15/20 | 19/39/115/115 | - |
| 21 | CLA | B | 804 | - | 1/1/15/20 | 13/39/115/115 | - |
| 21 | CLA | 5 | 605 | - | 1/1/9/20 | 6/10/82/115 | - |
| 29 | CHL | b | 308 | - | 3/3/17/26 | 6/24/122/137 | - |
| 21 | CLA | A | 818 | - | 1/1/12/20 | 7/24/100/115 | - |
| 21 | CLA | 3 | 403 | - | 1/1/13/20 | 8/27/103/115 | - |
| 28 | LMG | 2 | 615 | - | - | 1/4/24/70 | 0/1/1/1 |
| 21 | CLA | A | 829 | - | 1/1/15/20 | 9/39/115/115 | - |
| 21 | CLA | 2 | 603 | - | 1/1/11/20 | 7/15/91/115 | - |
| 21 | CLA | A | 806 | - | 1/1/15/20 | 18/39/115/115 | - |
| 21 | CLA | B | 835 | - | 1/1/15/20 | 6/39/115/115 | - |
| 21 | CLA | B | 818 | - | 1/1/13/20 | 9/31/107/115 | - |
| 21 | CLA | 5 | 610 | - | 1/1/10/20 | 0/4/80/115 | - |
| 24 | BCR | F | 301 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | DGD | B | 847 | - | - | 16/55/95/95 | 0/2/2/2 |
| 21 | CLA | L | 303 | - | 1/1/11/20 | 3/15/91/115 | - |
| 21 | CLA | H | 201 | 8 | 1/1/11/20 | 6/15/91/115 | - |
| 24 | BCR | B | 845 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 1 | 314 | - | 1/1/10/20 | 1/4/80/115 | - |
| 23 | LHG | A | 855 | - | - | 7/53/53/53 | - |
| 29 | CHL | 9 | 606 | 19 | 3/3/16/26 | 5/15/113/137 | - |
| 21 | CLA | c | 604 | - | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | 7 | 410 | - | 1/1/10/20 | 5/13/89/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | BCR | 3 | 418 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | BCR | L | 305 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 826 | - | 1/1/15/20 | 8/39/115/115 | - |
| 21 | CLA | F | 302 | - | 1/1/14/20 | 11/35/111/115 | - |
| 21 | CLA | 3 | 408 | 17 | 1/1/13/20 | 6/32/108/115 | - |
| 30 | LUT | 9 | 614 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | B | 840 | 23 | 1/1/15/20 | 4/39/115/115 | - |
| 21 | CLA | 7 | 414 | - | 1/1/10/20 | 1/8/84/115 | - |
| 21 | CLA | B | 809 | - | 1/1/14/20 | 13/35/111/115 | - |
| 21 | CLA | b | 313 | 20 | 1/1/11/20 | 8/15/91/115 | - |
| 21 | CLA | c | 610 | 20 | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | K | 204 | 11 | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | 8 | 618 | - | 1/1/10/20 | 4/10/86/115 | - |
| 21 | CLA | B | 825 | - | 1/1/15/20 | 9/39/115/115 | - |
| 21 | CLA | A | 819 | - | 1/1/15/20 | 15/39/115/115 | - |
| 21 | CLA | 5 | 609 | - | 1/1/11/20 | 5/11/87/115 | - |
| 23 | LHG | A | 844 | - | - | 8/53/53/53 | - |
| 21 | CLA | 1 | 312 | 15 | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | A | 824 | - | 1/1/13/20 | 11/27/103/115 | - |
| 21 | CLA | A | 807 | 1 | 1/1/15/20 | 11/39/115/115 | - |
| 29 | CHL | c | 601 | 20 | 3/3/16/26 | 6/19/117/137 | - |
| 21 | CLA | B | 807 | - | 1/1/15/20 | 17/39/115/115 | - |
| 29 | CHL | 5 | 606 | - | 3/3/16/26 | 5/15/113/137 | - |
| 21 | CLA | B | 803 | - | 1/1/13/20 | 7/27/103/115 | - |
| 24 | BCR | 3 | 419 | - | - | 8/29/63/63 | 0/2/2/2 |
| 21 | CLA | 1 | 313 | 15 | 1/1/11/20 | 5/15/91/115 | - |
| 22 | PQN | B | 841 | - | - | 1/23/43/43 | 0/2/2/2 |
| 30 | LUT | 6 | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 9 | 612 | 19 | 1/1/11/20 | 4/15/91/115 | - |
| 29 | CHL | 9 | 607 | - | 3/3/16/26 | 9/15/113/137 | - |
| 21 | CLA | L | 304 | - | 1/1/10/20 | 3/12/88/115 | - |
| 24 | BCR | A | 850 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | c | 614 | - | 1/1/11/20 | 5/15/91/115 | - |
| 21 | CLA | 4 | 610 | 23 | 1/1/11/20 | 2/15/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 6 | 612 | - | 1/1/11/20 | 7/15/91/115 | - |
| 21 | CLA | 7 | 407 | 17 | - | 5/13/89/115 | - |
| 23 | LHG | 5 | 617 | - | - | 6/32/32/53 | - |
| 31 | XAT | c | 617 | - | - | 1/31/93/93 | 0/4/4/4 |
| 21 | CLA | 4 | 601 | 18 | 1/1/11/20 | 3/15/91/115 | - |
| 21 | CLA | A | 820 | - | 1/1/11/20 | 2/13/89/115 | - |
| 21 | CLA | A | 805 | - | 1/1/13/20 | 6/27/103/115 | - |
| 24 | BCR | 7 | 418 | - | - | 6/29/63/63 | 0/2/2/2 |
| 29 | CHL | 4 | 606 | - | 3/3/16/26 | 4/15/113/137 | - |
| 21 | CLA | B | 838 | - | 1/1/15/20 | 9/39/115/115 | - |
| 21 | CLA | 9 | 611 | 23 | 1/1/13/20 | 9/30/106/115 | - |
| 21 | CLA | B | 833 | - | 1/1/11/20 | 2/15/91/115 | - |
| 21 | CLA | 4 | 612 | - | 1/1/13/20 | 7/27/103/115 | - |
| 21 | CLA | 1 | 309 | 15 | 1/1/10/20 | 2/10/86/115 | - |
| 21 | CLA | O | 202 | - | 1/1/9/20 | 2/6/78/115 | - |
| 21 | CLA | 5 | 608 | 15 | 1/1/10/20 | 2/8/84/115 | - |
| 29 | CHL | c | 608 | - | 3/3/16/26 | 8/15/113/137 | - |
| 21 | CLA | 8 | 608 | 18 | 1/1/10/20 | 5/9/87/115 | - |
| 24 | BCR | A | 847 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | 8 | 609 | 23 | 1/1/11/20 | 7/15/91/115 | - |
| 29 | CHL | b | 310 | - | 3/3/17/26 | 1/22/120/137 | - |
| 21 | CLA | 3 | 405 | - | 1/1/10/20 | 3/10/86/115 | - |
| 21 | CLA | G | 204 | 7 | 1/1/11/20 | 4/13/89/115 | - |
| 21 | CLA | B | 823 | - | 1/1/15/20 | 10/39/115/115 | - |
| 21 | CLA | A | 837 | - | 1/1/12/20 | 9/23/99/115 | - |
| 21 | CLA | 4 | 609 | 18 | - | 10/24/100/115 | - |
| 24 | BCR | M | 101 | - | - | 8/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 810 | - | 1/1/11/20 | 4/15/91/115 | - |
| 29 | CHL | b | 302 | 20 | 3/3/16/26 | 4/15/113/137 | - |
| 21 | CLA | 6 | 604 | - | 1/1/11/20 | 4/15/91/115 | - |
| 21 | CLA | B | 829 | - | 1/1/11/20 | 1/15/91/115 | - |
| 21 | CLA | a | 610 | 20 | 1/1/11/20 | 4/15/91/115 | - |
| 21 | CLA | A | 801 | - | - | 7/24/100/115 | - |
| 21 | CLA | 5 | 613 | - | 1/1/10/20 | 1/4/80/115 | - |
| 21 | CLA | F | 305 | 6 | 1/1/10/20 | 2/10/86/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 8 | 603 | - | 1/1/11/20 | 3/13/89/115 | - |
| 21 | CLA | K | 201 | 11 | 1/1/11/20 | 6/17/93/115 | - |
| 30 | LUT | 7 | 415 | - | - | 6/29/67/67 | 0/2/2/2 |
| 29 | CHL | 1 | 302 | 15 | 3/3/17/26 | 7/21/119/137 | - |
| 21 | CLA | A | 812 | - | 1/1/15/20 | 4/39/115/115 | - |
| 21 | CLA | A | 831 | - | 1/1/13/20 | 6/27/103/115 | - |
| 21 | CLA | A | 808 | - | 1/1/11/20 | 2/15/91/115 | - |
| 21 | CLA | 3 | 404 | - | 1/1/11/20 | 0/9/85/115 | - |
| 21 | CLA | B | 828 | - | 1/1/12/20 | 7/24/100/115 | - |
| 21 | CLA | B | 820 | - | 1/1/11/20 | 4/17/93/115 | - |
| 29 | CHL | 4 | 605 | - | 3/3/15/26 | 2/10/106/137 | - |
| 21 | CLA | A | 823 | - | 1/1/13/20 | 8/29/105/115 | - |
| 29 | CHL | 6 | 607 | - | 3/3/17/26 | 4/21/119/137 | - |
| 24 | BCR | 2 | 618 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | B | 814 | - | 1/1/14/20 | 9/33/109/115 | - |
| 21 | CLA | A | 834 | - | 1/1/15/20 | 10/39/115/115 | - |
| 23 | LHG | 6 | 619 | - | - | 3/39/39/53 | - |
| 21 | CLA | 2 | 609 | 16 | 1/1/11/20 | 9/22/98/115 | - |
| 21 | CLA | B | 811 | - | 1/1/11/20 | 3/15/91/115 | - |
| 21 | CLA | B | 822 | - | 1/1/11/20 | 4/15/91/115 | - |
| 21 | CLA | 7 | 402 | - | 1/1/11/20 | 9/15/91/115 | - |
| 21 | CLA | a | 614 | - | 1/1/10/20 | 2/10/86/115 | - |
| 21 | CLA | A | 839 | - | 1/1/11/20 | 0/15/91/115 | - |
| 25 | SF4 | C | 101 | 3 | - | - | 0/6/5/5 |
| 21 | CLA | K | 203 | - | 1/1/11/20 | 4/13/89/115 | - |
| 26 | LMU | A | 856 | - | - | 3/21/61/61 | 0/2/2/2 |
| 31 | XAT | a | 618 | - | - | 1/31/93/93 | 0/4/4/4 |
| 31 | XAT | 9 | 616 | - | - | 8/31/93/93 | 0/4/4/4 |
| 29 | CHL | a | 606 | - | 3/3/16/26 | 3/15/113/137 | - |
| 21 | CLA | c | 611 | 23 | 1/1/13/20 | 11/31/107/115 | - |
| 21 | CLA | B | 824 | - | 1/1/15/20 | 8/39/115/115 | - |
| 21 | CLA | 7 | 404 | - | 1/1/10/20 | 2/10/86/115 | - |
| 30 | LUT | 8 | 614 | - | - | 4/29/67/67 | 0/2/2/2 |
| 31 | XAT | 8 | 615 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | 7 | 411 | - | 1/1/13/20 | 8/25/101/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 29 | CHL | b | 307 | - | 3/3/16/26 | 2/15/113/137 | - |
| 21 | CLA | 9 | 613 | - | 1/1/12/20 | 7/25/101/115 | - |
| 29 | CHL | 9 | 605 | 19 | 3/3/16/26 | 4/15/113/137 | - |
| 29 | CHL | 9 | 609 | - | 3/3/16/26 | 4/15/113/137 | - |
| 30 | LUT | 5 | 615 | - | - | 7/29/67/67 | 0/2/2/2 |
| 21 | CLA | B | 836 | - | 1/1/15/20 | 14/39/115/115 | - |
| 21 | CLA | c | 602 | 20 | 1/1/14/20 | 7/33/109/115 | - |
| 23 | LHG | a | 617 | - | - | 10/53/53/53 | - |
| 29 | CHL | a | 605 | 20 | 3/3/16/26 | 4/13/111/137 | - |
| 24 | BCR | 6 | 618 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | BCR | 4 | 617 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 9 | 602 | 19 | 1/1/12/20 | 4/25/101/115 | - |
| 21 | CLA | 1 | 303 | 15 | 1/1/14/20 | 17/35/111/115 | - |
| 30 | LUT | 1 | 317 | - | - | 3/29/67/67 | 0/2/2/2 |
| 30 | LUT | 2 | 616 | - | - | 4/29/67/67 | 0/2/2/2 |
| 21 | CLA | A | 836 | 1 | 1/1/11/20 | 2/15/91/115 | - |
| 21 | CLA | B | 813 | - | 1/1/11/20 | 2/13/89/115 | - |
| 24 | BCR | J | 103 | - | - | 3/29/63/63 | 0/2/2/2 |
| 21 | CLA | b | 303 | 20 | 1/1/13/20 | 10/32/108/115 | - |
| 21 | CLA | 1 | 316 | 15 | 1/1/11/20 | 3/11/87/115 | - |
| 21 | CLA | 3 | 413 | - | 1/1/10/20 | 2/8/84/115 | - |
| 21 | CLA | 3 | 414 | - | 1/1/8/20 | 2/2/74/115 | - |
| 24 | BCR | B | 842 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | 3 | 401 | - | 1/1/10/20 | 1/8/84/115 | - |
| 24 | BCR | K | 205 | - | - | 3/29/63/63 | 0/2/2/2 |

All (3213) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | a | 601 | CHL | C2C-C3C | 12.04 | 1.48 | 1.36 |
| 29 | c | 605 | CHL | C2C-C3C | 12.02 | 1.48 | 1.36 |
| 29 | 9 | 601 | CHL | C2C-C3C | 12.00 | 1.48 | 1.36 |
| 29 | a | 606 | CHL | C2C-C3C | 11.98 | 1.48 | 1.36 |
| 29 | a | 609 | CHL | C2C-C3C | 11.97 | 1.48 | 1.36 |
| 29 | 8 | 606 | CHL | C2C-C3C | 11.94 | 1.47 | 1.36 |
| 29 | a | 605 | CHL | C2C-C3C | 11.82 | 1.47 | 1.36 |
| 29 | 6 | 614 | CHL | C2C-C3C | 11.82 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | c | 607 | CHL | C2C-C3C | 11.81 | 1.47 | 1.36 |
| 29 | 5 | 606 | CHL | C2C-C3C | 11.78 | 1.47 | 1.36 |
| 29 | 6 | 607 | CHL | C2C-C3C | 11.74 | 1.47 | 1.36 |
| 29 | b | 306 | CHL | C2C-C3C | 11.73 | 1.47 | 1.36 |
| 29 | 8 | 613 | CHL | C2C-C3C | 11.72 | 1.47 | 1.36 |
| 29 | b | 302 | CHL | C2C-C3C | 11.71 | 1.47 | 1.36 |
| 29 | 9 | 609 | CHL | C2C-C3C | 11.66 | 1.47 | 1.36 |
| 29 | c | 606 | CHL | C2C-C3C | 11.64 | 1.47 | 1.36 |
| 29 | c | 608 | CHL | C2C-C3C | 11.61 | 1.47 | 1.36 |
| 29 | b | 310 | CHL | C2C-C3C | 11.59 | 1.47 | 1.36 |
| 29 | 6 | 606 | CHL | C2C-C3C | 11.57 | 1.47 | 1.36 |
| 29 | a | 607 | CHL | C2C-C3C | 11.56 | 1.47 | 1.36 |
| 29 | 9 | 605 | CHL | C2C-C3C | 11.55 | 1.47 | 1.36 |
| 29 | 9 | 608 | CHL | C2C-C3C | 11.51 | 1.47 | 1.36 |
| 29 | 6 | 605 | CHL | C2C-C3C | 11.47 | 1.47 | 1.36 |
| 29 | 9 | 607 | CHL | C2C-C3C | 11.46 | 1.47 | 1.36 |
| 29 | 1 | 302 | CHL | C2C-C3C | 11.44 | 1.47 | 1.36 |
| 29 | b | 308 | CHL | C2C-C3C | 11.44 | 1.47 | 1.36 |
| 29 | 2 | 607 | CHL | C2C-C3C | 11.44 | 1.47 | 1.36 |
| 29 | 6 | 602 | CHL | C2C-C3C | 11.42 | 1.47 | 1.36 |
| 29 | 2 | 602 | CHL | C2C-C3C | 11.39 | 1.47 | 1.36 |
| 29 | 2 | 606 | CHL | C2C-C3C | 11.36 | 1.47 | 1.36 |
| 29 | c | 601 | CHL | C2C-C3C | 11.36 | 1.47 | 1.36 |
| 29 | 5 | 601 | CHL | C2C-C3C | 11.34 | 1.47 | 1.36 |
| 29 | a | 608 | CHL | C2C-C3C | 11.34 | 1.47 | 1.36 |
| 29 | 2 | 614 | CHL | C2C-C3C | 11.33 | 1.47 | 1.36 |
| 29 | 1 | 307 | CHL | C2C-C3C | 11.33 | 1.47 | 1.36 |
| 29 | 2 | 605 | CHL | C2C-C3C | 11.31 | 1.47 | 1.36 |
| 29 | 8 | 607 | CHL | C2C-C3C | 11.29 | 1.47 | 1.36 |
| 29 | 2 | 601 | CHL | C2C-C3C | 11.25 | 1.47 | 1.36 |
| 29 | b | 307 | CHL | C2C-C3C | 11.25 | 1.47 | 1.36 |
| 29 | b | 309 | CHL | C2C-C3C | 11.24 | 1.47 | 1.36 |
| 29 | 4 | 606 | CHL | C2C-C3C | 11.22 | 1.47 | 1.36 |
| 29 | 9 | 606 | CHL | C2C-C3C | 11.20 | 1.47 | 1.36 |
| 29 | 4 | 607 | CHL | C2C-C3C | 11.12 | 1.47 | 1.36 |
| 29 | 4 | 614 | CHL | C2C-C3C | 11.12 | 1.47 | 1.36 |
| 29 | a | 601 | CHL | C1A-CHA | 8.87 | 1.50 | 1.40 |
| 29 | a | 606 | CHL | C1A-CHA | 8.84 | 1.50 | 1.40 |
| 29 | a | 605 | CHL | C1A-CHA | 8.78 | 1.50 | 1.40 |
| 29 | 9 | 601 | CHL | C1A-CHA | 8.71 | 1.49 | 1.40 |
| 29 | b | 302 | CHL | C1A-CHA | 8.67 | 1.49 | 1.40 |
| 29 | 7 | 406 | CHL | C3B-C4B | 8.55 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | c | 606 | CHL | C3B-C4B | 8.52 | 1.49 | 1.41 |
| 29 | c | 608 | CHL | C1A-CHA | 8.49 | 1.49 | 1.40 |
| 29 | b | 309 | CHL | C3B-C4B | 8.48 | 1.49 | 1.41 |
| 29 | 6 | 605 | CHL | C3B-C4B | 8.47 | 1.49 | 1.41 |
| 29 | 2 | 602 | CHL | C3B-C4B | 8.46 | 1.49 | 1.41 |
| 29 | a | 605 | CHL | C3B-C4B | 8.46 | 1.49 | 1.41 |
| 29 | c | 605 | CHL | C3B-C4B | 8.45 | 1.49 | 1.41 |
| 29 | a | 606 | CHL | C3B-C4B | 8.45 | 1.49 | 1.41 |
| 29 | 6 | 614 | CHL | C3B-C4B | 8.44 | 1.49 | 1.41 |
| 29 | 8 | 606 | CHL | C3B-C4B | 8.44 | 1.49 | 1.41 |
| 29 | 5 | 606 | CHL | C3B-C4B | 8.43 | 1.49 | 1.41 |
| 29 | 9 | 605 | CHL | C3B-C4B | 8.42 | 1.49 | 1.41 |
| 29 | 4 | 605 | CHL | C4B-C3B | 8.40 | 1.49 | 1.39 |
| 29 | 6 | 606 | CHL | C3B-C4B | 8.40 | 1.49 | 1.41 |
| 29 | 8 | 605 | CHL | C4B-C3B | 8.40 | 1.49 | 1.39 |
| 29 | 2 | 605 | CHL | C3B-C4B | 8.38 | 1.49 | 1.41 |
| 29 | 6 | 601 | CHL | C1A-CHA | 8.38 | 1.49 | 1.40 |
| 29 | c | 609 | CHL | C3B-C4B | 8.38 | 1.49 | 1.41 |
| 29 | b | 307 | CHL | C3B-C4B | 8.36 | 1.49 | 1.41 |
| 29 | 8 | 605 | CHL | C1B-C2B | 8.36 | 1.49 | 1.39 |
| 29 | a | 609 | CHL | C3B-C4B | 8.34 | 1.49 | 1.41 |
| 29 | 9 | 601 | CHL | C3B-C4B | 8.34 | 1.49 | 1.41 |
| 29 | c | 608 | CHL | C3B-C4B | 8.33 | 1.49 | 1.41 |
| 29 | 6 | 602 | CHL | C3B-C4B | 8.32 | 1.49 | 1.41 |
| 29 | 5 | 601 | CHL | C3B-C4B | 8.32 | 1.49 | 1.41 |
| 29 | 9 | 607 | CHL | C1A-CHA | 8.32 | 1.49 | 1.40 |
| 29 | 5 | 606 | CHL | C1A-CHA | 8.29 | 1.49 | 1.40 |
| 29 | 1 | 307 | CHL | C3B-C4B | 8.29 | 1.49 | 1.41 |
| 29 | 2 | 614 | CHL | C3B-C4B | 8.28 | 1.49 | 1.41 |
| 29 | c | 607 | CHL | C3B-C4B | 8.28 | 1.49 | 1.41 |
| 29 | b | 302 | CHL | C1B-C2B | 8.28 | 1.49 | 1.39 |
| 29 | 6 | 601 | CHL | C1B-C2B | 8.27 | 1.49 | 1.39 |
| 29 | 6 | 607 | CHL | C3B-C4B | 8.27 | 1.49 | 1.41 |
| 29 | 9 | 606 | CHL | C3B-C4B | 8.26 | 1.49 | 1.41 |
| 29 | a | 608 | CHL | C3B-C4B | 8.25 | 1.49 | 1.41 |
| 29 | c | 607 | CHL | C1B-C2B | 8.25 | 1.48 | 1.39 |
| 29 | 4 | 606 | CHL | C3B-C4B | 8.24 | 1.49 | 1.41 |
| 29 | 8 | 613 | CHL | C3B-C4B | 8.23 | 1.49 | 1.41 |
| 29 | b | 306 | CHL | C3B-C4B | 8.23 | 1.49 | 1.41 |
| 29 | 2 | 606 | CHL | C3B-C4B | 8.23 | 1.49 | 1.41 |
| 29 | a | 607 | CHL | C3B-C4B | 8.22 | 1.49 | 1.41 |
| 29 | a | 605 | CHL | C1B-C2B | 8.22 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | c | 609 | CHL | C1A-CHA | 8.21 | 1.49 | 1.40 |
| 29 | 6 | 601 | CHL | C3B-C4B | 8.21 | 1.49 | 1.41 |
| 29 | 6 | 606 | CHL | C1A-CHA | 8.21 | 1.49 | 1.40 |
| 29 | 5 | 606 | CHL | C1B-C2B | 8.20 | 1.48 | 1.39 |
| 29 | c | 609 | CHL | C1B-C2B | 8.18 | 1.48 | 1.39 |
| 29 | 2 | 607 | CHL | C3B-C4B | 8.17 | 1.49 | 1.41 |
| 29 | 9 | 601 | CHL | C1B-C2B | 8.17 | 1.48 | 1.39 |
| 29 | c | 605 | CHL | C1A-CHA | 8.17 | 1.49 | 1.40 |
| 29 | 6 | 602 | CHL | C1A-CHA | 8.16 | 1.49 | 1.40 |
| 29 | 4 | 607 | CHL | C3B-C4B | 8.16 | 1.49 | 1.41 |
| 29 | 5 | 601 | CHL | C1B-C2B | 8.15 | 1.48 | 1.39 |
| 29 | a | 608 | CHL | C1B-C2B | 8.14 | 1.48 | 1.39 |
| 29 | 9 | 605 | CHL | C1B-C2B | 8.14 | 1.48 | 1.39 |
| 29 | 4 | 605 | CHL | C1B-C2B | 8.14 | 1.48 | 1.39 |
| 29 | b | 302 | CHL | C3B-C4B | 8.13 | 1.49 | 1.41 |
| 29 | a | 601 | CHL | C3B-C4B | 8.13 | 1.49 | 1.41 |
| 29 | 9 | 608 | CHL | C3B-C4B | 8.13 | 1.49 | 1.41 |
| 29 | a | 601 | CHL | C1B-C2B | 8.12 | 1.48 | 1.39 |
| 29 | c | 605 | CHL | C1B-C2B | 8.12 | 1.48 | 1.39 |
| 29 | 8 | 606 | CHL | C1B-C2B | 8.12 | 1.48 | 1.39 |
| 29 | b | 308 | CHL | C1A-CHA | 8.11 | 1.49 | 1.40 |
| 29 | c | 606 | CHL | C1B-C2B | 8.11 | 1.48 | 1.39 |
| 29 | 6 | 614 | CHL | C1B-C2B | 8.10 | 1.48 | 1.39 |
| 29 | 9 | 609 | CHL | C3B-C4B | 8.10 | 1.49 | 1.41 |
| 29 | 4 | 614 | CHL | C3B-C4B | 8.10 | 1.49 | 1.41 |
| 29 | 8 | 607 | CHL | C3B-C4B | 8.08 | 1.49 | 1.41 |
| 29 | 7 | 406 | CHL | C1B-C2B | 8.08 | 1.48 | 1.39 |
| 29 | c | 606 | CHL | C1A-CHA | 8.08 | 1.49 | 1.40 |
| 29 | 2 | 601 | CHL | C3B-C4B | 8.08 | 1.49 | 1.41 |
| 29 | 1 | 302 | CHL | C3B-C4B | 8.07 | 1.49 | 1.41 |
| 29 | 4 | 614 | CHL | C1B-C2B | 8.07 | 1.48 | 1.39 |
| 29 | c | 607 | CHL | C1A-CHA | 8.07 | 1.49 | 1.40 |
| 29 | 2 | 606 | CHL | C1A-CHA | 8.07 | 1.49 | 1.40 |
| 29 | 6 | 607 | CHL | C1B-C2B | 8.07 | 1.48 | 1.39 |
| 29 | b | 306 | CHL | C1B-C2B | 8.07 | 1.48 | 1.39 |
| 29 | 9 | 606 | CHL | C1B-C2B | 8.06 | 1.48 | 1.39 |
| 29 | b | 308 | CHL | C3B-C4B | 8.05 | 1.49 | 1.41 |
| 29 | 9 | 609 | CHL | C1B-C2B | 8.05 | 1.48 | 1.39 |
| 29 | c | 601 | CHL | C1A-CHA | 8.04 | 1.49 | 1.40 |
| 29 | 8 | 607 | CHL | C1B-C2B | 8.03 | 1.48 | 1.39 |
| 29 | a | 607 | CHL | C1B-C2B | 8.03 | 1.48 | 1.39 |
| 29 | a | 608 | CHL | C1A-CHA | 8.03 | 1.49 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 9 | 607 | CHL | C1B-C2B | 8.03 | 1.48 | 1.39 |
| 29 | 8 | 607 | CHL | C1A-CHA | 8.03 | 1.49 | 1.40 |
| 29 | 8 | 606 | CHL | C1A-CHA | 8.02 | 1.49 | 1.40 |
| 29 | 4 | 607 | CHL | C1A-CHA | 8.01 | 1.49 | 1.40 |
| 29 | 8 | 605 | CHL | C1A-CHA | 8.01 | 1.49 | 1.40 |
| 29 | c | 601 | CHL | C1B-C2B | 8.00 | 1.48 | 1.39 |
| 29 | 8 | 613 | CHL | C1B-C2B | 8.00 | 1.48 | 1.39 |
| 29 | c | 608 | CHL | C1B-C2B | 8.00 | 1.48 | 1.39 |
| 29 | 1 | 302 | CHL | C1B-C2B | 7.99 | 1.48 | 1.39 |
| 29 | 6 | 606 | CHL | C1B-C2B | 7.99 | 1.48 | 1.39 |
| 29 | 9 | 606 | CHL | C1A-CHA | 7.98 | 1.49 | 1.40 |
| 29 | 9 | 607 | CHL | C3B-C4B | 7.97 | 1.49 | 1.41 |
| 29 | 5 | 601 | CHL | C1A-CHA | 7.97 | 1.49 | 1.40 |
| 29 | a | 607 | CHL | C1A-CHA | 7.96 | 1.49 | 1.40 |
| 29 | 9 | 605 | CHL | C1A-CHA | 7.95 | 1.49 | 1.40 |
| 29 | 6 | 605 | CHL | C1B-C2B | 7.95 | 1.48 | 1.39 |
| 29 | 4 | 606 | CHL | C1B-C2B | 7.94 | 1.48 | 1.39 |
| 29 | 2 | 614 | CHL | C1B-C2B | 7.93 | 1.48 | 1.39 |
| 29 | 9 | 609 | CHL | C1A-CHA | 7.93 | 1.49 | 1.40 |
| 29 | 1 | 307 | CHL | C1B-C2B | 7.93 | 1.48 | 1.39 |
| 29 | 2 | 606 | CHL | C1B-C2B | 7.92 | 1.48 | 1.39 |
| 29 | 1 | 302 | CHL | C1A-CHA | 7.92 | 1.49 | 1.40 |
| 29 | 3 | 407 | CHL | C3B-C4B | 7.92 | 1.49 | 1.41 |
| 29 | 2 | 601 | CHL | C1B-C2B | 7.92 | 1.48 | 1.39 |
| 29 | b | 310 | CHL | C3B-C4B | 7.92 | 1.49 | 1.41 |
| 29 | 6 | 607 | CHL | C1A-CHA | 7.91 | 1.49 | 1.40 |
| 29 | b | 309 | CHL | C1A-CHA | 7.90 | 1.49 | 1.40 |
| 29 | 9 | 608 | CHL | C1B-C2B | 7.88 | 1.48 | 1.39 |
| 29 | b | 308 | CHL | C1B-C2B | 7.88 | 1.48 | 1.39 |
| 29 | 4 | 606 | CHL | C1A-CHA | 7.87 | 1.48 | 1.40 |
| 29 | 7 | 406 | CHL | C1A-CHA | 7.86 | 1.48 | 1.40 |
| 29 | 1 | 307 | CHL | C1A-CHA | 7.86 | 1.48 | 1.40 |
| 29 | c | 601 | CHL | C3B-C4B | 7.85 | 1.49 | 1.41 |
| 29 | a | 609 | CHL | C1B-C2B | 7.85 | 1.48 | 1.39 |
| 29 | 4 | 614 | CHL | C1A-CHA | 7.83 | 1.48 | 1.40 |
| 29 | 6 | 614 | CHL | C1A-CHA | 7.83 | 1.48 | 1.40 |
| 29 | 3 | 407 | CHL | C1B-C2B | 7.83 | 1.48 | 1.39 |
| 29 | b | 307 | CHL | C1B-C2B | 7.83 | 1.48 | 1.39 |
| 29 | 6 | 602 | CHL | C1B-C2B | 7.83 | 1.48 | 1.39 |
| 29 | a | 609 | CHL | C1D-C2D | 7.82 | 1.48 | 1.39 |
| 29 | 4 | 605 | CHL | C1A-CHA | 7.82 | 1.48 | 1.40 |
| 29 | 3 | 407 | CHL | C1A-CHA | 7.81 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 310 | CHL | C1B-C2B | 7.80 | 1.48 | 1.39 |
| 29 | 8 | 613 | CHL | C1A-CHA | 7.78 | 1.48 | 1.40 |
| 29 | 9 | 608 | CHL | C1A-CHA | 7.75 | 1.48 | 1.40 |
| 29 | 7 | 406 | CHL | C1D-C2D | 7.75 | 1.48 | 1.39 |
| 29 | 2 | 605 | CHL | C1A-CHA | 7.75 | 1.48 | 1.40 |
| 29 | b | 309 | CHL | C1B-C2B | 7.73 | 1.48 | 1.39 |
| 29 | b | 306 | CHL | C1A-CHA | 7.72 | 1.48 | 1.40 |
| 29 | a | 609 | CHL | C1A-CHA | 7.71 | 1.48 | 1.40 |
| 29 | 6 | 605 | CHL | C1D-C2D | 7.69 | 1.48 | 1.39 |
| 29 | a | 606 | CHL | C1B-C2B | 7.69 | 1.48 | 1.39 |
| 29 | 6 | 605 | CHL | C1A-CHA | 7.67 | 1.48 | 1.40 |
| 29 | 2 | 605 | CHL | C1B-C2B | 7.66 | 1.48 | 1.39 |
| 29 | 2 | 607 | CHL | C1B-C2B | 7.65 | 1.48 | 1.39 |
| 29 | 2 | 602 | CHL | C1B-C2B | 7.64 | 1.48 | 1.39 |
| 29 | c | 605 | CHL | C1D-C2D | 7.64 | 1.48 | 1.39 |
| 29 | 4 | 607 | CHL | C1B-C2B | 7.63 | 1.48 | 1.39 |
| 29 | 2 | 607 | CHL | C1A-CHA | 7.61 | 1.48 | 1.40 |
| 29 | 6 | 614 | CHL | C1D-C2D | 7.60 | 1.48 | 1.39 |
| 29 | 2 | 602 | CHL | C1A-CHA | 7.60 | 1.48 | 1.40 |
| 29 | 8 | 606 | CHL | C1D-C2D | 7.59 | 1.48 | 1.39 |
| 29 | b | 310 | CHL | C1A-CHA | 7.59 | 1.48 | 1.40 |
| 29 | 2 | 601 | CHL | C1A-CHA | 7.56 | 1.48 | 1.40 |
| 29 | 2 | 614 | CHL | C1A-CHA | 7.54 | 1.48 | 1.40 |
| 29 | a | 605 | CHL | C1D-C2D | 7.51 | 1.48 | 1.39 |
| 29 | b | 307 | CHL | C1A-CHA | 7.51 | 1.48 | 1.40 |
| 29 | c | 607 | CHL | C1D-C2D | 7.50 | 1.48 | 1.39 |
| 29 | c | 606 | CHL | C1D-C2D | 7.50 | 1.48 | 1.39 |
| 29 | 8 | 613 | CHL | C1D-C2D | 7.48 | 1.48 | 1.39 |
| 29 | 5 | 601 | CHL | C1D-C2D | 7.47 | 1.48 | 1.39 |
| 29 | a | 607 | CHL | C1D-C2D | 7.47 | 1.48 | 1.39 |
| 29 | 5 | 606 | CHL | C1D-C2D | 7.46 | 1.48 | 1.39 |
| 29 | 9 | 605 | CHL | C1D-C2D | 7.45 | 1.48 | 1.39 |
| 21 | 7 | 407 | CLA | C1D-ND | 7.45 | 1.47 | 1.37 |
| 29 | 8 | 607 | CHL | C1D-C2D | 7.45 | 1.48 | 1.39 |
| 29 | 6 | 607 | CHL | C1D-C2D | 7.41 | 1.48 | 1.39 |
| 29 | 9 | 609 | CHL | C1D-C2D | 7.41 | 1.48 | 1.39 |
| 29 | 6 | 601 | CHL | C1D-C2D | 7.41 | 1.48 | 1.39 |
| 29 | 8 | 605 | CHL | C1D-C2D | 7.40 | 1.48 | 1.39 |
| 29 | b | 302 | CHL | C1D-C2D | 7.40 | 1.48 | 1.39 |
| 29 | c | 608 | CHL | C1D-C2D | 7.39 | 1.48 | 1.39 |
| 29 | 6 | 606 | CHL | C1D-C2D | 7.39 | 1.48 | 1.39 |
| 29 | a | 601 | CHL | C1D-C2D | 7.39 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 310 | CHL | C1D-C2D | 7.38 | 1.47 | 1.39 |
| 29 | 4 | 605 | CHL | C1D-C2D | 7.35 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | C1D-C2D | 7.34 | 1.47 | 1.39 |
| 29 | b | 306 | CHL | C1D-C2D | 7.33 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | C1D-C2D | 7.33 | 1.47 | 1.39 |
| 29 | a | 606 | CHL | C1D-C2D | 7.30 | 1.47 | 1.39 |
| 29 | 1 | 302 | CHL | C1D-C2D | 7.28 | 1.47 | 1.39 |
| 29 | 9 | 607 | CHL | C1D-C2D | 7.28 | 1.47 | 1.39 |
| 29 | b | 308 | CHL | C1D-C2D | 7.27 | 1.47 | 1.39 |
| 29 | 9 | 606 | CHL | C1D-C2D | 7.27 | 1.47 | 1.39 |
| 29 | a | 608 | CHL | C1D-C2D | 7.26 | 1.47 | 1.39 |
| 29 | c | 609 | CHL | C1D-C2D | 7.26 | 1.47 | 1.39 |
| 29 | 1 | 307 | CHL | C1D-C2D | 7.26 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | C1D-C2D | 7.25 | 1.47 | 1.39 |
| 29 | 2 | 605 | CHL | C1D-C2D | 7.24 | 1.47 | 1.39 |
| 29 | 4 | 614 | CHL | C1D-C2D | 7.21 | 1.47 | 1.39 |
| 29 | 3 | 407 | CHL | C2A-C3A | -7.20 | 1.48 | 1.54 |
| 29 | 9 | 608 | CHL | C1D-C2D | 7.16 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | C1D-C2D | 7.14 | 1.47 | 1.39 |
| 29 | 2 | 601 | CHL | C1D-C2D | 7.11 | 1.47 | 1.39 |
| 29 | 2 | 602 | CHL | C1D-C2D | 7.10 | 1.47 | 1.39 |
| 29 | 3 | 407 | CHL | C1D-C2D | 7.07 | 1.47 | 1.39 |
| 29 | c | 601 | CHL | C1D-C2D | 7.07 | 1.47 | 1.39 |
| 29 | 2 | 607 | CHL | C1D-C2D | 7.06 | 1.47 | 1.39 |
| 29 | 2 | 606 | CHL | C1D-C2D | 6.95 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | C1D-C2D | 6.95 | 1.47 | 1.39 |
| 29 | 9 | 601 | CHL | C1D-C2D | 6.93 | 1.47 | 1.39 |
| 29 | 6 | 602 | CHL | C1D-C2D | 6.80 | 1.47 | 1.39 |
| 29 | 4 | 614 | CHL | C2A-C3A | -6.08 | 1.49 | 1.54 |
| 29 | a | 605 | CHL | C3B-C2B | 5.91 | 1.48 | 1.40 |
| 29 | 9 | 606 | CHL | C3A-C2A | -5.89 | 1.49 | 1.54 |
| 29 | c | 609 | CHL | C3B-C2B | 5.88 | 1.48 | 1.40 |
| 21 | A | 801 | CLA | C1D-ND | 5.85 | 1.45 | 1.37 |
| 29 | 6 | 614 | CHL | C3B-C2B | 5.85 | 1.48 | 1.40 |
| 29 | 8 | 605 | CHL | C3A-C2A | -5.84 | 1.49 | 1.54 |
| 29 | c | 605 | CHL | C3B-C2B | 5.83 | 1.48 | 1.40 |
| 29 | a | 609 | CHL | C3B-C2B | 5.82 | 1.48 | 1.40 |
| 29 | b | 307 | CHL | C3A-C2A | -5.81 | 1.49 | 1.54 |
| 29 | c | 607 | CHL | C3B-C2B | 5.81 | 1.48 | 1.40 |
| 29 | 4 | 605 | CHL | C3A-C2A | -5.80 | 1.49 | 1.54 |
| 29 | 7 | 406 | CHL | C3B-C2B | 5.80 | 1.48 | 1.40 |
| 29 | 8 | 606 | CHL | C3B-C2B | 5.78 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 4 | 607 | CHL | C3A-C2A | -5.77 | 1.49 | 1.54 |
| 29 | 6 | 607 | CHL | C3B-C2B | 5.76 | 1.48 | 1.40 |
| 29 | b | 309 | CHL | C3A-C2A | -5.75 | 1.49 | 1.54 |
| 29 | 2 | 605 | CHL | C3A-C2A | -5.75 | 1.49 | 1.54 |
| 29 | 2 | 614 | CHL | C3A-C2A | -5.75 | 1.49 | 1.54 |
| 29 | 4 | 606 | CHL | C3A-C2A | -5.75 | 1.49 | 1.54 |
| 29 | 5 | 606 | CHL | C3B-C2B | 5.75 | 1.48 | 1.40 |
| 29 | b | 302 | CHL | C3B-C2B | 5.74 | 1.48 | 1.40 |
| 29 | 8 | 613 | CHL | C3B-C2B | 5.73 | 1.48 | 1.40 |
| 29 | a | 608 | CHL | C3A-C2A | -5.73 | 1.49 | 1.54 |
| 29 | 6 | 605 | CHL | C3A-C2A | -5.71 | 1.49 | 1.54 |
| 29 | 2 | 607 | CHL | C3A-C2A | -5.70 | 1.49 | 1.54 |
| 29 | 2 | 602 | CHL | C3A-C2A | -5.70 | 1.49 | 1.54 |
| 29 | 9 | 608 | CHL | C3A-C2A | -5.69 | 1.49 | 1.54 |
| 29 | a | 601 | CHL | C3B-C2B | 5.68 | 1.48 | 1.40 |
| 29 | b | 306 | CHL | C3B-C2B | 5.66 | 1.48 | 1.40 |
| 29 | a | 607 | CHL | C3A-C2A | -5.65 | 1.49 | 1.54 |
| 29 | 6 | 601 | CHL | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 29 | c | 606 | CHL | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 29 | 9 | 605 | CHL | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 29 | b | 308 | CHL | C3A-C2A | -5.65 | 1.49 | 1.54 |
| 29 | 9 | 601 | CHL | C3B-C2B | 5.64 | 1.48 | 1.40 |
| 29 | c | 608 | CHL | C3B-C2B | 5.64 | 1.48 | 1.40 |
| 29 | 9 | 609 | CHL | C3A-C2A | -5.64 | 1.49 | 1.54 |
| 29 | 2 | 601 | CHL | C3A-C2A | -5.63 | 1.49 | 1.54 |
| 29 | 9 | 607 | CHL | C3A-C2A | -5.61 | 1.49 | 1.54 |
| 29 | a | 608 | CHL | C3B-C2B | 5.60 | 1.47 | 1.40 |
| 29 | 6 | 602 | CHL | C3A-C2A | -5.59 | 1.49 | 1.54 |
| 29 | 5 | 601 | CHL | C3A-C2A | -5.58 | 1.49 | 1.54 |
| 29 | 1 | 302 | CHL | C3B-C2B | 5.57 | 1.47 | 1.40 |
| 29 | b | 310 | CHL | C3A-C2A | -5.55 | 1.49 | 1.54 |
| 29 | 2 | 606 | CHL | C3A-C2A | -5.55 | 1.49 | 1.54 |
| 29 | 6 | 606 | CHL | C3B-C2B | 5.54 | 1.47 | 1.40 |
| 29 | 5 | 601 | CHL | C3B-C2B | 5.53 | 1.47 | 1.40 |
| 29 | 6 | 606 | CHL | C3A-C2A | -5.53 | 1.49 | 1.54 |
| 29 | 6 | 605 | CHL | C3B-C2B | 5.52 | 1.47 | 1.40 |
| 29 | 2 | 614 | CHL | C3B-C2B | 5.52 | 1.47 | 1.40 |
| 29 | 8 | 607 | CHL | C3B-C2B | 5.50 | 1.47 | 1.40 |
| 29 | 2 | 601 | CHL | C3B-C2B | 5.50 | 1.47 | 1.40 |
| 29 | 4 | 614 | CHL | C3B-C2B | 5.49 | 1.47 | 1.40 |
| 29 | 8 | 613 | CHL | C2A-C3A | -5.49 | 1.50 | 1.54 |
| 29 | a | 607 | CHL | C3B-C2B | 5.48 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 606 | CHL | C3B-C2B | 5.46 | 1.47 | 1.40 |
| 29 | 9 | 609 | CHL | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 29 | a | 606 | CHL | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 29 | 1 | 307 | CHL | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 29 | 6 | 601 | CHL | C2C-C3C | 5.43 | 1.47 | 1.37 |
| 29 | b | 308 | CHL | C3B-C2B | 5.43 | 1.47 | 1.40 |
| 29 | 1 | 307 | CHL | C3A-C2A | -5.42 | 1.50 | 1.54 |
| 29 | b | 310 | CHL | C3B-C2B | 5.42 | 1.47 | 1.40 |
| 29 | 9 | 608 | CHL | C3B-C2B | 5.40 | 1.47 | 1.40 |
| 29 | c | 601 | CHL | C3A-C2A | -5.39 | 1.50 | 1.54 |
| 29 | b | 306 | CHL | C3A-C2A | -5.38 | 1.50 | 1.54 |
| 29 | 2 | 602 | CHL | C3B-C2B | 5.37 | 1.47 | 1.40 |
| 29 | 4 | 606 | CHL | C3B-C2B | 5.34 | 1.47 | 1.40 |
| 29 | 2 | 605 | CHL | C3B-C2B | 5.34 | 1.47 | 1.40 |
| 29 | 8 | 607 | CHL | C3A-C2A | -5.33 | 1.50 | 1.54 |
| 29 | 9 | 606 | CHL | C3B-C2B | 5.32 | 1.47 | 1.40 |
| 29 | 9 | 605 | CHL | C3A-C2A | -5.31 | 1.50 | 1.54 |
| 29 | 6 | 602 | CHL | C3B-C2B | 5.31 | 1.47 | 1.40 |
| 29 | b | 309 | CHL | C3B-C2B | 5.30 | 1.47 | 1.40 |
| 21 | B | 801 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 29 | c | 609 | CHL | C3A-C2A | -5.29 | 1.50 | 1.54 |
| 29 | a | 609 | CHL | CHD-C1D | 5.28 | 1.48 | 1.39 |
| 29 | c | 608 | CHL | C3A-C2A | -5.27 | 1.50 | 1.54 |
| 29 | 3 | 407 | CHL | C3B-C2B | 5.25 | 1.47 | 1.40 |
| 29 | c | 606 | CHL | C3A-C2A | -5.24 | 1.50 | 1.54 |
| 29 | 1 | 302 | CHL | C3A-C2A | -5.23 | 1.50 | 1.54 |
| 29 | 9 | 601 | CHL | C3A-C2A | -5.23 | 1.50 | 1.54 |
| 29 | 9 | 607 | CHL | C3B-C2B | 5.22 | 1.47 | 1.40 |
| 29 | 2 | 607 | CHL | C3B-C2B | 5.21 | 1.47 | 1.40 |
| 21 | A | 801 | CLA | O2D-CGD | 5.21 | 1.46 | 1.33 |
| 29 | c | 601 | CHL | C3B-C2B | 5.19 | 1.47 | 1.40 |
| 29 | 4 | 607 | CHL | C3B-C2B | 5.19 | 1.47 | 1.40 |
| 29 | b | 307 | CHL | C3B-C2B | 5.18 | 1.47 | 1.40 |
| 29 | 6 | 614 | CHL | O2D-CGD | 5.17 | 1.45 | 1.33 |
| 29 | a | 609 | CHL | O2D-CGD | 5.15 | 1.45 | 1.33 |
| 29 | 7 | 406 | CHL | C2A-C3A | -5.15 | 1.50 | 1.54 |
| 29 | 9 | 605 | CHL | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 29 | c | 609 | CHL | C2C-C3C | 5.14 | 1.47 | 1.37 |
| 29 | c | 608 | CHL | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 29 | b | 306 | CHL | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 29 | 9 | 607 | CHL | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 29 | 8 | 605 | CHL | O2D-CGD | 5.13 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 5 | 606 | CHL | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 29 | 9 | 609 | CHL | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 29 | 9 | 607 | CHL | OBD-CAD | 5.13 | 1.29 | 1.22 |
| 29 | 6 | 606 | CHL | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 29 | 6 | 605 | CHL | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 29 | c | 607 | CHL | C3A-C2A | -5.11 | 1.50 | 1.54 |
| 29 | 8 | 606 | CHL | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 29 | 8 | 613 | CHL | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 29 | 8 | 607 | CHL | OBD-CAD | 5.11 | 1.29 | 1.22 |
| 29 | a | 601 | CHL | C3A-C2A | -5.10 | 1.50 | 1.54 |
| 29 | b | 302 | CHL | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 29 | c | 606 | CHL | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 29 | 6 | 601 | CHL | C3A-C2A | -5.09 | 1.50 | 1.54 |
| 29 | a | 605 | CHL | OBD-CAD | 5.09 | 1.29 | 1.22 |
| 29 | 9 | 601 | CHL | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 29 | 9 | 606 | CHL | OBD-CAD | 5.08 | 1.29 | 1.22 |
| 29 | c | 607 | CHL | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 29 | c | 601 | CHL | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 29 | a | 607 | CHL | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 29 | 9 | 606 | CHL | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 29 | 6 | 601 | CHL | OBD-CAD | 5.07 | 1.29 | 1.22 |
| 29 | 8 | 605 | CHL | OBD-CAD | 5.07 | 1.28 | 1.22 |
| 29 | a | 609 | CHL | CHC-C4B | 5.07 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 29 | 4 | 614 | CHL | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 29 | 7 | 406 | CHL | CHD-C1D | 5.07 | 1.47 | 1.39 |
| 21 | B | 801 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 29 | 6 | 605 | CHL | OBD-CAD | 5.06 | 1.28 | 1.22 |
| 29 | 6 | 602 | CHL | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 29 | c | 608 | CHL | OBD-CAD | 5.06 | 1.28 | 1.22 |
| 29 | c | 605 | CHL | OBD-CAD | 5.06 | 1.28 | 1.22 |
| 29 | 2 | 605 | CHL | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 29 | 8 | 606 | CHL | OBD-CAD | 5.05 | 1.28 | 1.22 |
| 29 | 4 | 606 | CHL | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 29 | 6 | 614 | CHL | OBD-CAD | 5.05 | 1.28 | 1.22 |
| 29 | 4 | 607 | CHL | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 29 | b | 307 | CHL | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | C3A-C2A | -5.04 | 1.50 | 1.54 |
| 29 | 5 | 601 | CHL | OBD-CAD | 5.03 | 1.28 | 1.22 |
| 29 | a | 601 | CHL | OBD-CAD | 5.03 | 1.28 | 1.22 |
| 29 | 6 | 606 | CHL | OBD-CAD | 5.03 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 4 | 605 | CHL | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 29 | 9 | 608 | CHL | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 29 | 5 | 606 | CHL | OBD-CAD | 5.02 | 1.28 | 1.22 |
| 21 | 8 | 609 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 29 | c | 609 | CHL | C3D-C2D | 5.02 | 1.48 | 1.39 |
| 29 | 2 | 606 | CHL | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 29 | b | 308 | CHL | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 29 | a | 601 | CHL | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 29 | 9 | 605 | CHL | OBD-CAD | 5.01 | 1.28 | 1.22 |
| 29 | 1 | 307 | CHL | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 29 | a | 608 | CHL | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | OBD-CAD | 5.01 | 1.28 | 1.22 |
| 29 | 7 | 406 | CHL | OBD-CAD | 5.01 | 1.28 | 1.22 |
| 29 | b | 309 | CHL | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 29 | a | 601 | CHL | CHD-C1D | 5.01 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | OBD-CAD | 5.01 | 1.28 | 1.22 |
| 29 | c | 607 | CHL | OBD-CAD | 5.00 | 1.28 | 1.22 |
| 29 | c | 605 | CHL | CHD-C1D | 5.00 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | OBD-CAD | 5.00 | 1.28 | 1.22 |
| 29 | 7 | 406 | CHL | CHC-C4B | 5.00 | 1.47 | 1.39 |
| 29 | 8 | 613 | CHL | C3D-C2D | 5.00 | 1.48 | 1.39 |
| 29 | 8 | 613 | CHL | OBD-CAD | 4.99 | 1.28 | 1.22 |
| 29 | 9 | 601 | CHL | OBD-CAD | 4.99 | 1.28 | 1.22 |
| 29 | 2 | 602 | CHL | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 29 | 2 | 607 | CHL | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 29 | a | 607 | CHL | OBD-CAD | 4.99 | 1.28 | 1.22 |
| 29 | a | 609 | CHL | OBD-CAD | 4.98 | 1.28 | 1.22 |
| 29 | a | 606 | CHL | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 29 | 1 | 307 | CHL | OBD-CAD | 4.98 | 1.28 | 1.22 |
| 29 | c | 607 | CHL | C3D-C2D | 4.98 | 1.48 | 1.39 |
| 29 | b | 306 | CHL | OBD-CAD | 4.97 | 1.28 | 1.22 |
| 29 | c | 606 | CHL | OBD-CAD | 4.97 | 1.28 | 1.22 |
| 29 | 8 | 605 | CHL | C2C-C3C | 4.97 | 1.47 | 1.37 |
| 29 | a | 605 | CHL | CHD-C1D | 4.96 | 1.47 | 1.39 |
| 29 | 4 | 614 | CHL | OBD-CAD | 4.96 | 1.28 | 1.22 |
| 29 | a | 609 | CHL | C3D-C2D | 4.96 | 1.48 | 1.39 |
| 29 | c | 601 | CHL | OBD-CAD | 4.96 | 1.28 | 1.22 |
| 29 | 8 | 607 | CHL | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 29 | 4 | 605 | CHL | C2C-C3C | 4.95 | 1.47 | 1.37 |
| 29 | c | 609 | CHL | CHC-C4B | 4.95 | 1.47 | 1.39 |
| 29 | 5 | 606 | CHL | C3A-C2A | -4.95 | 1.50 | 1.54 |
| 29 | 6 | 602 | CHL | OBD-CAD | 4.95 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 309 | CHL | OBD-CAD | 4.95 | 1.28 | 1.22 |
| 29 | 2 | 601 | CHL | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 29 | 7 | 406 | CHL | C3D-C2D | 4.94 | 1.48 | 1.39 |
| 29 | 2 | 602 | CHL | OBD-CAD | 4.94 | 1.28 | 1.22 |
| 21 | 3 | 409 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 29 | 5 | 601 | CHL | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 29 | b | 302 | CHL | C3D-C2D | 4.94 | 1.48 | 1.39 |
| 29 | 8 | 606 | CHL | CHD-C1D | 4.93 | 1.47 | 1.39 |
| 29 | 6 | 614 | CHL | C3D-C2D | 4.93 | 1.48 | 1.39 |
| 29 | 4 | 605 | CHL | OBD-CAD | 4.93 | 1.28 | 1.22 |
| 29 | 6 | 614 | CHL | C3A-C2A | -4.93 | 1.50 | 1.54 |
| 29 | c | 605 | CHL | C3D-C2D | 4.93 | 1.48 | 1.39 |
| 21 | B | 801 | CLA | CHC-C1C | 4.92 | 1.48 | 1.38 |
| 29 | 2 | 605 | CHL | OBD-CAD | 4.92 | 1.28 | 1.22 |
| 29 | 9 | 609 | CHL | OBD-CAD | 4.92 | 1.28 | 1.22 |
| 29 | c | 607 | CHL | CHD-C1D | 4.92 | 1.47 | 1.39 |
| 29 | a | 605 | CHL | C3D-C2D | 4.92 | 1.48 | 1.39 |
| 29 | 1 | 302 | CHL | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 29 | b | 306 | CHL | C3D-C2D | 4.91 | 1.48 | 1.39 |
| 29 | c | 609 | CHL | CHD-C1D | 4.91 | 1.47 | 1.39 |
| 29 | c | 605 | CHL | CHC-C4B | 4.91 | 1.47 | 1.39 |
| 29 | 1 | 302 | CHL | OBD-CAD | 4.91 | 1.28 | 1.22 |
| 29 | 8 | 606 | CHL | C3D-C2D | 4.91 | 1.48 | 1.39 |
| 29 | 6 | 614 | CHL | CHC-C4B | 4.91 | 1.47 | 1.39 |
| 29 | 9 | 608 | CHL | OBD-CAD | 4.91 | 1.28 | 1.22 |
| 29 | 6 | 601 | CHL | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 21 | 1 | 309 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 29 | a | 601 | CHL | C3D-C2D | 4.90 | 1.48 | 1.39 |
| 29 | 2 | 614 | CHL | C3D-C2D | 4.90 | 1.48 | 1.39 |
| 29 | 6 | 614 | CHL | CHD-C1D | 4.90 | 1.47 | 1.39 |
| 29 | b | 302 | CHL | OBD-CAD | 4.89 | 1.28 | 1.22 |
| 29 | 6 | 607 | CHL | CHC-C4B | 4.89 | 1.47 | 1.39 |
| 21 | 4 | 609 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 29 | b | 302 | CHL | CHD-C1D | 4.88 | 1.47 | 1.39 |
| 29 | 2 | 601 | CHL | OBD-CAD | 4.88 | 1.28 | 1.22 |
| 21 | 2 | 609 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 29 | 9 | 601 | CHL | C3D-C2D | 4.87 | 1.48 | 1.39 |
| 29 | a | 608 | CHL | OBD-CAD | 4.87 | 1.28 | 1.22 |
| 29 | 2 | 602 | CHL | C3D-C2D | 4.87 | 1.47 | 1.39 |
| 29 | a | 605 | CHL | C3A-C2A | -4.86 | 1.50 | 1.54 |
| 29 | 9 | 607 | CHL | C3D-C2D | 4.86 | 1.47 | 1.39 |
| 29 | 8 | 613 | CHL | CHC-C4B | 4.85 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 308 | CHL | OBD-CAD | 4.85 | 1.28 | 1.22 |
| 29 | a | 606 | CHL | OBD-CAD | 4.85 | 1.28 | 1.22 |
| 29 | b | 310 | CHL | C3D-C2D | 4.85 | 1.47 | 1.39 |
| 29 | 6 | 602 | CHL | C3D-C2D | 4.85 | 1.47 | 1.39 |
| 29 | a | 607 | CHL | C3D-C2D | 4.84 | 1.47 | 1.39 |
| 29 | c | 606 | CHL | CHC-C4B | 4.84 | 1.47 | 1.39 |
| 29 | 6 | 607 | CHL | CHD-C1D | 4.84 | 1.47 | 1.39 |
| 29 | 6 | 601 | CHL | CHC-C4B | 4.84 | 1.47 | 1.39 |
| 29 | 8 | 606 | CHL | CHC-C4B | 4.83 | 1.47 | 1.39 |
| 29 | c | 607 | CHL | CHC-C4B | 4.82 | 1.47 | 1.39 |
| 29 | c | 608 | CHL | C3D-C2D | 4.82 | 1.47 | 1.39 |
| 29 | 6 | 605 | CHL | CHD-C1D | 4.82 | 1.47 | 1.39 |
| 29 | 9 | 605 | CHL | C3D-C2D | 4.81 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | OBD-CAD | 4.81 | 1.28 | 1.22 |
| 29 | c | 609 | CHL | O2D-CGD | 4.80 | 1.46 | 1.30 |
| 29 | 8 | 606 | CHL | C3A-C2A | -4.80 | 1.50 | 1.54 |
| 29 | 6 | 606 | CHL | C3D-C2D | 4.80 | 1.47 | 1.39 |
| 29 | 6 | 607 | CHL | C3D-C2D | 4.80 | 1.47 | 1.39 |
| 29 | c | 609 | CHL | OBD-CAD | 4.80 | 1.28 | 1.22 |
| 29 | a | 605 | CHL | CHC-C4B | 4.80 | 1.47 | 1.39 |
| 29 | 9 | 607 | CHL | CHD-C1D | 4.80 | 1.47 | 1.39 |
| 21 | A | 801 | CLA | MG-ND | -4.80 | 1.96 | 2.05 |
| 29 | c | 608 | CHL | CHD-C1D | 4.79 | 1.47 | 1.39 |
| 29 | c | 606 | CHL | C3D-C2D | 4.79 | 1.47 | 1.39 |
| 29 | 5 | 606 | CHL | C3D-C2D | 4.79 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | OBD-CAD | 4.79 | 1.28 | 1.22 |
| 29 | 6 | 605 | CHL | C3D-C2D | 4.79 | 1.47 | 1.39 |
| 29 | b | 310 | CHL | OBD-CAD | 4.79 | 1.28 | 1.22 |
| 29 | 1 | 302 | CHL | C3D-C2D | 4.78 | 1.47 | 1.39 |
| 29 | 6 | 601 | CHL | CHD-C1D | 4.78 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | CHC-C4B | 4.78 | 1.47 | 1.39 |
| 29 | 6 | 601 | CHL | C3D-C2D | 4.78 | 1.47 | 1.39 |
| 29 | a | 606 | CHL | CHC-C4B | 4.78 | 1.47 | 1.39 |
| 29 | 2 | 607 | CHL | OBD-CAD | 4.78 | 1.28 | 1.22 |
| 29 | 9 | 606 | CHL | C3D-C2D | 4.77 | 1.47 | 1.39 |
| 29 | a | 609 | CHL | C3A-C2A | -4.77 | 1.50 | 1.54 |
| 29 | a | 605 | CHL | O2D-CGD | 4.77 | 1.45 | 1.30 |
| 29 | 6 | 602 | CHL | CHC-C4B | 4.77 | 1.47 | 1.39 |
| 21 | 7 | 407 | CLA | O2D-CGD | 4.77 | 1.45 | 1.30 |
| 29 | 7 | 406 | CHL | O2D-CGD | 4.77 | 1.45 | 1.30 |
| 29 | 6 | 605 | CHL | CHC-C4B | 4.76 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | C3D-C2D | 4.75 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 310 | CHL | CHD-C1D | 4.75 | 1.47 | 1.39 |
| 29 | b | 302 | CHL | C3A-C2A | -4.75 | 1.50 | 1.54 |
| 29 | 9 | 601 | CHL | CHC-C4B | 4.75 | 1.47 | 1.39 |
| 29 | b | 308 | CHL | C3D-C2D | 4.75 | 1.47 | 1.39 |
| 29 | 5 | 601 | CHL | C3D-C2D | 4.75 | 1.47 | 1.39 |
| 29 | 9 | 605 | CHL | CHD-C1D | 4.74 | 1.47 | 1.39 |
| 29 | 8 | 607 | CHL | C3D-C2D | 4.74 | 1.47 | 1.39 |
| 29 | 9 | 608 | CHL | C3D-C2D | 4.74 | 1.47 | 1.39 |
| 29 | 5 | 606 | CHL | CHC-C4B | 4.74 | 1.47 | 1.39 |
| 29 | 8 | 605 | CHL | C3D-C2D | 4.74 | 1.47 | 1.39 |
| 29 | 3 | 407 | CHL | O2D-CGD | 4.73 | 1.45 | 1.30 |
| 29 | 2 | 602 | CHL | CHC-C4B | 4.73 | 1.47 | 1.39 |
| 29 | b | 302 | CHL | CHC-C4B | 4.73 | 1.47 | 1.39 |
| 29 | 9 | 605 | CHL | CHC-C4B | 4.73 | 1.47 | 1.39 |
| 29 | 8 | 607 | CHL | CHD-C1D | 4.73 | 1.47 | 1.39 |
| 29 | 2 | 605 | CHL | CHC-C4B | 4.73 | 1.47 | 1.39 |
| 29 | a | 609 | CHL | CHB-C1B | 4.73 | 1.47 | 1.39 |
| 29 | a | 607 | CHL | CHD-C1D | 4.72 | 1.47 | 1.39 |
| 29 | 2 | 605 | CHL | C3D-C2D | 4.72 | 1.47 | 1.39 |
| 29 | 3 | 407 | CHL | C3D-C2D | 4.72 | 1.47 | 1.39 |
| 29 | 4 | 605 | CHL | C3D-C2D | 4.72 | 1.47 | 1.39 |
| 29 | c | 601 | CHL | C3D-C2D | 4.72 | 1.47 | 1.39 |
| 29 | b | 310 | CHL | O2D-CGD | 4.71 | 1.45 | 1.30 |
| 29 | 2 | 601 | CHL | C3D-C2D | 4.71 | 1.47 | 1.39 |
| 29 | a | 606 | CHL | CHD-C1D | 4.71 | 1.47 | 1.39 |
| 29 | 7 | 406 | CHL | CHB-C1B | 4.71 | 1.47 | 1.39 |
| 29 | c | 609 | CHL | CHB-C1B | 4.71 | 1.47 | 1.39 |
| 29 | c | 606 | CHL | CHD-C1D | 4.71 | 1.47 | 1.39 |
| 29 | 6 | 606 | CHL | CHC-C4B | 4.70 | 1.47 | 1.39 |
| 29 | 4 | 614 | CHL | C3D-C2D | 4.70 | 1.47 | 1.39 |
| 29 | 2 | 607 | CHL | CHC-C4B | 4.70 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | CHC-C4B | 4.70 | 1.47 | 1.39 |
| 29 | 2 | 606 | CHL | OBD-CAD | 4.69 | 1.28 | 1.22 |
| 29 | 8 | 613 | CHL | CHD-C1D | 4.69 | 1.47 | 1.39 |
| 29 | b | 306 | CHL | CHD-C1D | 4.69 | 1.47 | 1.39 |
| 21 | B | 801 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 29 | 5 | 606 | CHL | CHD-C1D | 4.68 | 1.47 | 1.39 |
| 29 | a | 601 | CHL | CHC-C4B | 4.68 | 1.47 | 1.39 |
| 29 | b | 308 | CHL | CHD-C1D | 4.68 | 1.47 | 1.39 |
| 29 | 2 | 605 | CHL | CHD-C1D | 4.67 | 1.47 | 1.39 |
| 29 | 9 | 609 | CHL | C3D-C2D | 4.67 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | C3D-C2D | 4.67 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | b | 306 | CHL | CHC-C4B | 4.66 | 1.47 | 1.39 |
| 29 | 9 | 609 | CHL | CHD-C1D | 4.66 | 1.47 | 1.39 |
| 29 | a | 608 | CHL | C3D-C2D | 4.65 | 1.47 | 1.39 |
| 29 | 1 | 307 | CHL | CHC-C4B | 4.65 | 1.47 | 1.39 |
| 29 | c | 605 | CHL | C3A-C2A | -4.64 | 1.50 | 1.54 |
| 29 | a | 607 | CHL | CHC-C4B | 4.63 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | CHD-C1D | 4.63 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | CHC-C4B | 4.63 | 1.47 | 1.39 |
| 29 | 9 | 606 | CHL | CHC-C4B | 4.63 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | C3D-C2D | 4.63 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | CHB-C4A | -4.63 | 1.33 | 1.38 |
| 29 | c | 608 | CHL | CHC-C4B | 4.62 | 1.47 | 1.39 |
| 29 | 2 | 606 | CHL | C3D-C2D | 4.62 | 1.47 | 1.39 |
| 29 | a | 609 | CHL | CHC-C1C | 4.62 | 1.48 | 1.39 |
| 29 | 9 | 606 | CHL | CHD-C1D | 4.62 | 1.47 | 1.39 |
| 29 | 8 | 605 | CHL | CHD-C1D | 4.62 | 1.47 | 1.39 |
| 29 | 2 | 607 | CHL | C3D-C2D | 4.62 | 1.47 | 1.39 |
| 21 | A | 830 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |
| 29 | b | 306 | CHL | O2A-CGA | 4.62 | 1.46 | 1.30 |
| 29 | a | 608 | CHL | CHC-C4B | 4.61 | 1.47 | 1.39 |
| 29 | a | 606 | CHL | O2A-CGA | 4.61 | 1.46 | 1.30 |
| 29 | 4 | 605 | CHL | CHC-C4B | 4.61 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | CHB-C4A | -4.61 | 1.33 | 1.38 |
| 29 | c | 607 | CHL | CHB-C1B | 4.60 | 1.47 | 1.39 |
| 29 | 1 | 307 | CHL | C3D-C2D | 4.60 | 1.47 | 1.39 |
| 29 | b | 302 | CHL | CHB-C1B | 4.60 | 1.47 | 1.39 |
| 29 | b | 308 | CHL | CHB-C4A | -4.60 | 1.33 | 1.38 |
| 29 | a | 608 | CHL | CHD-C1D | 4.60 | 1.47 | 1.39 |
| 29 | 5 | 601 | CHL | CHD-C1D | 4.59 | 1.47 | 1.39 |
| 29 | a | 605 | CHL | CHB-C1B | 4.59 | 1.47 | 1.39 |
| 29 | 6 | 606 | CHL | CHD-C1D | 4.59 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | CHC-C4B | 4.59 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | CHD-C1D | 4.58 | 1.47 | 1.39 |
| 29 | a | 609 | CHL | CHD-C4C | 4.58 | 1.48 | 1.39 |
| 29 | c | 605 | CHL | CHB-C1B | 4.58 | 1.47 | 1.39 |
| 29 | a | 605 | CHL | O2A-CGA | 4.58 | 1.45 | 1.30 |
| 29 | 9 | 608 | CHL | CHD-C1D | 4.57 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | CHC-C4B | 4.57 | 1.47 | 1.39 |
| 29 | 7 | 406 | CHL | CHD-C4C | 4.57 | 1.48 | 1.39 |
| 29 | 6 | 601 | CHL | CHB-C1B | 4.57 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | C3D-C2D | 4.57 | 1.47 | 1.39 |
| 29 | 2 | 607 | CHL | CHB-C4A | -4.56 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 8 | 607 | CHL | CHC-C4B | 4.56 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 29 | 5 | 601 | CHL | CHC-C4B | 4.56 | 1.47 | 1.39 |
| 29 | 1 | 307 | CHL | CHD-C1D | 4.56 | 1.47 | 1.39 |
| 29 | 6 | 607 | CHL | CHB-C1B | 4.56 | 1.47 | 1.39 |
| 29 | 6 | 614 | CHL | CHB-C1B | 4.56 | 1.47 | 1.39 |
| 29 | c | 605 | CHL | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 29 | 1 | 302 | CHL | CHC-C4B | 4.56 | 1.47 | 1.39 |
| 29 | 6 | 606 | CHL | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 29 | b | 307 | CHL | CHB-C4A | -4.56 | 1.33 | 1.38 |
| 29 | 5 | 601 | CHL | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 29 | 9 | 608 | CHL | CHC-C4B | 4.56 | 1.47 | 1.39 |
| 29 | 6 | 602 | CHL | CHB-C4A | -4.56 | 1.33 | 1.38 |
| 29 | 9 | 605 | CHL | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 29 | 8 | 606 | CHL | CHB-C1B | 4.55 | 1.47 | 1.39 |
| 29 | a | 608 | CHL | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 29 | 2 | 606 | CHL | CHC-C4B | 4.55 | 1.47 | 1.39 |
| 29 | 9 | 601 | CHL | CHD-C1D | 4.55 | 1.47 | 1.39 |
| 29 | 9 | 608 | CHL | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 29 | 9 | 609 | CHL | CHC-C4B | 4.55 | 1.47 | 1.39 |
| 29 | 8 | 606 | CHL | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 29 | 4 | 614 | CHL | CHC-C4B | 4.55 | 1.47 | 1.39 |
| 29 | 6 | 614 | CHL | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 29 | 4 | 614 | CHL | CHD-C1D | 4.55 | 1.47 | 1.39 |
| 29 | c | 607 | CHL | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 29 | 9 | 609 | CHL | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 29 | 8 | 605 | CHL | CHB-C1B | 4.54 | 1.47 | 1.39 |
| 29 | 8 | 605 | CHL | CHC-C4B | 4.54 | 1.47 | 1.39 |
| 29 | 5 | 606 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | 6 | 601 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | b | 307 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | b | 307 | CHL | CHD-C1D | 4.54 | 1.47 | 1.39 |
| 29 | a | 601 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | 6 | 605 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | c | 609 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 21 | 8 | 609 | CLA | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | 1 | 302 | CHL | CHD-C1D | 4.54 | 1.47 | 1.39 |
| 29 | c | 606 | CHL | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 29 | 9 | 607 | CHL | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 29 | a | 609 | CHL | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 29 | a | 601 | CHL | CHB-C1B | 4.53 | 1.47 | 1.39 |
| 29 | b | 310 | CHL | CHC-C4B | 4.53 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 614 | CHL | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 29 | c | 608 | CHL | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 29 | b | 308 | CHL | CHC-C4B | 4.53 | 1.47 | 1.39 |
| 29 | 2 | 606 | CHL | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 29 | c | 605 | CHL | CHD-C4C | 4.53 | 1.48 | 1.39 |
| 29 | a | 606 | CHL | C3D-C2D | 4.53 | 1.47 | 1.39 |
| 29 | 6 | 614 | CHL | CHD-C4C | 4.52 | 1.48 | 1.39 |
| 29 | 2 | 605 | CHL | O2A-CGA | 4.52 | 1.45 | 1.30 |
| 29 | 9 | 606 | CHL | O2A-CGA | 4.52 | 1.45 | 1.30 |
| 21 | 7 | 407 | CLA | O2A-CGA | 4.52 | 1.45 | 1.30 |
| 29 | 4 | 605 | CHL | CHD-C1D | 4.52 | 1.46 | 1.39 |
| 29 | 7 | 406 | CHL | CHC-C1C | 4.52 | 1.48 | 1.39 |
| 29 | 2 | 607 | CHL | CHD-C1D | 4.51 | 1.46 | 1.39 |
| 29 | 9 | 601 | CHL | CHB-C1B | 4.51 | 1.46 | 1.39 |
| 29 | c | 601 | CHL | CHD-C1D | 4.51 | 1.46 | 1.39 |
| 29 | a | 601 | CHL | CHD-C4C | 4.51 | 1.48 | 1.39 |
| 29 | b | 310 | CHL | CHB-C4A | -4.50 | 1.33 | 1.38 |
| 29 | a | 606 | CHL | CHB-C4A | -4.50 | 1.33 | 1.38 |
| 29 | 3 | 407 | CHL | CHB-C4A | -4.50 | 1.33 | 1.38 |
| 29 | 2 | 602 | CHL | CHB-C4A | -4.49 | 1.33 | 1.38 |
| 29 | 2 | 605 | CHL | CHB-C4A | -4.49 | 1.33 | 1.38 |
| 29 | 9 | 609 | CHL | CHB-C4A | -4.49 | 1.33 | 1.38 |
| 29 | 2 | 602 | CHL | CHD-C1D | 4.49 | 1.46 | 1.39 |
| 29 | 4 | 606 | CHL | CHB-C4A | -4.49 | 1.33 | 1.38 |
| 29 | 8 | 613 | CHL | CHB-C1B | 4.49 | 1.46 | 1.39 |
| 29 | 6 | 606 | CHL | CHB-C4A | -4.49 | 1.33 | 1.38 |
| 29 | a | 606 | CHL | CHD-C4C | 4.48 | 1.48 | 1.39 |
| 29 | 5 | 606 | CHL | CHB-C1B | 4.48 | 1.46 | 1.39 |
| 29 | b | 302 | CHL | O2A-CGA | 4.48 | 1.45 | 1.30 |
| 29 | 6 | 607 | CHL | CHD-C4C | 4.48 | 1.48 | 1.39 |
| 29 | 2 | 601 | CHL | CHC-C4B | 4.47 | 1.46 | 1.39 |
| 29 | 3 | 407 | CHL | CHD-C1D | 4.46 | 1.46 | 1.39 |
| 29 | 8 | 606 | CHL | CHD-C4C | 4.46 | 1.47 | 1.39 |
| 29 | b | 306 | CHL | CHB-C1B | 4.46 | 1.46 | 1.39 |
| 29 | 1 | 307 | CHL | CHB-C4A | -4.46 | 1.33 | 1.38 |
| 29 | 6 | 605 | CHL | CHB-C4A | -4.46 | 1.33 | 1.38 |
| 29 | c | 601 | CHL | CHB-C4A | -4.46 | 1.33 | 1.38 |
| 29 | b | 310 | CHL | CHD-C4C | 4.45 | 1.47 | 1.39 |
| 29 | b | 302 | CHL | CHD-C4C | 4.45 | 1.47 | 1.39 |
| 29 | 8 | 606 | CHL | CHC-C1C | 4.45 | 1.47 | 1.39 |
| 29 | 5 | 606 | CHL | CHD-C4C | 4.44 | 1.47 | 1.39 |
| 29 | a | 605 | CHL | CHD-C4C | 4.44 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | c | 607 | CHL | CHD-C4C | 4.44 | 1.47 | 1.39 |
| 29 | 9 | 605 | CHL | CHB-C1B | 4.43 | 1.46 | 1.39 |
| 29 | 6 | 614 | CHL | CHC-C1C | 4.43 | 1.47 | 1.39 |
| 29 | c | 605 | CHL | CHC-C1C | 4.42 | 1.47 | 1.39 |
| 29 | 2 | 606 | CHL | CHB-C4A | -4.42 | 1.33 | 1.38 |
| 29 | 2 | 601 | CHL | CHD-C1D | 4.42 | 1.46 | 1.39 |
| 29 | 4 | 605 | CHL | CHB-C4A | -4.41 | 1.33 | 1.38 |
| 29 | b | 309 | CHL | CHD-C1D | 4.41 | 1.46 | 1.39 |
| 21 | 8 | 608 | CLA | O1D-CGD | 4.41 | 1.36 | 1.20 |
| 29 | 9 | 608 | CHL | CHB-C4A | -4.41 | 1.33 | 1.38 |
| 29 | 9 | 607 | CHL | CHD-C4C | 4.40 | 1.47 | 1.39 |
| 29 | a | 608 | CHL | CHB-C1B | 4.40 | 1.46 | 1.39 |
| 29 | a | 607 | CHL | CHB-C4A | -4.40 | 1.33 | 1.38 |
| 29 | 9 | 606 | CHL | CHB-C1B | 4.40 | 1.46 | 1.39 |
| 29 | c | 608 | CHL | CHD-C4C | 4.40 | 1.47 | 1.39 |
| 29 | 4 | 614 | CHL | CHB-C4A | -4.40 | 1.33 | 1.38 |
| 29 | c | 606 | CHL | CHD-C4C | 4.40 | 1.47 | 1.39 |
| 29 | 3 | 407 | CHL | CHC-C4B | 4.39 | 1.46 | 1.39 |
| 29 | c | 608 | CHL | CHB-C4A | -4.39 | 1.33 | 1.38 |
| 29 | c | 609 | CHL | CHC-C1C | 4.39 | 1.47 | 1.39 |
| 29 | c | 601 | CHL | CHC-C4B | 4.39 | 1.46 | 1.39 |
| 29 | 9 | 607 | CHL | CHB-C1B | 4.39 | 1.46 | 1.39 |
| 29 | 8 | 613 | CHL | CHD-C4C | 4.39 | 1.47 | 1.39 |
| 29 | 1 | 302 | CHL | CHB-C1B | 4.38 | 1.46 | 1.39 |
| 29 | c | 606 | CHL | CHB-C1B | 4.38 | 1.46 | 1.39 |
| 29 | 9 | 605 | CHL | CHD-C4C | 4.38 | 1.47 | 1.39 |
| 29 | 5 | 601 | CHL | CHB-C4A | -4.38 | 1.33 | 1.38 |
| 21 | 4 | 608 | CLA | O1D-CGD | 4.38 | 1.36 | 1.20 |
| 29 | 2 | 601 | CHL | CHB-C1B | 4.37 | 1.46 | 1.39 |
| 29 | 6 | 602 | CHL | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 29 | 5 | 606 | CHL | CHC-C1C | 4.36 | 1.47 | 1.39 |
| 29 | 8 | 613 | CHL | CHC-C1C | 4.36 | 1.47 | 1.39 |
| 29 | 6 | 601 | CHL | CHD-C4C | 4.36 | 1.47 | 1.39 |
| 29 | c | 607 | CHL | CHC-C1C | 4.36 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | CHB-C4A | -4.35 | 1.33 | 1.38 |
| 29 | 6 | 605 | CHL | CHD-C4C | 4.35 | 1.47 | 1.39 |
| 29 | 6 | 601 | CHL | CHC-C1C | 4.35 | 1.47 | 1.39 |
| 29 | 9 | 601 | CHL | CHB-C4A | -4.35 | 1.33 | 1.38 |
| 29 | b | 308 | CHL | CHD-C4C | 4.34 | 1.47 | 1.39 |
| 29 | 6 | 602 | CHL | CHD-C1D | 4.34 | 1.46 | 1.39 |
| 29 | 9 | 601 | CHL | CHD-C4C | 4.34 | 1.47 | 1.39 |
| 29 | c | 601 | CHL | O2A-CGA | 4.34 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 9 | 607 | CHL | CHB-C4A | -4.34 | 1.33 | 1.38 |
| 29 | 8 | 607 | CHL | CHB-C1B | 4.33 | 1.46 | 1.39 |
| 29 | 6 | 605 | CHL | CHB-C1B | 4.33 | 1.46 | 1.39 |
| 29 | 2 | 601 | CHL | CHB-C4A | -4.33 | 1.33 | 1.38 |
| 29 | a | 605 | CHL | CHC-C1C | 4.33 | 1.47 | 1.39 |
| 29 | a | 607 | CHL | CHD-C4C | 4.33 | 1.47 | 1.39 |
| 29 | 2 | 614 | CHL | CHB-C1B | 4.32 | 1.46 | 1.39 |
| 29 | 8 | 607 | CHL | CHD-C4C | 4.32 | 1.47 | 1.39 |
| 29 | 1 | 302 | CHL | CHD-C4C | 4.32 | 1.47 | 1.39 |
| 29 | 9 | 605 | CHL | CHB-C4A | -4.32 | 1.33 | 1.38 |
| 29 | 2 | 605 | CHL | CHD-C4C | 4.32 | 1.47 | 1.39 |
| 29 | 2 | 602 | CHL | CHB-C1B | 4.31 | 1.46 | 1.39 |
| 29 | a | 606 | CHL | CHC-C1C | 4.31 | 1.47 | 1.39 |
| 29 | a | 608 | CHL | CHB-C4A | -4.31 | 1.33 | 1.38 |
| 29 | 1 | 302 | CHL | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 29 | 8 | 607 | CHL | CHB-C4A | -4.31 | 1.33 | 1.38 |
| 29 | 8 | 607 | CHL | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 29 | b | 310 | CHL | CHB-C1B | 4.30 | 1.46 | 1.39 |
| 29 | a | 605 | CHL | CHB-C4A | -4.30 | 1.33 | 1.38 |
| 29 | 4 | 614 | CHL | CHB-C1B | 4.30 | 1.46 | 1.39 |
| 29 | 6 | 606 | CHL | CHD-C4C | 4.30 | 1.47 | 1.39 |
| 29 | b | 308 | CHL | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 29 | 9 | 607 | CHL | CHC-C4B | 4.29 | 1.46 | 1.39 |
| 29 | c | 609 | CHL | CHD-C4C | 4.29 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 29 | b | 310 | CHL | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 29 | 6 | 602 | CHL | CHC-C1C | 4.29 | 1.47 | 1.39 |
| 29 | 8 | 605 | CHL | CHD-C4C | 4.29 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | CHC-C1C | 4.29 | 1.47 | 1.39 |
| 29 | 6 | 607 | CHL | CHC-C1C | 4.29 | 1.47 | 1.39 |
| 29 | 1 | 307 | CHL | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 29 | c | 606 | CHL | CHC-C1C | 4.28 | 1.47 | 1.39 |
| 29 | 1 | 302 | CHL | CHB-C4A | -4.28 | 1.33 | 1.38 |
| 29 | 6 | 601 | CHL | CHB-C4A | -4.28 | 1.33 | 1.38 |
| 29 | 3 | 407 | CHL | CHD-C4C | 4.28 | 1.47 | 1.39 |
| 29 | a | 601 | CHL | CHC-C1C | 4.28 | 1.47 | 1.39 |
| 29 | 5 | 601 | CHL | CHB-C1B | 4.28 | 1.46 | 1.39 |
| 29 | 1 | 307 | CHL | CHD-C4C | 4.28 | 1.47 | 1.39 |
| 29 | 2 | 601 | CHL | CHD-C4C | 4.27 | 1.47 | 1.39 |
| 29 | 2 | 602 | CHL | CHD-C4C | 4.27 | 1.47 | 1.39 |
| 29 | 2 | 602 | CHL | CHC-C1C | 4.27 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 9 | 609 | CHL | CHD-C4C | 4.27 | 1.47 | 1.39 |
| 29 | b | 306 | CHL | CHC-C1C | 4.27 | 1.47 | 1.39 |
| 21 | B | 801 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 29 | 4 | 614 | CHL | CHD-C4C | 4.27 | 1.47 | 1.39 |
| 29 | 2 | 607 | CHL | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 29 | 9 | 606 | CHL | CHD-C4C | 4.26 | 1.47 | 1.39 |
| 29 | b | 306 | CHL | CHD-C4C | 4.26 | 1.47 | 1.39 |
| 29 | 2 | 601 | CHL | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 29 | 4 | 606 | CHL | CHD-C4C | 4.26 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | CHD-C1D | 4.26 | 1.46 | 1.39 |
| 29 | 9 | 605 | CHL | CHC-C1C | 4.25 | 1.47 | 1.39 |
| 29 | 4 | 605 | CHL | CHB-C1B | 4.25 | 1.46 | 1.39 |
| 29 | 5 | 601 | CHL | CHD-C4C | 4.25 | 1.47 | 1.39 |
| 29 | a | 607 | CHL | CHB-C1B | 4.25 | 1.46 | 1.39 |
| 29 | 2 | 606 | CHL | CHB-C1B | 4.25 | 1.46 | 1.39 |
| 29 | 2 | 607 | CHL | CHC-C1C | 4.25 | 1.47 | 1.39 |
| 29 | 5 | 606 | CHL | CHB-C4A | -4.24 | 1.33 | 1.38 |
| 29 | c | 608 | CHL | CHC-C1C | 4.24 | 1.47 | 1.39 |
| 29 | 4 | 605 | CHL | CHD-C4C | 4.24 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | CHD-C4C | 4.24 | 1.47 | 1.39 |
| 29 | b | 306 | CHL | CHB-C4A | -4.24 | 1.33 | 1.38 |
| 29 | b | 302 | CHL | CHC-C1C | 4.24 | 1.47 | 1.39 |
| 29 | 2 | 606 | CHL | CHD-C1D | 4.24 | 1.46 | 1.39 |
| 29 | 2 | 614 | CHL | CHD-C4C | 4.23 | 1.47 | 1.39 |
| 29 | 6 | 605 | CHL | CHC-C1C | 4.23 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | CHD-C4C | 4.23 | 1.47 | 1.39 |
| 29 | 6 | 606 | CHL | CHC-C1C | 4.23 | 1.47 | 1.39 |
| 29 | 9 | 608 | CHL | CHD-C4C | 4.23 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 29 | 9 | 606 | CHL | CHB-C4A | -4.23 | 1.33 | 1.38 |
| 29 | 2 | 605 | CHL | CHC-C1C | 4.23 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | CHB-C1B | 4.23 | 1.46 | 1.39 |
| 29 | a | 608 | CHL | CHD-C4C | 4.22 | 1.47 | 1.39 |
| 29 | 9 | 601 | CHL | CHC-C1C | 4.22 | 1.47 | 1.39 |
| 29 | c | 608 | CHL | CHB-C1B | 4.22 | 1.46 | 1.39 |
| 21 | 4 | 609 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 29 | 1 | 307 | CHL | CHB-C1B | 4.20 | 1.46 | 1.39 |
| 29 | 8 | 613 | CHL | CHB-C4A | -4.20 | 1.33 | 1.38 |
| 29 | c | 601 | CHL | CHD-C4C | 4.20 | 1.47 | 1.39 |
| 29 | b | 307 | CHL | CHB-C1B | 4.20 | 1.46 | 1.39 |
| 29 | a | 609 | CHL | CHB-C4A | -4.19 | 1.33 | 1.38 |
| 29 | 4 | 607 | CHL | CHC-C1C | 4.19 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 27 | B | 847 | DGD | O1G-C1A | 4.18 | 1.45 | 1.33 |
| 29 | b | 302 | CHL | CHB-C4A | -4.18 | 1.33 | 1.38 |
| 29 | b | 308 | CHL | CHB-C1B | 4.18 | 1.46 | 1.39 |
| 29 | 6 | 602 | CHL | CHD-C4C | 4.18 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | CHC-C1C | 4.17 | 1.47 | 1.39 |
| 21 | B | 801 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 29 | 9 | 608 | CHL | CHB-C1B | 4.17 | 1.46 | 1.39 |
| 29 | 2 | 606 | CHL | CHD-C4C | 4.17 | 1.47 | 1.39 |
| 29 | c | 605 | CHL | CHB-C4A | -4.17 | 1.33 | 1.38 |
| 29 | 9 | 609 | CHL | CHB-C1B | 4.17 | 1.46 | 1.39 |
| 29 | 2 | 607 | CHL | CHB-C1B | 4.17 | 1.46 | 1.39 |
| 29 | 6 | 606 | CHL | CHB-C1B | 4.16 | 1.46 | 1.39 |
| 29 | a | 601 | CHL | CHB-C4A | -4.16 | 1.33 | 1.38 |
| 29 | 1 | 307 | CHL | CHC-C1C | 4.16 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | CHB-C1B | 4.16 | 1.46 | 1.39 |
| 29 | 9 | 606 | CHL | CHC-C1C | 4.15 | 1.47 | 1.39 |
| 29 | b | 309 | CHL | CHB-C1B | 4.15 | 1.46 | 1.39 |
| 29 | 2 | 605 | CHL | CHB-C1B | 4.15 | 1.46 | 1.39 |
| 29 | 4 | 607 | CHL | CHD-C4C | 4.15 | 1.47 | 1.39 |
| 29 | a | 608 | CHL | CHC-C1C | 4.15 | 1.47 | 1.39 |
| 29 | 4 | 606 | CHL | CHC-C1C | 4.14 | 1.47 | 1.39 |
| 29 | c | 601 | CHL | CHB-C1B | 4.14 | 1.46 | 1.39 |
| 29 | 2 | 602 | CHL | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 29 | a | 606 | CHL | C3A-C2A | -4.14 | 1.51 | 1.54 |
| 29 | a | 607 | CHL | CHC-C1C | 4.14 | 1.47 | 1.39 |
| 29 | c | 606 | CHL | CHB-C4A | -4.14 | 1.33 | 1.38 |
| 29 | 2 | 606 | CHL | CHC-C1C | 4.13 | 1.47 | 1.39 |
| 29 | 4 | 605 | CHL | CHC-C1C | 4.13 | 1.47 | 1.39 |
| 29 | 8 | 607 | CHL | CHC-C1C | 4.13 | 1.47 | 1.39 |
| 29 | 3 | 407 | CHL | CHB-C1B | 4.13 | 1.46 | 1.39 |
| 29 | 8 | 606 | CHL | CHB-C4A | -4.13 | 1.33 | 1.38 |
| 29 | b | 310 | CHL | CHC-C1C | 4.13 | 1.47 | 1.39 |
| 29 | 7 | 406 | CHL | CHB-C4A | -4.12 | 1.33 | 1.38 |
| 29 | 6 | 614 | CHL | CHB-C4A | -4.12 | 1.33 | 1.38 |
| 29 | 2 | 607 | CHL | CHD-C4C | 4.12 | 1.47 | 1.39 |
| 21 | A | 801 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 29 | a | 606 | CHL | CHB-C1B | 4.11 | 1.46 | 1.39 |
| 29 | 8 | 605 | CHL | CHC-C1C | 4.11 | 1.47 | 1.39 |
| 21 | A | 830 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | CHB-C4A | -4.10 | 1.33 | 1.38 |
| 29 | 9 | 609 | CHL | CHC-C1C | 4.10 | 1.47 | 1.39 |
| 29 | b | 308 | CHL | CHC-C1C | 4.09 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | 6 | 602 | CHL | CHB-C1B | 4.09 | 1.46 | 1.39 |
| 29 | 1 | 302 | CHL | CHC-C1C | 4.08 | 1.47 | 1.39 |
| 29 | c | 607 | CHL | CHB-C4A | -4.07 | 1.33 | 1.38 |
| 29 | c | 601 | CHL | CHC-C1C | 4.05 | 1.47 | 1.39 |
| 21 | B | 801 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 29 | 2 | 601 | CHL | CHC-C1C | 4.05 | 1.47 | 1.39 |
| 29 | 5 | 601 | CHL | CHC-C1C | 4.05 | 1.47 | 1.39 |
| 29 | 9 | 608 | CHL | CHC-C1C | 4.05 | 1.47 | 1.39 |
| 29 | 4 | 614 | CHL | CHC-C1C | 4.04 | 1.47 | 1.39 |
| 21 | 3 | 409 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 27 | B | 847 | DGD | O2G-C1B | 4.03 | 1.45 | 1.34 |
| 29 | 2 | 614 | CHL | CHC-C1C | 4.01 | 1.47 | 1.39 |
| 29 | 9 | 607 | CHL | CHC-C1C | 3.98 | 1.47 | 1.39 |
| 29 | c | 605 | CHL | CHA-CBD | -3.92 | 1.48 | 1.52 |
| 29 | 3 | 407 | CHL | CHC-C1C | 3.91 | 1.46 | 1.39 |
| 21 | 7 | 407 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 29 | c | 609 | CHL | CHB-C4A | -3.87 | 1.34 | 1.38 |
| 21 | B | 801 | CLA | C3D-C2D | 3.86 | 1.49 | 1.39 |
| 21 | B | 801 | CLA | OBD-CAD | 3.81 | 1.29 | 1.22 |
| 21 | 7 | 407 | CLA | MG-NC | 3.81 | 2.15 | 2.06 |
| 29 | 8 | 605 | CHL | CHB-C4A | -3.80 | 1.34 | 1.38 |
| 21 | 7 | 407 | CLA | C3D-C4D | -3.78 | 1.35 | 1.44 |
| 21 | O | 204 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 21 | 7 | 407 | CLA | C4C-C3C | 3.73 | 1.51 | 1.45 |
| 21 | 5 | 612 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 21 | 3 | 409 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 21 | 8 | 609 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 21 | A | 830 | CLA | C1D-ND | 3.71 | 1.42 | 1.37 |
| 21 | 2 | 609 | CLA | C1D-ND | 3.71 | 1.42 | 1.37 |
| 21 | B | 801 | CLA | CHC-C4B | 3.69 | 1.47 | 1.39 |
| 21 | 4 | 609 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 21 | 1 | 309 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 21 | 7 | 402 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 21 | 6 | 608 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 29 | a | 606 | CHL | CHA-CBD | -3.65 | 1.47 | 1.51 |
| 21 | G | 204 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 21 | A | 818 | CLA | C1D-ND | 3.64 | 1.42 | 1.37 |
| 21 | 7 | 413 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 21 | 7 | 407 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 21 | 7 | 412 | CLA | C4B-NB | 3.62 | 1.42 | 1.37 |
| 21 | 5 | 604 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 21 | 6 | 612 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 604 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 21 | A | 837 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 21 | 7 | 411 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 21 | 7 | 404 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 21 | 7 | 414 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 21 | A | 839 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 21 | a | 612 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 21 | b | 315 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 21 | B | 811 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 21 | 1 | 316 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 21 | a | 611 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 21 | c | 612 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 21 | 6 | 610 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | 5 | 613 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | 5 | 603 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | 8 | 612 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | 7 | 412 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | 7 | 409 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | c | 604 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | 6 | 609 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 21 | A | 818 | CLA | C4B-NB | 3.56 | 1.42 | 1.37 |
| 21 | 6 | 613 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 21 | 6 | 611 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 21 | b | 304 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 21 | 8 | 618 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 21 | 4 | 611 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 5 | 614 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 8 | 603 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 8 | 601 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 1 | 314 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 7 | 408 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 5 | 605 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 5 | 611 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 21 | 6 | 603 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 21 | 4 | 609 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 21 | 5 | 608 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 21 | 7 | 410 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 21 | 5 | 610 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 21 | 7 | 405 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 21 | a | 614 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 21 | B | 816 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 21 | 8 | 611 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 825 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 21 | A | 841 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 21 | 3 | 410 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | 8 | 608 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | A | 838 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | 1 | 315 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | 1 | 305 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | 8 | 604 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | b | 314 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 21 | 1 | 308 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 21 | B | 826 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 21 | 7 | 403 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 21 | b | 313 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 21 | G | 203 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | 8 | 610 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | B | 804 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | B | 837 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | 4 | 601 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | 7 | 407 | CLA | CHC-C1C | 3.49 | 1.45 | 1.38 |
| 21 | F | 304 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | a | 604 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 21 | 2 | 603 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | b | 312 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | c | 610 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | F | 302 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | 3 | 406 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | K | 201 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | B | 839 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 21 | 9 | 613 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | a | 603 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | A | 827 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | 4 | 603 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | b | 305 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | 3 | 412 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | a | 613 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 21 | B | 801 | CLA | CHB-C1B | 3.46 | 1.47 | 1.39 |
| 21 | 5 | 607 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | c | 613 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | a | 602 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | 1 | 313 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | 9 | 603 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | B | 829 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 401 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | L | 302 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | a | 610 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 21 | b | 303 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 29 | 2 | 602 | CHL | CHA-CBD | -3.44 | 1.47 | 1.51 |
| 21 | A | 802 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 21 | 2 | 604 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 21 | 1 | 311 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 21 | 3 | 402 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | B | 823 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | 1 | 312 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | K | 204 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | 2 | 611 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | A | 828 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | B | 815 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | 4 | 610 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 21 | G | 202 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 21 | 3 | 415 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 21 | 4 | 609 | CLA | CHC-C1C | 3.42 | 1.45 | 1.38 |
| 21 | c | 611 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 21 | J | 102 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 21 | 8 | 602 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 21 | 4 | 604 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | 2 | 612 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | B | 809 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | K | 203 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | B | 819 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | B | 835 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | 3 | 413 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | 3 | 404 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | 1 | 310 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 21 | O | 202 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | B | 820 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | B | 814 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | O | 201 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | 4 | 613 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | b | 311 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | B | 830 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | A | 803 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 21 | A | 824 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 29 | 2 | 614 | CHL | CHA-CBD | -3.40 | 1.47 | 1.51 |
| 21 | A | 822 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 822 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | A | 834 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | A | 804 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | H | 201 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | 3 | 405 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | L | 304 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | c | 603 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | B | 810 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | 3 | 411 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | B | 803 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | 3 | 414 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 21 | A | 816 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 21 | c | 614 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 21 | 3 | 409 | CLA | CHC-C1C | 3.38 | 1.45 | 1.38 |
| 21 | A | 836 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 21 | A | 835 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 21 | B | 805 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 21 | 2 | 610 | CLA | C1D-ND | 3.38 | 1.42 | 1.37 |
| 21 | A | 825 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | A | 833 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | 5 | 602 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | 2 | 613 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | 3 | 403 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | A | 821 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | A | 813 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | O | 203 | CLA | C1D-ND | 3.37 | 1.42 | 1.37 |
| 21 | 1 | 306 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | 1 | 304 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | A | 808 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | 9 | 610 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | A | 823 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | K | 202 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | A | 852 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 29 | a | 609 | CHL | CHA-CBD | -3.36 | 1.47 | 1.51 |
| 21 | A | 826 | CLA | C1D-ND | 3.36 | 1.42 | 1.37 |
| 21 | 3 | 408 | CLA | C1D-ND | 3.35 | 1.42 | 1.37 |
| 29 | 2 | 601 | CHL | CHA-CBD | -3.35 | 1.47 | 1.51 |
| 21 | 4 | 612 | CLA | C1D-ND | 3.35 | 1.42 | 1.37 |
| 21 | A | 820 | CLA | C1D-ND | 3.35 | 1.42 | 1.37 |
| 21 | B | 833 | CLA | C1D-ND | 3.35 | 1.42 | 1.37 |
| 21 | 6 | 603 | CLA | C4B-NB | 3.35 | 1.42 | 1.37 |
| 21 | F | 305 | CLA | C1D-ND | 3.35 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | c | 602 | CLA | C1D-ND | 3.35 | 1.42 | 1.37 |
| 21 | A | 815 | CLA | C1D-ND | 3.34 | 1.42 | 1.37 |
| 21 | 9 | 612 | CLA | C1D-ND | 3.34 | 1.42 | 1.37 |
| 21 | A | 809 | CLA | C1D-ND | 3.34 | 1.42 | 1.37 |
| 21 | 9 | 611 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | 9 | 604 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | A | 817 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | 2 | 608 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | B | 811 | CLA | C4B-NB | 3.33 | 1.42 | 1.37 |
| 21 | A | 805 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | B | 834 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | B | 812 | CLA | C1D-ND | 3.33 | 1.42 | 1.37 |
| 21 | B | 832 | CLA | C1D-ND | 3.32 | 1.42 | 1.37 |
| 21 | A | 807 | CLA | C1D-ND | 3.32 | 1.42 | 1.37 |
| 21 | B | 817 | CLA | C1D-ND | 3.32 | 1.42 | 1.37 |
| 21 | B | 807 | CLA | C1D-ND | 3.32 | 1.42 | 1.37 |
| 21 | A | 840 | CLA | C1D-ND | 3.32 | 1.42 | 1.37 |
| 21 | 4 | 608 | CLA | C1D-ND | 3.32 | 1.42 | 1.37 |
| 21 | A | 819 | CLA | C1D-ND | 3.31 | 1.42 | 1.37 |
| 21 | A | 831 | CLA | C1D-ND | 3.31 | 1.42 | 1.37 |
| 21 | B | 838 | CLA | C1D-ND | 3.31 | 1.42 | 1.37 |
| 21 | 6 | 612 | CLA | C4B-NB | 3.31 | 1.42 | 1.37 |
| 21 | 4 | 602 | CLA | C1D-ND | 3.30 | 1.42 | 1.37 |
| 29 | 5 | 601 | CHL | CHA-CBD | -3.30 | 1.47 | 1.51 |
| 21 | B | 840 | CLA | C1D-ND | 3.30 | 1.42 | 1.37 |
| 21 | B | 836 | CLA | C1D-ND | 3.30 | 1.42 | 1.37 |
| 21 | B | 808 | CLA | C1D-ND | 3.29 | 1.42 | 1.37 |
| 21 | B | 827 | CLA | C1D-ND | 3.29 | 1.42 | 1.37 |
| 29 | a | 607 | CHL | CHA-CBD | -3.29 | 1.47 | 1.51 |
| 21 | A | 842 | CLA | C1D-ND | 3.29 | 1.42 | 1.37 |
| 21 | 9 | 602 | CLA | C1D-ND | 3.29 | 1.42 | 1.37 |
| 21 | 1 | 303 | CLA | C1D-ND | 3.29 | 1.42 | 1.37 |
| 21 | A | 814 | CLA | C1D-ND | 3.28 | 1.42 | 1.37 |
| 21 | B | 806 | CLA | C1D-ND | 3.28 | 1.42 | 1.37 |
| 29 | c | 607 | CHL | CHA-CBD | -3.28 | 1.47 | 1.51 |
| 21 | A | 832 | CLA | C1D-ND | 3.28 | 1.42 | 1.37 |
| 21 | 5 | 609 | CLA | C1D-ND | 3.28 | 1.42 | 1.37 |
| 21 | B | 831 | CLA | C4B-NB | 3.28 | 1.42 | 1.37 |
| 21 | A | 812 | CLA | C1D-ND | 3.27 | 1.42 | 1.37 |
| 21 | A | 810 | CLA | C1D-ND | 3.27 | 1.42 | 1.37 |
| 21 | B | 813 | CLA | C1D-ND | 3.27 | 1.42 | 1.37 |
| 29 | b | 307 | CHL | CHA-CBD | -3.26 | 1.47 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 828 | CLA | C1D-ND | 3.25 | 1.42 | 1.37 |
| 29 | 4 | 605 | CHL | CHA-CBD | -3.25 | 1.47 | 1.51 |
| 21 | L | 303 | CLA | C1D-ND | 3.25 | 1.42 | 1.37 |
| 21 | B | 824 | CLA | C1D-ND | 3.25 | 1.42 | 1.37 |
| 21 | 9 | 612 | CLA | C4B-NB | 3.25 | 1.42 | 1.37 |
| 29 | 9 | 606 | CHL | CHA-CBD | -3.24 | 1.47 | 1.51 |
| 21 | B | 821 | CLA | C1D-ND | 3.24 | 1.42 | 1.37 |
| 21 | 1 | 312 | CLA | C4B-NB | 3.24 | 1.42 | 1.37 |
| 29 | 8 | 613 | CHL | CHA-CBD | -3.23 | 1.47 | 1.51 |
| 21 | b | 312 | CLA | C4B-NB | 3.23 | 1.42 | 1.37 |
| 21 | 7 | 401 | CLA | C1D-ND | 3.23 | 1.42 | 1.37 |
| 21 | 7 | 408 | CLA | C4B-NB | 3.23 | 1.42 | 1.37 |
| 21 | B | 818 | CLA | C1D-ND | 3.23 | 1.42 | 1.37 |
| 21 | 3 | 406 | CLA | CAB-C3B | -3.23 | 1.44 | 1.50 |
| 21 | A | 806 | CLA | C1D-ND | 3.22 | 1.42 | 1.37 |
| 21 | 1 | 311 | CLA | CAB-C3B | -3.22 | 1.44 | 1.50 |
| 29 | 2 | 607 | CHL | CHA-CBD | -3.22 | 1.47 | 1.51 |
| 21 | 6 | 604 | CLA | C4B-NB | 3.21 | 1.42 | 1.37 |
| 21 | A | 811 | CLA | C1D-ND | 3.21 | 1.42 | 1.37 |
| 29 | 2 | 606 | CHL | CHA-CBD | -3.21 | 1.47 | 1.51 |
| 21 | 3 | 404 | CLA | CAB-C3B | -3.21 | 1.44 | 1.50 |
| 21 | B | 810 | CLA | CAB-C3B | -3.21 | 1.44 | 1.50 |
| 21 | 9 | 603 | CLA | C4B-NB | 3.20 | 1.42 | 1.37 |
| 29 | b | 310 | CHL | CHA-CBD | -3.20 | 1.47 | 1.51 |
| 21 | 2 | 603 | CLA | C4B-NB | 3.19 | 1.42 | 1.37 |
| 21 | B | 802 | CLA | C1D-ND | 3.19 | 1.42 | 1.37 |
| 21 | 5 | 614 | CLA | CAB-C3B | -3.19 | 1.44 | 1.50 |
| 29 | 7 | 406 | CHL | CHA-CBD | -3.19 | 1.47 | 1.51 |
| 21 | 7 | 403 | CLA | CAB-C3B | -3.18 | 1.44 | 1.50 |
| 21 | A | 839 | CLA | C4B-NB | 3.18 | 1.42 | 1.37 |
| 29 | 6 | 605 | CHL | CHA-CBD | -3.18 | 1.47 | 1.51 |
| 21 | B | 829 | CLA | C4B-NB | 3.18 | 1.42 | 1.37 |
| 21 | 5 | 603 | CLA | C4B-NB | 3.18 | 1.42 | 1.37 |
| 21 | 3 | 408 | CLA | C4B-NB | 3.18 | 1.42 | 1.37 |
| 29 | 4 | 606 | CHL | CHA-CBD | -3.17 | 1.47 | 1.51 |
| 21 | 1 | 316 | CLA | CAB-C3B | -3.17 | 1.44 | 1.50 |
| 21 | 5 | 614 | CLA | C4B-NB | 3.17 | 1.42 | 1.37 |
| 21 | B | 815 | CLA | C4B-NB | 3.16 | 1.42 | 1.37 |
| 21 | 8 | 612 | CLA | C4B-NB | 3.16 | 1.42 | 1.37 |
| 21 | K | 203 | CLA | CAB-C3B | -3.16 | 1.44 | 1.50 |
| 21 | A | 833 | CLA | C4B-NB | 3.15 | 1.42 | 1.37 |
| 21 | a | 612 | CLA | C4B-NB | 3.15 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 831 | CLA | C1D-ND | 3.15 | 1.42 | 1.37 |
| 21 | 4 | 603 | CLA | C4B-NB | 3.15 | 1.42 | 1.37 |
| 21 | 3 | 411 | CLA | C4B-NB | 3.15 | 1.42 | 1.37 |
| 21 | 5 | 612 | CLA | C4B-NB | 3.14 | 1.42 | 1.37 |
| 21 | 7 | 410 | CLA | C4B-NB | 3.14 | 1.42 | 1.37 |
| 21 | 5 | 613 | CLA | CAB-C3B | -3.14 | 1.44 | 1.50 |
| 21 | 1 | 314 | CLA | CAB-C3B | -3.14 | 1.44 | 1.50 |
| 21 | 6 | 611 | CLA | C4B-NB | 3.14 | 1.42 | 1.37 |
| 21 | 8 | 603 | CLA | C4B-NB | 3.14 | 1.42 | 1.37 |
| 21 | c | 612 | CLA | C4B-NB | 3.13 | 1.42 | 1.37 |
| 21 | 7 | 405 | CLA | CAB-C3B | -3.13 | 1.44 | 1.50 |
| 21 | 3 | 403 | CLA | C4B-NB | 3.13 | 1.42 | 1.37 |
| 21 | A | 829 | CLA | C1D-ND | 3.13 | 1.42 | 1.37 |
| 21 | A | 823 | CLA | C4B-NB | 3.13 | 1.42 | 1.37 |
| 21 | F | 304 | CLA | C4B-NB | 3.13 | 1.42 | 1.37 |
| 21 | a | 613 | CLA | C4B-NB | 3.13 | 1.42 | 1.37 |
| 29 | 1 | 307 | CHL | CHA-CBD | -3.12 | 1.48 | 1.51 |
| 21 | B | 821 | CLA | C4B-NB | 3.12 | 1.42 | 1.37 |
| 21 | 7 | 402 | CLA | C4B-NB | 3.12 | 1.42 | 1.37 |
| 21 | 5 | 610 | CLA | CAB-C3B | -3.12 | 1.44 | 1.50 |
| 21 | 8 | 601 | CLA | C4B-NB | 3.12 | 1.42 | 1.37 |
| 21 | 8 | 611 | CLA | C4B-NB | 3.12 | 1.42 | 1.37 |
| 29 | c | 601 | CHL | CHA-CBD | -3.12 | 1.48 | 1.51 |
| 21 | 3 | 410 | CLA | C4B-NB | 3.12 | 1.42 | 1.37 |
| 21 | c | 614 | CLA | C4B-NB | 3.12 | 1.42 | 1.37 |
| 29 | 4 | 607 | CHL | CHA-CBD | -3.11 | 1.48 | 1.51 |
| 29 | 2 | 605 | CHL | CHA-CBD | -3.11 | 1.48 | 1.51 |
| 21 | 5 | 611 | CLA | C4B-NB | 3.11 | 1.41 | 1.37 |
| 21 | 7 | 411 | CLA | C4B-NB | 3.11 | 1.41 | 1.37 |
| 29 | 8 | 607 | CHL | CHA-CBD | -3.11 | 1.48 | 1.51 |
| 21 | B | 804 | CLA | C4B-NB | 3.11 | 1.41 | 1.37 |
| 21 | 7 | 413 | CLA | C4B-NB | 3.11 | 1.41 | 1.37 |
| 21 | a | 611 | CLA | C4B-NB | 3.11 | 1.41 | 1.37 |
| 29 | 9 | 608 | CHL | CHA-CBD | -3.10 | 1.48 | 1.51 |
| 21 | b | 313 | CLA | C4B-NB | 3.10 | 1.41 | 1.37 |
| 21 | 1 | 315 | CLA | C4B-NB | 3.10 | 1.41 | 1.37 |
| 21 | 6 | 608 | CLA | C4B-NB | 3.10 | 1.41 | 1.37 |
| 21 | A | 802 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | 6 | 613 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | 7 | 409 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | B | 810 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | 2 | 613 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 4 | 612 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | a | 603 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | 1 | 316 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | 7 | 414 | CLA | C4B-NB | 3.09 | 1.41 | 1.37 |
| 21 | a | 614 | CLA | C4B-NB | 3.08 | 1.41 | 1.37 |
| 21 | 5 | 607 | CLA | C4B-NB | 3.08 | 1.41 | 1.37 |
| 21 | 3 | 413 | CLA | C4B-NB | 3.08 | 1.41 | 1.37 |
| 29 | b | 306 | CHL | CHA-CBD | -3.08 | 1.48 | 1.51 |
| 21 | G | 203 | CLA | C4B-NB | 3.08 | 1.41 | 1.37 |
| 21 | 5 | 608 | CLA | CAB-C3B | -3.08 | 1.44 | 1.50 |
| 21 | B | 820 | CLA | C4B-NB | 3.07 | 1.41 | 1.37 |
| 21 | A | 841 | CLA | C4B-NB | 3.07 | 1.41 | 1.37 |
| 21 | 1 | 304 | CLA | C4B-NB | 3.07 | 1.41 | 1.37 |
| 21 | B | 839 | CLA | C4B-NB | 3.07 | 1.41 | 1.37 |
| 21 | 7 | 401 | CLA | C4B-NB | 3.07 | 1.41 | 1.37 |
| 29 | 4 | 614 | CHL | CHA-CBD | -3.07 | 1.48 | 1.51 |
| 29 | 9 | 605 | CHL | CHA-CBD | -3.07 | 1.48 | 1.51 |
| 21 | 8 | 610 | CLA | C4B-NB | 3.07 | 1.41 | 1.37 |
| 21 | 8 | 608 | CLA | C4B-NB | 3.06 | 1.41 | 1.37 |
| 21 | A | 820 | CLA | C4B-NB | 3.06 | 1.41 | 1.37 |
| 21 | 7 | 403 | CLA | C4B-NB | 3.06 | 1.41 | 1.37 |
| 29 | c | 609 | CHL | CHA-CBD | -3.05 | 1.48 | 1.51 |
| 21 | A | 836 | CLA | C4B-NB | 3.05 | 1.41 | 1.37 |
| 21 | 1 | 308 | CLA | C4B-NB | 3.05 | 1.41 | 1.37 |
| 21 | 1 | 309 | CLA | C3A-C2A | -3.05 | 1.51 | 1.54 |
| 21 | 4 | 601 | CLA | C4B-NB | 3.05 | 1.41 | 1.37 |
| 21 | G | 204 | CLA | C4B-NB | 3.04 | 1.41 | 1.37 |
| 21 | 3 | 414 | CLA | C4B-NB | 3.04 | 1.41 | 1.37 |
| 21 | O | 204 | CLA | C4B-NB | 3.04 | 1.41 | 1.37 |
| 21 | 7 | 405 | CLA | C4B-NB | 3.04 | 1.41 | 1.37 |
| 21 | G | 202 | CLA | C4B-NB | 3.04 | 1.41 | 1.37 |
| 21 | b | 315 | CLA | C4B-NB | 3.04 | 1.41 | 1.37 |
| 21 | 1 | 314 | CLA | C4B-NB | 3.03 | 1.41 | 1.37 |
| 21 | 3 | 412 | CLA | C4B-NB | 3.03 | 1.41 | 1.37 |
| 21 | b | 314 | CLA | C4B-NB | 3.03 | 1.41 | 1.37 |
| 21 | 5 | 604 | CLA | C4B-NB | 3.03 | 1.41 | 1.37 |
| 29 | 6 | 607 | CHL | CHA-CBD | -3.03 | 1.48 | 1.51 |
| 21 | 5 | 609 | CLA | C4B-NB | 3.03 | 1.41 | 1.37 |
| 21 | B | 809 | CLA | C4B-NB | 3.03 | 1.41 | 1.37 |
| 21 | 5 | 613 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 21 | a | 610 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 21 | b | 305 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 610 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 21 | 4 | 613 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 21 | a | 602 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 29 | 8 | 606 | CHL | CHA-CBD | -3.02 | 1.48 | 1.51 |
| 21 | 5 | 610 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 21 | 8 | 604 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 21 | 7 | 407 | CLA | CHC-C4B | 3.02 | 1.46 | 1.39 |
| 21 | 5 | 608 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 29 | b | 309 | CHL | CHA-CBD | -3.02 | 1.48 | 1.51 |
| 24 | A | 850 | BCR | C23-C22 | -3.02 | 1.39 | 1.46 |
| 21 | A | 804 | CLA | C4B-NB | 3.02 | 1.41 | 1.37 |
| 24 | A | 848 | BCR | C23-C22 | -3.02 | 1.39 | 1.46 |
| 21 | 2 | 612 | CLA | C4B-NB | 3.01 | 1.41 | 1.37 |
| 21 | c | 603 | CLA | C4B-NB | 3.01 | 1.41 | 1.37 |
| 29 | 6 | 614 | CHL | CHA-CBD | -3.01 | 1.48 | 1.51 |
| 21 | A | 822 | CLA | C4B-NB | 3.00 | 1.41 | 1.37 |
| 21 | 1 | 313 | CLA | C4B-NB | 3.00 | 1.41 | 1.37 |
| 24 | F | 301 | BCR | C8-C9 | -3.00 | 1.39 | 1.46 |
| 21 | 8 | 602 | CLA | C4B-NB | 3.00 | 1.41 | 1.37 |
| 21 | c | 604 | CLA | C4B-NB | 3.00 | 1.41 | 1.37 |
| 21 | K | 204 | CLA | C4B-NB | 3.00 | 1.41 | 1.37 |
| 21 | 6 | 609 | CLA | C4B-NB | 2.99 | 1.41 | 1.37 |
| 21 | A | 805 | CLA | C4B-NB | 2.99 | 1.41 | 1.37 |
| 21 | L | 302 | CLA | C4B-NB | 2.99 | 1.41 | 1.37 |
| 21 | b | 303 | CLA | C4B-NB | 2.99 | 1.41 | 1.37 |
| 24 | A | 848 | BCR | C8-C9 | -2.99 | 1.39 | 1.46 |
| 21 | 7 | 404 | CLA | C4B-NB | 2.99 | 1.41 | 1.37 |
| 24 | A | 849 | BCR | C8-C9 | -2.99 | 1.39 | 1.46 |
| 21 | 4 | 609 | CLA | C1B-C2B | 2.99 | 1.50 | 1.43 |
| 21 | 2 | 611 | CLA | C4B-NB | 2.98 | 1.41 | 1.37 |
| 21 | 3 | 409 | CLA | C1B-C2B | 2.98 | 1.50 | 1.43 |
| 21 | B | 803 | CLA | C4B-NB | 2.98 | 1.41 | 1.37 |
| 24 | A | 850 | BCR | C8-C9 | -2.98 | 1.39 | 1.46 |
| 30 | 7 | 415 | LUT | C8-C9 | -2.98 | 1.39 | 1.46 |
| 21 | B | 802 | CLA | C4B-NB | 2.98 | 1.41 | 1.37 |
| 21 | 2 | 608 | CLA | C4B-NB | 2.98 | 1.41 | 1.37 |
| 29 | 1 | 302 | CHL | CHA-CBD | -2.97 | 1.48 | 1.51 |
| 21 | 5 | 605 | CLA | C4B-NB | 2.97 | 1.41 | 1.37 |
| 21 | 9 | 611 | CLA | C4B-NB | 2.97 | 1.41 | 1.37 |
| 21 | H | 201 | CLA | C4B-NB | 2.97 | 1.41 | 1.37 |
| 21 | 9 | 602 | CLA | C4B-NB | 2.97 | 1.41 | 1.37 |
| 21 | A | 837 | CLA | C4B-NB | 2.97 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 602 | CLA | C4B-NB | 2.96 | 1.41 | 1.37 |
| 21 | 7 | 407 | CLA | C1B-C2B | 2.96 | 1.50 | 1.43 |
| 21 | 2 | 609 | CLA | C1B-C2B | 2.96 | 1.50 | 1.43 |
| 21 | A | 852 | CLA | C4B-NB | 2.95 | 1.41 | 1.37 |
| 21 | B | 801 | CLA | C1B-NB | -2.95 | 1.34 | 1.37 |
| 21 | 3 | 406 | CLA | C4B-NB | 2.95 | 1.41 | 1.37 |
| 29 | 6 | 602 | CHL | CHA-CBD | -2.95 | 1.48 | 1.51 |
| 29 | 9 | 609 | CHL | CHA-CBD | -2.95 | 1.48 | 1.51 |
| 21 | B | 814 | CLA | C4B-NB | 2.95 | 1.41 | 1.37 |
| 21 | c | 611 | CLA | C4B-NB | 2.95 | 1.41 | 1.37 |
| 21 | A | 830 | CLA | C1B-C2B | 2.95 | 1.50 | 1.43 |
| 24 | A | 854 | BCR | C23-C22 | -2.95 | 1.39 | 1.46 |
| 21 | A | 834 | CLA | C4B-NB | 2.95 | 1.41 | 1.37 |
| 29 | b | 308 | CHL | CHA-CBD | -2.94 | 1.48 | 1.51 |
| 24 | J | 101 | BCR | C8-C9 | -2.94 | 1.39 | 1.46 |
| 21 | O | 202 | CLA | C4B-NB | 2.94 | 1.41 | 1.37 |
| 29 | 8 | 605 | CHL | CHA-CBD | -2.94 | 1.48 | 1.51 |
| 24 | A | 847 | BCR | C23-C22 | -2.94 | 1.39 | 1.46 |
| 21 | 1 | 306 | CLA | C4B-NB | 2.94 | 1.41 | 1.37 |
| 21 | A | 819 | CLA | C4B-NB | 2.93 | 1.41 | 1.37 |
| 24 | F | 303 | BCR | C8-C9 | -2.93 | 1.39 | 1.46 |
| 30 | b | 317 | LUT | C8-C9 | -2.93 | 1.39 | 1.46 |
| 21 | 1 | 309 | CLA | C1B-C2B | 2.93 | 1.50 | 1.43 |
| 21 | a | 604 | CLA | C4B-NB | 2.93 | 1.41 | 1.37 |
| 24 | A | 854 | BCR | C8-C9 | -2.93 | 1.39 | 1.46 |
| 21 | c | 613 | CLA | C4B-NB | 2.92 | 1.41 | 1.37 |
| 21 | 3 | 415 | CLA | C4B-NB | 2.92 | 1.41 | 1.37 |
| 24 | A | 847 | BCR | C8-C9 | -2.92 | 1.39 | 1.46 |
| 24 | A | 849 | BCR | C23-C22 | -2.92 | 1.39 | 1.46 |
| 21 | B | 838 | CLA | C4B-NB | 2.92 | 1.41 | 1.37 |
| 29 | 5 | 606 | CHL | CHA-CBD | -2.92 | 1.48 | 1.51 |
| 24 | L | 305 | BCR | C23-C22 | -2.92 | 1.39 | 1.46 |
| 21 | A | 829 | CLA | C4B-NB | 2.92 | 1.41 | 1.37 |
| 21 | 2 | 604 | CLA | C4B-NB | 2.92 | 1.41 | 1.37 |
| 21 | A | 831 | CLA | C4B-NB | 2.91 | 1.41 | 1.37 |
| 21 | B | 828 | CLA | C4B-NB | 2.91 | 1.41 | 1.37 |
| 21 | 3 | 405 | CLA | C4B-NB | 2.91 | 1.41 | 1.37 |
| 21 | 4 | 611 | CLA | C4B-NB | 2.91 | 1.41 | 1.37 |
| 24 | L | 301 | BCR | C8-C9 | -2.91 | 1.39 | 1.46 |
| 24 | 3 | 419 | BCR | C8-C9 | -2.91 | 1.39 | 1.46 |
| 24 | B | 845 | BCR | C8-C9 | -2.91 | 1.39 | 1.46 |
| 21 | 8 | 609 | CLA | C1B-C2B | 2.90 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | M | 101 | BCR | C8-C9 | -2.90 | 1.39 | 1.46 |
| 21 | B | 807 | CLA | C4B-NB | 2.90 | 1.41 | 1.37 |
| 21 | B | 806 | CLA | C4B-NB | 2.90 | 1.41 | 1.37 |
| 21 | B | 818 | CLA | C4B-NB | 2.90 | 1.41 | 1.37 |
| 21 | B | 837 | CLA | C4B-NB | 2.90 | 1.41 | 1.37 |
| 21 | 8 | 618 | CLA | C4B-NB | 2.90 | 1.41 | 1.37 |
| 24 | I | 101 | BCR | C23-C22 | -2.89 | 1.39 | 1.46 |
| 21 | b | 311 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 24 | B | 845 | BCR | C23-C22 | -2.89 | 1.39 | 1.46 |
| 21 | A | 835 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 21 | c | 610 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 30 | 9 | 615 | LUT | C8-C9 | -2.89 | 1.39 | 1.46 |
| 21 | c | 602 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 21 | 1 | 303 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 24 | L | 305 | BCR | C8-C9 | -2.89 | 1.39 | 1.46 |
| 21 | 4 | 604 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 21 | 3 | 402 | CLA | C4B-NB | 2.89 | 1.41 | 1.37 |
| 29 | a | 608 | CHL | CHA-CBD | -2.89 | 1.48 | 1.51 |
| 21 | 3 | 404 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | B | 817 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | 9 | 604 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 29 | 9 | 607 | CHL | CHA-CBD | -2.88 | 1.48 | 1.51 |
| 21 | B | 826 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 24 | L | 301 | BCR | C23-C22 | -2.88 | 1.39 | 1.46 |
| 21 | F | 302 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | B | 812 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | A | 811 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | A | 824 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | 9 | 613 | CLA | C4B-NB | 2.88 | 1.41 | 1.37 |
| 21 | B | 816 | CLA | C4B-NB | 2.87 | 1.41 | 1.37 |
| 29 | c | 606 | CHL | CHA-CBD | -2.87 | 1.48 | 1.51 |
| 21 | A | 806 | CLA | C4B-NB | 2.87 | 1.41 | 1.37 |
| 21 | A | 810 | CLA | C4B-NB | 2.87 | 1.41 | 1.37 |
| 21 | B | 827 | CLA | C4B-NB | 2.87 | 1.41 | 1.37 |
| 24 | B | 842 | BCR | C23-C22 | -2.87 | 1.39 | 1.46 |
| 21 | 3 | 409 | CLA | CHC-C4B | 2.87 | 1.45 | 1.39 |
| 30 | 8 | 614 | LUT | C8-C9 | -2.87 | 1.39 | 1.46 |
| 21 | 1 | 305 | CLA | C4B-NB | 2.87 | 1.41 | 1.37 |
| 21 | b | 304 | CLA | C4B-NB | 2.87 | 1.41 | 1.37 |
| 21 | 8 | 618 | CLA | C1B-C2B | 2.87 | 1.49 | 1.43 |
| 21 | A | 840 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | 1 | 311 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 842 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | J | 102 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | 4 | 608 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | B | 833 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | O | 203 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | A | 832 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | B | 830 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 21 | 9 | 610 | CLA | C4B-NB | 2.86 | 1.41 | 1.37 |
| 24 | A | 846 | BCR | C8-C9 | -2.85 | 1.39 | 1.46 |
| 21 | A | 808 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 21 | 4 | 610 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 24 | F | 301 | BCR | C23-C22 | -2.85 | 1.39 | 1.46 |
| 21 | B | 832 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 21 | 4 | 602 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 29 | 6 | 606 | CHL | CHA-CBD | -2.85 | 1.48 | 1.51 |
| 21 | 4 | 609 | CLA | CHC-C4B | 2.85 | 1.45 | 1.39 |
| 21 | A | 828 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 21 | 1 | 309 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 24 | 3 | 418 | BCR | C8-C9 | -2.85 | 1.39 | 1.46 |
| 21 | A | 815 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 21 | A | 826 | CLA | C4B-NB | 2.85 | 1.41 | 1.37 |
| 24 | 2 | 618 | BCR | C8-C9 | -2.84 | 1.39 | 1.46 |
| 21 | K | 201 | CLA | C4B-NB | 2.84 | 1.41 | 1.37 |
| 21 | B | 819 | CLA | C4B-NB | 2.84 | 1.41 | 1.37 |
| 29 | c | 608 | CHL | CHA-CBD | -2.84 | 1.48 | 1.51 |
| 24 | I | 101 | BCR | C8-C9 | -2.84 | 1.39 | 1.46 |
| 21 | A | 817 | CLA | C4B-NB | 2.84 | 1.41 | 1.37 |
| 24 | G | 205 | BCR | C8-C9 | -2.84 | 1.39 | 1.46 |
| 30 | c | 615 | LUT | C8-C9 | -2.84 | 1.39 | 1.46 |
| 21 | A | 830 | CLA | C4B-NB | 2.83 | 1.41 | 1.37 |
| 21 | A | 812 | CLA | C4B-NB | 2.83 | 1.41 | 1.37 |
| 21 | K | 203 | CLA | C4B-NB | 2.83 | 1.41 | 1.37 |
| 21 | A | 809 | CLA | C4B-NB | 2.83 | 1.41 | 1.37 |
| 21 | 7 | 404 | CLA | C1B-C2B | 2.83 | 1.49 | 1.43 |
| 24 | 4 | 617 | BCR | C8-C9 | -2.82 | 1.39 | 1.46 |
| 24 | B | 842 | BCR | C8-C9 | -2.82 | 1.39 | 1.46 |
| 21 | K | 202 | CLA | C4B-NB | 2.82 | 1.41 | 1.37 |
| 21 | 1 | 310 | CLA | C4B-NB | 2.82 | 1.41 | 1.37 |
| 21 | B | 823 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 21 | B | 836 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 24 | G | 201 | BCR | C8-C9 | -2.81 | 1.39 | 1.46 |
| 21 | L | 303 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | O | 201 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 21 | 8 | 609 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 21 | A | 825 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 21 | B | 805 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 21 | B | 822 | CLA | C4B-NB | 2.81 | 1.41 | 1.37 |
| 21 | B | 801 | CLA | C1B-C2B | 2.80 | 1.49 | 1.43 |
| 21 | A | 813 | CLA | C4B-NB | 2.80 | 1.41 | 1.37 |
| 21 | 7 | 408 | CLA | C1B-C2B | 2.80 | 1.49 | 1.43 |
| 21 | A | 816 | CLA | C4B-NB | 2.80 | 1.41 | 1.37 |
| 21 | B | 824 | CLA | C4B-NB | 2.80 | 1.41 | 1.37 |
| 24 | A | 846 | BCR | C23-C22 | -2.80 | 1.40 | 1.46 |
| 21 | F | 305 | CLA | C4B-NB | 2.80 | 1.41 | 1.37 |
| 21 | G | 202 | CLA | C1B-C2B | 2.80 | 1.49 | 1.43 |
| 21 | 6 | 604 | CLA | C1B-C2B | 2.79 | 1.49 | 1.43 |
| 21 | A | 814 | CLA | C4B-NB | 2.79 | 1.41 | 1.37 |
| 30 | 9 | 614 | LUT | C8-C9 | -2.79 | 1.40 | 1.46 |
| 24 | L | 306 | BCR | C8-C9 | -2.79 | 1.40 | 1.46 |
| 21 | 7 | 412 | CLA | C1B-C2B | 2.79 | 1.49 | 1.43 |
| 21 | A | 803 | CLA | C4B-NB | 2.79 | 1.41 | 1.37 |
| 21 | A | 827 | CLA | C4B-NB | 2.79 | 1.41 | 1.37 |
| 21 | B | 834 | CLA | C4B-NB | 2.79 | 1.41 | 1.37 |
| 21 | A | 801 | CLA | C4B-NB | 2.79 | 1.41 | 1.37 |
| 24 | 3 | 419 | BCR | C23-C22 | -2.78 | 1.40 | 1.46 |
| 21 | 3 | 401 | CLA | C4B-NB | 2.78 | 1.41 | 1.37 |
| 21 | 3 | 405 | CLA | C1B-C2B | 2.78 | 1.49 | 1.43 |
| 30 | 2 | 616 | LUT | C8-C9 | -2.78 | 1.40 | 1.46 |
| 24 | F | 303 | BCR | C23-C22 | -2.78 | 1.40 | 1.46 |
| 24 | 6 | 618 | BCR | C23-C22 | -2.78 | 1.40 | 1.46 |
| 21 | A | 838 | CLA | C4B-NB | 2.78 | 1.41 | 1.37 |
| 30 | 4 | 615 | LUT | C8-C9 | -2.78 | 1.40 | 1.46 |
| 24 | G | 205 | BCR | C23-C22 | -2.78 | 1.40 | 1.46 |
| 24 | 7 | 418 | BCR | C23-C22 | -2.78 | 1.40 | 1.46 |
| 21 | A | 821 | CLA | C4B-NB | 2.78 | 1.41 | 1.37 |
| 21 | B | 808 | CLA | C4B-NB | 2.78 | 1.41 | 1.37 |
| 29 | a | 601 | CHL | CHA-CBD | -2.78 | 1.48 | 1.51 |
| 24 | G | 201 | BCR | C23-C22 | -2.77 | 1.40 | 1.46 |
| 21 | 2 | 610 | CLA | C4B-NB | 2.77 | 1.41 | 1.37 |
| 30 | 6 | 616 | LUT | C8-C9 | -2.77 | 1.40 | 1.46 |
| 30 | 5 | 615 | LUT | C8-C9 | -2.77 | 1.40 | 1.46 |
| 21 | 9 | 613 | CLA | C1B-C2B | 2.77 | 1.49 | 1.43 |
| 30 | c | 616 | LUT | C8-C9 | -2.77 | 1.40 | 1.46 |
| 21 | B | 811 | CLA | C1B-C2B | 2.77 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | J | 103 | BCR | C8-C9 | -2.77 | 1.40 | 1.46 |
| 21 | 5 | 613 | CLA | C4B-C3B | 2.76 | 1.49 | 1.43 |
| 21 | 5 | 608 | CLA | C4B-C3B | 2.76 | 1.49 | 1.43 |
| 24 | 4 | 617 | BCR | C23-C22 | -2.76 | 1.40 | 1.46 |
| 21 | a | 614 | CLA | C1B-C2B | 2.76 | 1.49 | 1.43 |
| 21 | 4 | 613 | CLA | C1B-C2B | 2.76 | 1.49 | 1.43 |
| 21 | 7 | 405 | CLA | C1B-C2B | 2.76 | 1.49 | 1.43 |
| 21 | 7 | 409 | CLA | C1B-C2B | 2.76 | 1.49 | 1.43 |
| 21 | 5 | 614 | CLA | C1B-C2B | 2.76 | 1.49 | 1.43 |
| 21 | c | 613 | CLA | C1B-C2B | 2.76 | 1.49 | 1.43 |
| 21 | 5 | 604 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 21 | 6 | 612 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 29 | 3 | 407 | CHL | CHA-CBD | -2.75 | 1.48 | 1.51 |
| 21 | 8 | 610 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 21 | 2 | 609 | CLA | C4B-NB | 2.75 | 1.41 | 1.37 |
| 21 | A | 807 | CLA | C4B-NB | 2.75 | 1.41 | 1.37 |
| 21 | 4 | 604 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 21 | 5 | 610 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 21 | 8 | 612 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 21 | 6 | 603 | CLA | C1B-C2B | 2.75 | 1.49 | 1.43 |
| 24 | M | 101 | BCR | C23-C22 | -2.74 | 1.40 | 1.46 |
| 21 | 7 | 405 | CLA | C4B-C3B | 2.74 | 1.49 | 1.43 |
| 21 | b | 304 | CLA | C1B-C2B | 2.74 | 1.49 | 1.43 |
| 24 | J | 103 | BCR | C23-C22 | -2.74 | 1.40 | 1.46 |
| 24 | 7 | 417 | BCR | C8-C9 | -2.74 | 1.40 | 1.46 |
| 21 | G | 204 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 24 | L | 306 | BCR | C23-C22 | -2.73 | 1.40 | 1.46 |
| 21 | B | 813 | CLA | C4B-NB | 2.73 | 1.41 | 1.37 |
| 21 | 5 | 612 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 21 | 3 | 401 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 21 | K | 203 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 21 | 5 | 613 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 21 | 6 | 610 | CLA | C1B-C2B | 2.73 | 1.49 | 1.43 |
| 21 | 7 | 403 | CLA | C1B-C2B | 2.72 | 1.49 | 1.43 |
| 24 | J | 101 | BCR | C23-C22 | -2.72 | 1.40 | 1.46 |
| 24 | 6 | 618 | BCR | C8-C9 | -2.72 | 1.40 | 1.46 |
| 24 | 7 | 417 | BCR | C23-C22 | -2.72 | 1.40 | 1.46 |
| 21 | A | 817 | CLA | C1B-C2B | 2.72 | 1.49 | 1.43 |
| 21 | O | 201 | CLA | C1B-C2B | 2.72 | 1.49 | 1.43 |
| 21 | 5 | 614 | CLA | C4B-C3B | 2.72 | 1.49 | 1.43 |
| 21 | 5 | 608 | CLA | C1B-C2B | 2.71 | 1.49 | 1.43 |
| 21 | 6 | 613 | CLA | C1B-C2B | 2.71 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | a | 615 | LUT | C8-C9 | -2.71 | 1.40 | 1.46 |
| 24 | J | 101 | BCR | C21-C22 | 2.71 | 1.42 | 1.35 |
| 21 | 5 | 607 | CLA | C1B-C2B | 2.71 | 1.49 | 1.43 |
| 21 | B | 835 | CLA | C4B-NB | 2.71 | 1.41 | 1.37 |
| 21 | c | 603 | CLA | C1B-C2B | 2.71 | 1.49 | 1.43 |
| 21 | 6 | 611 | CLA | C1B-C2B | 2.71 | 1.49 | 1.43 |
| 21 | 1 | 316 | CLA | C4B-C3B | 2.71 | 1.49 | 1.43 |
| 24 | 7 | 418 | BCR | C8-C9 | -2.71 | 1.40 | 1.46 |
| 30 | a | 616 | LUT | C8-C9 | -2.71 | 1.40 | 1.46 |
| 24 | O | 205 | BCR | C23-C22 | -2.71 | 1.40 | 1.46 |
| 21 | 5 | 611 | CLA | C1B-C2B | 2.71 | 1.49 | 1.43 |
| 21 | L | 304 | CLA | C4B-NB | 2.70 | 1.41 | 1.37 |
| 21 | 1 | 314 | CLA | C4B-C3B | 2.70 | 1.49 | 1.43 |
| 21 | c | 611 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | B | 814 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | 5 | 605 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | 7 | 411 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | B | 825 | CLA | C4B-NB | 2.70 | 1.41 | 1.37 |
| 21 | a | 611 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | a | 604 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | A | 810 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | 6 | 608 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | 2 | 610 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | b | 305 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | A | 834 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | b | 312 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | 1 | 314 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | 7 | 413 | CLA | C1B-C2B | 2.70 | 1.49 | 1.43 |
| 21 | B | 826 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 21 | 8 | 603 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 21 | b | 315 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 24 | 8 | 616 | BCR | C8-C9 | -2.69 | 1.40 | 1.46 |
| 21 | G | 203 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 21 | A | 838 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 21 | B | 810 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 29 | 6 | 601 | CHL | CHA-CBD | -2.69 | 1.48 | 1.51 |
| 24 | 3 | 418 | BCR | C23-C22 | -2.69 | 1.40 | 1.46 |
| 21 | 3 | 406 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 21 | 8 | 601 | CLA | C1B-C2B | 2.69 | 1.49 | 1.43 |
| 21 | A | 835 | CLA | C3B-C4B | 2.69 | 1.50 | 1.42 |
| 21 | F | 305 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | 7 | 410 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 311 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | 5 | 602 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | B | 829 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | B | 823 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | 4 | 610 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | a | 612 | CLA | C1B-C2B | 2.68 | 1.49 | 1.43 |
| 21 | 7 | 403 | CLA | C4B-C3B | 2.67 | 1.49 | 1.43 |
| 21 | 5 | 610 | CLA | C4B-C3B | 2.67 | 1.49 | 1.43 |
| 30 | 1 | 317 | LUT | C8-C9 | -2.67 | 1.40 | 1.46 |
| 21 | B | 810 | CLA | C4B-C3B | 2.67 | 1.49 | 1.43 |
| 21 | O | 202 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | A | 801 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | c | 614 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 30 | b | 316 | LUT | C8-C9 | -2.67 | 1.40 | 1.46 |
| 21 | 7 | 407 | CLA | CMD-C2D | -2.67 | 1.45 | 1.50 |
| 21 | L | 302 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | 3 | 402 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | B | 802 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | a | 613 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | b | 314 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | A | 833 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | 8 | 608 | CLA | C1B-C2B | 2.67 | 1.49 | 1.43 |
| 21 | c | 604 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | B | 840 | CLA | C4B-NB | 2.66 | 1.41 | 1.37 |
| 21 | A | 835 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | H | 201 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 1 | 316 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | L | 304 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | A | 807 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 30 | 5 | 615 | LUT | C10-C9 | 2.66 | 1.42 | 1.35 |
| 21 | 1 | 308 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 5 | 603 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 8 | 611 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | a | 602 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 8 | 604 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | b | 313 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 1 | 315 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 9 | 603 | CLA | C1B-C2B | 2.66 | 1.49 | 1.43 |
| 21 | 1 | 311 | CLA | C4B-C3B | 2.66 | 1.49 | 1.43 |
| 21 | B | 827 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | B | 819 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | A | 804 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | a | 610 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | A | 824 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | 3 | 413 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | 4 | 611 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | a | 603 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 29 | b | 302 | CHL | CHA-CBD | -2.65 | 1.48 | 1.51 |
| 21 | B | 805 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 21 | B | 809 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 7 | 402 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 1 | 306 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 24 | O | 205 | BCR | C8-C9 | -2.64 | 1.40 | 1.46 |
| 21 | A | 806 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | A | 827 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | B | 837 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 2 | 611 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 9 | 611 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 5 | 609 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 3 | 404 | CLA | C4B-C3B | 2.64 | 1.49 | 1.43 |
| 21 | B | 839 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 1 | 303 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | B | 825 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | 3 | 410 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | A | 841 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 21 | B | 821 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | 2 | 613 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | B | 830 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | 4 | 603 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 30 | 3 | 416 | LUT | C8-C9 | -2.63 | 1.40 | 1.46 |
| 21 | A | 840 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | c | 612 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | 4 | 602 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | O | 203 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | B | 840 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | K | 204 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | 1 | 313 | CLA | C1B-C2B | 2.63 | 1.49 | 1.43 |
| 21 | 1 | 310 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 21 | 2 | 604 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 24 | A | 850 | BCR | C19-C18 | -2.62 | 1.40 | 1.46 |
| 30 | 7 | 415 | LUT | C10-C9 | 2.62 | 1.41 | 1.35 |
| 21 | 3 | 414 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 21 | 3 | 412 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 21 | B | 822 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 824 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 21 | J | 102 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 21 | O | 204 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 21 | A | 831 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | 9 | 604 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | K | 201 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | 4 | 612 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 24 | 2 | 618 | BCR | C23-C22 | -2.61 | 1.40 | 1.46 |
| 21 | B | 834 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | 7 | 401 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | b | 303 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | 3 | 406 | CLA | C4B-C3B | 2.61 | 1.49 | 1.43 |
| 21 | 7 | 414 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | B | 835 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | 4 | 608 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 21 | A | 816 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 24 | J | 103 | BCR | C10-C9 | 2.60 | 1.41 | 1.35 |
| 21 | A | 802 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | B | 806 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | A | 829 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | 2 | 612 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | A | 822 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | A | 820 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | B | 804 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | A | 808 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 21 | A | 813 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 21 | 1 | 312 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 21 | L | 303 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 21 | K | 202 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 21 | 2 | 608 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 24 | A | 848 | BCR | C19-C18 | -2.59 | 1.40 | 1.46 |
| 21 | A | 812 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 21 | 1 | 304 | CLA | C1B-C2B | 2.59 | 1.49 | 1.43 |
| 21 | O | 204 | CLA | CHC-C1C | 2.58 | 1.43 | 1.38 |
| 21 | B | 820 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 21 | 6 | 609 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 21 | 8 | 602 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 21 | A | 803 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 21 | B | 801 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 21 | 3 | 409 | CLA | C4B-NB | -2.57 | 1.34 | 1.37 |
| 21 | c | 610 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 24 | 8 | 616 | BCR | C23-C22 | -2.57 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | F | 301 | BCR | C12-C13 | -2.57 | 1.40 | 1.46 |
| 21 | A | 811 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 21 | 1 | 305 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 21 | B | 803 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 21 | B | 836 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 21 | 9 | 602 | CLA | C1B-C2B | 2.56 | 1.49 | 1.43 |
| 21 | A | 828 | CLA | C1B-C2B | 2.56 | 1.49 | 1.43 |
| 21 | A | 842 | CLA | C1B-C2B | 2.56 | 1.49 | 1.43 |
| 21 | 9 | 612 | CLA | C3B-C4B | 2.56 | 1.50 | 1.42 |
| 24 | A | 848 | BCR | C12-C13 | -2.56 | 1.40 | 1.46 |
| 21 | b | 311 | CLA | C1B-C2B | 2.55 | 1.49 | 1.43 |
| 21 | 3 | 404 | CLA | C1B-C2B | 2.55 | 1.49 | 1.43 |
| 21 | A | 823 | CLA | C1B-C2B | 2.55 | 1.49 | 1.43 |
| 21 | A | 821 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 21 | A | 825 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 21 | B | 838 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 21 | B | 815 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 31 | 6 | 617 | XAT | C34-C33 | 2.54 | 1.41 | 1.35 |
| 21 | K | 203 | CLA | C4B-C3B | 2.54 | 1.49 | 1.43 |
| 21 | c | 602 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 21 | A | 839 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 21 | B | 832 | CLA | C1B-C2B | 2.54 | 1.49 | 1.43 |
| 24 | A | 849 | BCR | C12-C13 | -2.54 | 1.40 | 1.46 |
| 21 | A | 814 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | 3 | 403 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | A | 818 | CLA | C3B-C4B | 2.53 | 1.50 | 1.42 |
| 21 | F | 302 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | 4 | 601 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | B | 831 | CLA | C3B-C4B | 2.53 | 1.50 | 1.42 |
| 21 | B | 807 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | 3 | 411 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | A | 815 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 21 | F | 304 | CLA | C1B-C2B | 2.52 | 1.49 | 1.43 |
| 21 | A | 802 | CLA | C3B-C4B | 2.52 | 1.50 | 1.42 |
| 21 | A | 832 | CLA | C1B-C2B | 2.52 | 1.49 | 1.43 |
| 21 | 3 | 408 | CLA | C3B-C4B | 2.52 | 1.50 | 1.42 |
| 21 | A | 826 | CLA | C1B-C2B | 2.52 | 1.49 | 1.43 |
| 21 | 1 | 312 | CLA | C3B-C4B | 2.51 | 1.50 | 1.42 |
| 21 | B | 812 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 21 | B | 801 | CLA | C4B-NB | -2.51 | 1.34 | 1.37 |
| 21 | B | 813 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 31 | 2 | 617 | XAT | C32-C33 | -2.51 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 817 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 24 | A | 854 | BCR | C19-C18 | -2.50 | 1.40 | 1.46 |
| 21 | A | 852 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 31 | 9 | 616 | XAT | C10-C9 | 2.50 | 1.41 | 1.35 |
| 21 | 9 | 610 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 21 | A | 835 | CLA | CHC-C1C | 2.50 | 1.43 | 1.38 |
| 30 | b | 317 | LUT | C12-C13 | -2.49 | 1.40 | 1.46 |
| 31 | 4 | 616 | XAT | C28-C29 | -2.49 | 1.40 | 1.46 |
| 21 | 3 | 415 | CLA | C1B-C2B | 2.49 | 1.49 | 1.43 |
| 21 | 9 | 612 | CLA | C1B-C2B | 2.49 | 1.49 | 1.43 |
| 21 | B | 818 | CLA | C1B-C2B | 2.49 | 1.49 | 1.43 |
| 21 | A | 837 | CLA | C1B-C2B | 2.49 | 1.49 | 1.43 |
| 21 | B | 833 | CLA | C1B-C2B | 2.48 | 1.48 | 1.43 |
| 24 | A | 854 | BCR | C12-C13 | -2.48 | 1.40 | 1.46 |
| 31 | 3 | 417 | XAT | C28-C29 | -2.47 | 1.40 | 1.46 |
| 24 | F | 303 | BCR | C12-C13 | -2.47 | 1.40 | 1.46 |
| 21 | A | 836 | CLA | C1B-C2B | 2.47 | 1.48 | 1.43 |
| 21 | A | 805 | CLA | C1B-C2B | 2.47 | 1.48 | 1.43 |
| 24 | L | 305 | BCR | C12-C13 | -2.47 | 1.40 | 1.46 |
| 21 | 4 | 609 | CLA | C4B-NB | -2.47 | 1.34 | 1.37 |
| 21 | 8 | 603 | CLA | C3B-C4B | 2.47 | 1.49 | 1.42 |
| 21 | B | 815 | CLA | C3B-C4B | 2.46 | 1.49 | 1.42 |
| 21 | A | 836 | CLA | C3B-C4B | 2.46 | 1.49 | 1.42 |
| 29 | 9 | 601 | CHL | CHA-CBD | -2.46 | 1.48 | 1.51 |
| 24 | L | 305 | BCR | C19-C18 | -2.46 | 1.40 | 1.46 |
| 21 | 3 | 408 | CLA | C1B-C2B | 2.46 | 1.48 | 1.43 |
| 31 | 6 | 617 | XAT | C10-C9 | 2.46 | 1.41 | 1.35 |
| 31 | 6 | 617 | XAT | C32-C33 | -2.46 | 1.40 | 1.46 |
| 21 | B | 801 | CLA | C1C-C2C | 2.46 | 1.49 | 1.44 |
| 21 | 2 | 603 | CLA | C1B-C2B | 2.46 | 1.48 | 1.43 |
| 30 | 8 | 614 | LUT | C34-C33 | 2.46 | 1.41 | 1.35 |
| 24 | M | 101 | BCR | C21-C22 | 2.45 | 1.41 | 1.35 |
| 21 | A | 809 | CLA | C1B-C2B | 2.45 | 1.48 | 1.43 |
| 21 | B | 804 | CLA | C3B-C4B | 2.45 | 1.49 | 1.42 |
| 30 | 7 | 415 | LUT | C12-C13 | -2.45 | 1.40 | 1.46 |
| 24 | M | 101 | BCR | C10-C9 | 2.45 | 1.41 | 1.35 |
| 30 | 1 | 317 | LUT | C10-C9 | 2.45 | 1.41 | 1.35 |
| 24 | L | 301 | BCR | C12-C13 | -2.45 | 1.40 | 1.46 |
| 31 | 3 | 417 | XAT | C12-C13 | -2.45 | 1.40 | 1.46 |
| 30 | 3 | 416 | LUT | C28-C29 | -2.45 | 1.40 | 1.46 |
| 21 | F | 304 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |
| 21 | 3 | 411 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | b | 317 | LUT | C32-C33 | -2.44 | 1.40 | 1.46 |
| 24 | B | 845 | BCR | C19-C18 | -2.44 | 1.40 | 1.46 |
| 30 | c | 615 | LUT | C12-C13 | -2.44 | 1.40 | 1.46 |
| 24 | A | 847 | BCR | C19-C18 | -2.44 | 1.40 | 1.46 |
| 31 | 9 | 616 | XAT | C14-C13 | 2.44 | 1.41 | 1.35 |
| 21 | B | 831 | CLA | C1B-C2B | 2.44 | 1.48 | 1.43 |
| 31 | 4 | 616 | XAT | C32-C33 | -2.44 | 1.40 | 1.46 |
| 24 | L | 301 | BCR | C19-C18 | -2.44 | 1.40 | 1.46 |
| 24 | F | 301 | BCR | C19-C18 | -2.44 | 1.40 | 1.46 |
| 24 | 8 | 616 | BCR | C14-C13 | 2.44 | 1.41 | 1.35 |
| 24 | 8 | 616 | BCR | C17-C18 | 2.43 | 1.41 | 1.35 |
| 31 | c | 617 | XAT | C12-C13 | -2.43 | 1.40 | 1.46 |
| 21 | c | 614 | CLA | C3B-C4B | 2.43 | 1.49 | 1.42 |
| 31 | 1 | 318 | XAT | C12-C13 | -2.43 | 1.40 | 1.46 |
| 31 | 3 | 417 | XAT | C32-C33 | -2.43 | 1.40 | 1.46 |
| 21 | a | 603 | CLA | C3B-C4B | 2.43 | 1.49 | 1.42 |
| 31 | 8 | 615 | XAT | C10-C9 | 2.43 | 1.41 | 1.35 |
| 31 | 9 | 616 | XAT | C34-C33 | 2.43 | 1.41 | 1.35 |
| 21 | 8 | 601 | CLA | C3B-C4B | 2.43 | 1.49 | 1.42 |
| 30 | 9 | 614 | LUT | C32-C33 | -2.43 | 1.40 | 1.46 |
| 24 | A | 847 | BCR | C12-C13 | -2.43 | 1.40 | 1.46 |
| 21 | a | 612 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 31 | 9 | 616 | XAT | C30-C29 | 2.42 | 1.41 | 1.35 |
| 31 | 4 | 616 | XAT | C12-C13 | -2.42 | 1.40 | 1.46 |
| 31 | 5 | 616 | XAT | C32-C33 | -2.42 | 1.40 | 1.46 |
| 21 | B | 801 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 31 | 1 | 318 | XAT | C28-C29 | -2.41 | 1.40 | 1.46 |
| 30 | 8 | 614 | LUT | C14-C13 | 2.41 | 1.41 | 1.35 |
| 24 | G | 201 | BCR | C19-C18 | -2.41 | 1.40 | 1.46 |
| 24 | J | 101 | BCR | C12-C13 | -2.41 | 1.40 | 1.46 |
| 21 | 8 | 602 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 21 | A | 819 | CLA | C1B-C2B | 2.41 | 1.48 | 1.43 |
| 21 | B | 820 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 30 | 6 | 616 | LUT | C30-C29 | 2.41 | 1.41 | 1.35 |
| 21 | 3 | 409 | CLA | C4D-CHA | 2.41 | 1.46 | 1.38 |
| 21 | 8 | 602 | CLA | CHC-C1C | 2.41 | 1.43 | 1.38 |
| 24 | G | 201 | BCR | C12-C13 | -2.41 | 1.40 | 1.46 |
| 21 | B | 828 | CLA | C1B-C2B | 2.41 | 1.48 | 1.43 |
| 21 | G | 203 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 30 | 1 | 317 | LUT | C14-C13 | 2.40 | 1.41 | 1.35 |
| 21 | A | 841 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 24 | G | 205 | BCR | C12-C13 | -2.40 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 612 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 21 | a | 602 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 21 | 7 | 412 | CLA | CHC-C1C | 2.40 | 1.43 | 1.38 |
| 31 | 1 | 318 | XAT | C32-C33 | -2.40 | 1.40 | 1.46 |
| 21 | 1 | 309 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 21 | b | 303 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 30 | 9 | 614 | LUT | C12-C13 | -2.40 | 1.40 | 1.46 |
| 30 | 8 | 614 | LUT | C12-C13 | -2.40 | 1.40 | 1.46 |
| 24 | M | 101 | BCR | C17-C18 | 2.40 | 1.41 | 1.35 |
| 21 | 7 | 413 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 21 | 5 | 612 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 21 | O | 204 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 24 | A | 846 | BCR | C19-C18 | -2.39 | 1.40 | 1.46 |
| 30 | 3 | 416 | LUT | C32-C33 | -2.39 | 1.40 | 1.46 |
| 21 | 6 | 613 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 32 | 9 | 617 | NEX | C28-C29 | -2.39 | 1.40 | 1.46 |
| 31 | 8 | 615 | XAT | C34-C33 | 2.39 | 1.41 | 1.35 |
| 31 | 2 | 617 | XAT | C8-C9 | -2.39 | 1.40 | 1.46 |
| 24 | B | 845 | BCR | C12-C13 | -2.39 | 1.40 | 1.46 |
| 21 | B | 816 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |
| 31 | 5 | 616 | XAT | C28-C29 | -2.39 | 1.40 | 1.46 |
| 21 | 5 | 602 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 24 | A | 850 | BCR | C12-C13 | -2.38 | 1.40 | 1.46 |
| 30 | 2 | 616 | LUT | C32-C33 | -2.38 | 1.40 | 1.46 |
| 30 | 9 | 615 | LUT | C12-C13 | -2.38 | 1.40 | 1.46 |
| 21 | 4 | 601 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 21 | B | 808 | CLA | C1B-C2B | 2.38 | 1.48 | 1.43 |
| 24 | A | 846 | BCR | C12-C13 | -2.38 | 1.40 | 1.46 |
| 31 | 6 | 617 | XAT | C14-C13 | 2.38 | 1.41 | 1.35 |
| 24 | 2 | 618 | BCR | C21-C22 | 2.38 | 1.41 | 1.35 |
| 31 | 2 | 617 | XAT | C12-C13 | -2.38 | 1.40 | 1.46 |
| 21 | 7 | 414 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 21 | 1 | 308 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 30 | a | 616 | LUT | C14-C13 | 2.38 | 1.41 | 1.35 |
| 21 | 5 | 602 | CLA | CHC-C1C | 2.38 | 1.43 | 1.38 |
| 30 | 1 | 317 | LUT | C30-C29 | 2.38 | 1.41 | 1.35 |
| 31 | 2 | 617 | XAT | C28-C29 | -2.38 | 1.40 | 1.46 |
| 21 | 5 | 611 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 21 | 7 | 410 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 21 | A | 818 | CLA | C1B-C2B | 2.38 | 1.48 | 1.43 |
| 30 | 1 | 317 | LUT | C34-C33 | 2.38 | 1.41 | 1.35 |
| 21 | b | 311 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | b | 312 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 21 | 2 | 603 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 21 | 9 | 603 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 24 | O | 205 | BCR | C14-C13 | 2.38 | 1.41 | 1.35 |
| 30 | 4 | 615 | LUT | C10-C9 | 2.38 | 1.41 | 1.35 |
| 31 | 4 | 616 | XAT | C8-C9 | -2.37 | 1.40 | 1.46 |
| 30 | 9 | 615 | LUT | C32-C33 | -2.37 | 1.40 | 1.46 |
| 21 | a | 610 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 30 | 4 | 615 | LUT | C32-C33 | -2.37 | 1.40 | 1.46 |
| 31 | 8 | 615 | XAT | C14-C13 | 2.37 | 1.41 | 1.35 |
| 24 | M | 101 | BCR | C14-C13 | 2.37 | 1.41 | 1.35 |
| 21 | B | 833 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 30 | 9 | 615 | LUT | C28-C29 | -2.37 | 1.40 | 1.46 |
| 31 | 5 | 616 | XAT | C12-C13 | -2.37 | 1.40 | 1.46 |
| 21 | 2 | 612 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 24 | 7 | 418 | BCR | C21-C22 | 2.37 | 1.41 | 1.35 |
| 21 | B | 808 | CLA | CMB-C2B | -2.37 | 1.45 | 1.50 |
| 29 | a | 605 | CHL | CHA-CBD | -2.36 | 1.48 | 1.51 |
| 30 | 4 | 615 | LUT | C28-C29 | -2.36 | 1.40 | 1.46 |
| 24 | G | 205 | BCR | C19-C18 | -2.36 | 1.40 | 1.46 |
| 21 | b | 313 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 21 | A | 837 | CLA | CHC-C1C | 2.36 | 1.43 | 1.38 |
| 21 | 7 | 413 | CLA | CHC-C1C | 2.36 | 1.43 | 1.38 |
| 21 | c | 612 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 21 | 8 | 604 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 31 | c | 617 | XAT | C8-C9 | -2.36 | 1.40 | 1.46 |
| 30 | c | 616 | LUT | C12-C13 | -2.36 | 1.40 | 1.46 |
| 31 | 6 | 617 | XAT | C28-C29 | -2.36 | 1.40 | 1.46 |
| 31 | 7 | 416 | XAT | C14-C13 | 2.36 | 1.41 | 1.35 |
| 21 | 9 | 602 | CLA | CHC-C1C | 2.36 | 1.43 | 1.38 |
| 24 | 3 | 418 | BCR | C12-C13 | -2.36 | 1.40 | 1.46 |
| 21 | F | 302 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 24 | O | 205 | BCR | C21-C22 | 2.36 | 1.41 | 1.35 |
| 21 | 1 | 309 | CLA | C4D-CHA | 2.36 | 1.46 | 1.38 |
| 21 | 6 | 611 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 24 | J | 103 | BCR | C21-C22 | 2.36 | 1.41 | 1.35 |
| 21 | B | 802 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 30 | b | 316 | LUT | C34-C33 | 2.35 | 1.41 | 1.35 |
| 31 | 8 | 615 | XAT | C30-C29 | 2.35 | 1.41 | 1.35 |
| 24 | 8 | 616 | BCR | C21-C22 | 2.35 | 1.41 | 1.35 |
| 24 | B | 842 | BCR | C19-C18 | -2.35 | 1.40 | 1.46 |
| 31 | 3 | 417 | XAT | C8-C9 | -2.35 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | B | 842 | BCR | C12-C13 | -2.35 | 1.40 | 1.46 |
| 21 | b | 303 | CLA | CHC-C1C | 2.35 | 1.43 | 1.38 |
| 24 | O | 205 | BCR | C17-C18 | 2.35 | 1.41 | 1.35 |
| 21 | 4 | 611 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 21 | 7 | 411 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 32 | b | 318 | NEX | C12-C13 | -2.35 | 1.40 | 1.46 |
| 31 | 7 | 416 | XAT | C34-C33 | 2.35 | 1.41 | 1.35 |
| 21 | A | 805 | CLA | CHC-C1C | 2.35 | 1.43 | 1.38 |
| 21 | 3 | 412 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 31 | a | 618 | XAT | C12-C13 | -2.35 | 1.40 | 1.46 |
| 30 | 8 | 614 | LUT | C30-C29 | 2.35 | 1.41 | 1.35 |
| 21 | 3 | 410 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 21 | a | 614 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 21 | B | 828 | CLA | CMB-C2B | -2.35 | 1.46 | 1.50 |
| 21 | B | 803 | CLA | CHC-C1C | 2.35 | 1.43 | 1.38 |
| 24 | 7 | 417 | BCR | C17-C18 | 2.35 | 1.41 | 1.35 |
| 21 | 4 | 612 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 30 | a | 615 | LUT | C30-C29 | 2.34 | 1.41 | 1.35 |
| 30 | a | 616 | LUT | C30-C29 | 2.34 | 1.41 | 1.35 |
| 21 | 6 | 610 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 21 | 5 | 609 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 21 | A | 823 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 30 | 6 | 616 | LUT | C10-C9 | 2.34 | 1.41 | 1.35 |
| 24 | 7 | 418 | BCR | C14-C13 | 2.34 | 1.41 | 1.35 |
| 31 | c | 617 | XAT | C28-C29 | -2.34 | 1.40 | 1.46 |
| 24 | 7 | 417 | BCR | C21-C22 | 2.34 | 1.41 | 1.35 |
| 21 | A | 820 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 21 | B | 836 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 30 | c | 616 | LUT | C32-C33 | -2.34 | 1.40 | 1.46 |
| 31 | 1 | 318 | XAT | C8-C9 | -2.34 | 1.40 | 1.46 |
| 21 | 8 | 611 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 24 | 6 | 618 | BCR | C17-C18 | 2.34 | 1.41 | 1.35 |
| 21 | A | 839 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 21 | 6 | 603 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 21 | A | 809 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 21 | 8 | 610 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 30 | 4 | 615 | LUT | C34-C33 | 2.33 | 1.41 | 1.35 |
| 21 | 2 | 611 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 24 | 8 | 616 | BCR | C10-C9 | 2.33 | 1.41 | 1.35 |
| 21 | b | 311 | CLA | CHC-C1C | 2.33 | 1.43 | 1.38 |
| 21 | 3 | 413 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 21 | 5 | 604 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | 6 | 618 | BCR | C10-C9 | 2.33 | 1.41 | 1.35 |
| 21 | c | 603 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 30 | 2 | 616 | LUT | C28-C29 | -2.33 | 1.41 | 1.46 |
| 21 | b | 315 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 32 | b | 318 | NEX | C28-C29 | -2.33 | 1.41 | 1.46 |
| 21 | 7 | 401 | CLA | CHC-C1C | 2.33 | 1.43 | 1.38 |
| 24 | F | 303 | BCR | C17-C18 | 2.33 | 1.41 | 1.35 |
| 24 | 7 | 417 | BCR | C10-C9 | 2.33 | 1.41 | 1.35 |
| 21 | b | 314 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 30 | 7 | 415 | LUT | C30-C29 | 2.33 | 1.41 | 1.35 |
| 21 | 1 | 313 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 24 | 3 | 418 | BCR | C19-C18 | -2.33 | 1.41 | 1.46 |
| 21 | 9 | 610 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 21 | 7 | 412 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 21 | A | 829 | CLA | CMD-C2D | -2.33 | 1.46 | 1.50 |
| 29 | 3 | 407 | CHL | OBD-CAD | 2.33 | 1.25 | 1.22 |
| 21 | 9 | 602 | CLA | CMD-C2D | -2.33 | 1.46 | 1.50 |
| 21 | 7 | 409 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 32 | c | 618 | NEX | C30-C29 | 2.33 | 1.41 | 1.35 |
| 21 | 4 | 608 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 21 | a | 613 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 30 | 1 | 317 | LUT | C28-C29 | -2.33 | 1.41 | 1.46 |
| 30 | 1 | 317 | LUT | C32-C33 | -2.33 | 1.41 | 1.46 |
| 30 | c | 616 | LUT | C14-C13 | 2.33 | 1.41 | 1.35 |
| 21 | b | 315 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | a | 602 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 24 | O | 205 | BCR | C10-C9 | 2.32 | 1.41 | 1.35 |
| 21 | c | 611 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 21 | 7 | 410 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | A | 809 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | 5 | 607 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 24 | 2 | 618 | BCR | C14-C13 | 2.32 | 1.41 | 1.35 |
| 30 | a | 616 | LUT | C34-C33 | 2.32 | 1.41 | 1.35 |
| 21 | b | 312 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 24 | 6 | 618 | BCR | C21-C22 | 2.32 | 1.41 | 1.35 |
| 21 | B | 802 | CLA | CMC-C2C | -2.32 | 1.46 | 1.50 |
| 21 | 5 | 613 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | 7 | 414 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | A | 837 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 32 | b | 318 | NEX | C32-C33 | -2.32 | 1.41 | 1.46 |
| 21 | 3 | 414 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 32 | 9 | 617 | NEX | C34-C33 | 2.32 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 315 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 31 | 7 | 416 | XAT | C12-C13 | -2.32 | 1.41 | 1.46 |
| 21 | 2 | 608 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | a | 610 | CLA | CHC-C1C | 2.32 | 1.43 | 1.38 |
| 21 | A | 805 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 30 | b | 317 | LUT | C28-C29 | -2.32 | 1.41 | 1.46 |
| 30 | a | 615 | LUT | C10-C9 | 2.32 | 1.41 | 1.35 |
| 30 | b | 316 | LUT | C10-C9 | 2.31 | 1.41 | 1.35 |
| 21 | 3 | 403 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | 4 | 617 | BCR | C12-C13 | -2.31 | 1.41 | 1.46 |
| 21 | 5 | 609 | CLA | CHC-C1C | 2.31 | 1.43 | 1.38 |
| 21 | a | 612 | CLA | CHC-C1C | 2.31 | 1.43 | 1.38 |
| 31 | c | 617 | XAT | C32-C33 | -2.31 | 1.41 | 1.46 |
| 21 | 4 | 603 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 30 | 9 | 614 | LUT | C34-C33 | 2.31 | 1.41 | 1.35 |
| 21 | c | 604 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | A | 849 | BCR | C19-C18 | -2.31 | 1.41 | 1.46 |
| 24 | 6 | 618 | BCR | C14-C13 | 2.31 | 1.41 | 1.35 |
| 32 | c | 618 | NEX | C14-C13 | 2.31 | 1.41 | 1.35 |
| 31 | a | 618 | XAT | C8-C9 | -2.31 | 1.41 | 1.46 |
| 24 | 3 | 419 | BCR | C14-C13 | 2.31 | 1.41 | 1.35 |
| 31 | 7 | 416 | XAT | C30-C29 | 2.31 | 1.41 | 1.35 |
| 21 | 3 | 415 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 21 | 9 | 602 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 24 | 2 | 618 | BCR | C12-C13 | -2.31 | 1.41 | 1.46 |
| 21 | 4 | 608 | CLA | CHC-C1C | 2.31 | 1.43 | 1.38 |
| 21 | B | 816 | CLA | CMB-C2B | -2.31 | 1.46 | 1.50 |
| 30 | a | 616 | LUT | C32-C33 | -2.31 | 1.41 | 1.46 |
| 30 | 4 | 615 | LUT | C14-C13 | 2.31 | 1.41 | 1.35 |
| 24 | I | 101 | BCR | C17-C18 | 2.31 | 1.41 | 1.35 |
| 21 | A | 852 | CLA | CHC-C1C | 2.31 | 1.43 | 1.38 |
| 21 | 6 | 608 | CLA | CHC-C1C | 2.31 | 1.43 | 1.38 |
| 24 | I | 101 | BCR | C10-C9 | 2.31 | 1.41 | 1.35 |
| 30 | 6 | 616 | LUT | C34-C33 | 2.31 | 1.41 | 1.35 |
| 21 | 9 | 610 | CLA | CHC-C1C | 2.31 | 1.43 | 1.38 |
| 31 | a | 618 | XAT | C14-C13 | 2.31 | 1.41 | 1.35 |
| 31 | a | 618 | XAT | C30-C29 | 2.31 | 1.41 | 1.35 |
| 24 | L | 306 | BCR | C21-C22 | 2.30 | 1.41 | 1.35 |
| 21 | B | 801 | CLA | C4C-C3C | 2.30 | 1.48 | 1.45 |
| 30 | 5 | 615 | LUT | C32-C33 | -2.30 | 1.41 | 1.46 |
| 24 | I | 101 | BCR | C19-C18 | -2.30 | 1.41 | 1.46 |
| 30 | 7 | 415 | LUT | C28-C29 | -2.30 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | 7 | 416 | XAT | C8-C9 | -2.30 | 1.41 | 1.46 |
| 21 | A | 802 | CLA | CHC-C1C | 2.30 | 1.43 | 1.38 |
| 21 | A | 826 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 30 | 9 | 614 | LUT | C28-C29 | -2.30 | 1.41 | 1.46 |
| 32 | b | 318 | NEX | C30-C29 | 2.30 | 1.41 | 1.35 |
| 24 | 7 | 418 | BCR | C10-C9 | 2.30 | 1.41 | 1.35 |
| 21 | A | 824 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 21 | a | 613 | CLA | CHC-C1C | 2.30 | 1.43 | 1.38 |
| 21 | A | 852 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 30 | 2 | 616 | LUT | C14-C13 | 2.30 | 1.41 | 1.35 |
| 30 | 5 | 615 | LUT | C34-C33 | 2.30 | 1.41 | 1.35 |
| 21 | 4 | 602 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 32 | 9 | 617 | NEX | C32-C33 | -2.30 | 1.41 | 1.46 |
| 21 | b | 314 | CLA | CHC-C1C | 2.30 | 1.43 | 1.38 |
| 21 | 6 | 608 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 21 | 5 | 605 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 21 | 8 | 612 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 24 | 3 | 419 | BCR | C21-C22 | 2.30 | 1.41 | 1.35 |
| 21 | 5 | 607 | CLA | CHC-C1C | 2.30 | 1.43 | 1.38 |
| 21 | L | 303 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 30 | 3 | 416 | LUT | C34-C33 | 2.30 | 1.41 | 1.35 |
| 30 | a | 615 | LUT | C34-C33 | 2.30 | 1.41 | 1.35 |
| 30 | a | 616 | LUT | C10-C9 | 2.30 | 1.41 | 1.35 |
| 21 | a | 611 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 21 | A | 801 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 24 | L | 306 | BCR | C10-C9 | 2.30 | 1.41 | 1.35 |
| 21 | B | 822 | CLA | CMD-C2D | -2.29 | 1.46 | 1.50 |
| 30 | a | 616 | LUT | C12-C13 | -2.29 | 1.41 | 1.46 |
| 30 | c | 615 | LUT | C30-C29 | 2.29 | 1.41 | 1.35 |
| 21 | K | 201 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 24 | 7 | 417 | BCR | C14-C13 | 2.29 | 1.41 | 1.35 |
| 30 | 2 | 616 | LUT | C10-C9 | 2.29 | 1.41 | 1.35 |
| 31 | a | 618 | XAT | C34-C33 | 2.29 | 1.41 | 1.35 |
| 31 | 7 | 416 | XAT | C32-C33 | -2.29 | 1.41 | 1.46 |
| 21 | 7 | 402 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 30 | 3 | 416 | LUT | C30-C29 | 2.29 | 1.41 | 1.35 |
| 21 | B | 838 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 21 | 5 | 611 | CLA | CHC-C1C | 2.29 | 1.43 | 1.38 |
| 21 | 7 | 409 | CLA | CHC-C1C | 2.29 | 1.43 | 1.38 |
| 24 | J | 103 | BCR | C14-C13 | 2.29 | 1.41 | 1.35 |
| 30 | 2 | 616 | LUT | C12-C13 | -2.29 | 1.41 | 1.46 |
| 30 | c | 615 | LUT | C28-C29 | -2.29 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | O | 202 | CLA | CHC-C1C | 2.29 | 1.43 | 1.38 |
| 24 | 7 | 418 | BCR | C17-C18 | 2.29 | 1.41 | 1.35 |
| 21 | 3 | 402 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 24 | 3 | 419 | BCR | C17-C18 | 2.29 | 1.41 | 1.35 |
| 24 | J | 101 | BCR | C19-C18 | -2.29 | 1.41 | 1.46 |
| 32 | c | 618 | NEX | C34-C33 | 2.29 | 1.41 | 1.35 |
| 21 | 9 | 611 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 21 | A | 832 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 21 | H | 201 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 21 | 6 | 610 | CLA | CHC-C1C | 2.29 | 1.43 | 1.38 |
| 30 | b | 316 | LUT | C14-C13 | 2.29 | 1.41 | 1.35 |
| 21 | B | 803 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 24 | J | 103 | BCR | C17-C18 | 2.29 | 1.41 | 1.35 |
| 21 | 3 | 409 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 21 | 2 | 604 | CLA | MG-NB | -2.29 | 2.01 | 2.05 |
| 24 | B | 842 | BCR | C14-C13 | 2.28 | 1.41 | 1.35 |
| 21 | 2 | 609 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 30 | c | 615 | LUT | C34-C33 | 2.28 | 1.41 | 1.35 |
| 21 | B | 815 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | B | 833 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | 6 | 613 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | A | 836 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | 7 | 408 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | B | 824 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | a | 604 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | A | 823 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 30 | a | 615 | LUT | C14-C13 | 2.28 | 1.41 | 1.35 |
| 31 | 7 | 416 | XAT | C10-C9 | 2.28 | 1.41 | 1.35 |
| 30 | 6 | 616 | LUT | C14-C13 | 2.28 | 1.41 | 1.35 |
| 21 | 7 | 404 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 30 | 2 | 616 | LUT | C34-C33 | 2.28 | 1.41 | 1.35 |
| 21 | 6 | 609 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 30 | 5 | 615 | LUT | C30-C29 | 2.28 | 1.41 | 1.35 |
| 24 | 4 | 617 | BCR | C19-C18 | -2.28 | 1.41 | 1.46 |
| 24 | F | 303 | BCR | C21-C22 | 2.28 | 1.41 | 1.35 |
| 21 | B | 812 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | 8 | 611 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | A | 822 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | A | 818 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | 2 | 613 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | A | 830 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | G | 202 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 306 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | 8 | 618 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 21 | A | 826 | CLA | CHC-C1C | 2.28 | 1.43 | 1.38 |
| 21 | A | 819 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 24 | 4 | 617 | BCR | C14-C13 | 2.27 | 1.41 | 1.35 |
| 21 | A | 832 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | 3 | 415 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | 2 | 608 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 3 | 408 | CLA | CMB-C2B | -2.27 | 1.46 | 1.50 |
| 21 | O | 202 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 30 | 2 | 616 | LUT | C30-C29 | 2.27 | 1.41 | 1.35 |
| 30 | 3 | 416 | LUT | C10-C9 | 2.27 | 1.41 | 1.35 |
| 21 | J | 102 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 4 | 604 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 30 | 4 | 615 | LUT | C30-C29 | 2.27 | 1.41 | 1.35 |
| 21 | A | 833 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 8 | 604 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | A | 815 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 24 | J | 101 | BCR | C14-C13 | 2.27 | 1.41 | 1.35 |
| 32 | 9 | 617 | NEX | C14-C13 | 2.27 | 1.41 | 1.35 |
| 21 | 6 | 611 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | 7 | 405 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 24 | G | 205 | BCR | C17-C18 | 2.27 | 1.41 | 1.35 |
| 21 | B | 807 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | c | 604 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | A | 816 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 8 | 608 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | A | 818 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 21 | 1 | 305 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 7 | 401 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | B | 804 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 30 | b | 316 | LUT | C32-C33 | -2.27 | 1.41 | 1.46 |
| 30 | c | 615 | LUT | C32-C33 | -2.27 | 1.41 | 1.46 |
| 21 | b | 305 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | B | 809 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 4 | 610 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 21 | 8 | 601 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | 8 | 603 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 21 | 6 | 604 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 30 | 5 | 615 | LUT | C12-C13 | -2.27 | 1.41 | 1.46 |
| 21 | 4 | 602 | CLA | CHC-C1C | 2.27 | 1.43 | 1.38 |
| 24 | L | 306 | BCR | C14-C13 | 2.27 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 1 | 317 | LUT | C12-C13 | -2.27 | 1.41 | 1.46 |
| 21 | B | 835 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 21 | 1 | 305 | CLA | CHC-C1C | 2.26 | 1.43 | 1.38 |
| 24 | I | 101 | BCR | C14-C13 | 2.26 | 1.41 | 1.35 |
| 21 | B | 807 | CLA | CMB-C2B | -2.26 | 1.46 | 1.50 |
| 21 | B | 839 | CLA | CMB-C2B | -2.26 | 1.46 | 1.50 |
| 21 | 3 | 404 | CLA | CMB-C2B | -2.26 | 1.46 | 1.50 |
| 24 | A | 846 | BCR | C21-C22 | 2.26 | 1.41 | 1.35 |
| 21 | c | 610 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 24 | L | 306 | BCR | C12-C13 | -2.26 | 1.41 | 1.46 |
| 32 | b | 318 | NEX | C34-C33 | 2.26 | 1.41 | 1.35 |
| 21 | L | 303 | CLA | CHC-C1C | 2.26 | 1.43 | 1.38 |
| 21 | 1 | 310 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 30 | c | 616 | LUT | C28-C29 | -2.26 | 1.41 | 1.46 |
| 21 | L | 302 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 21 | c | 613 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 21 | A | 814 | CLA | MG-NB | -2.26 | 2.01 | 2.05 |
| 21 | B | 816 | CLA | MG-NB | -2.26 | 2.01 | 2.05 |
| 21 | 8 | 612 | CLA | CHC-C1C | 2.26 | 1.43 | 1.38 |
| 21 | K | 204 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 21 | A | 818 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 31 | a | 618 | XAT | C32-C33 | -2.26 | 1.41 | 1.46 |
| 21 | 1 | 309 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 31 | 6 | 617 | XAT | C30-C29 | 2.26 | 1.41 | 1.35 |
| 30 | b | 316 | LUT | C28-C29 | -2.26 | 1.41 | 1.46 |
| 21 | 2 | 604 | CLA | CHC-C1C | 2.26 | 1.43 | 1.38 |
| 21 | 5 | 610 | CLA | CHC-C1C | 2.26 | 1.43 | 1.38 |
| 21 | 5 | 614 | CLA | CHC-C1C | 2.26 | 1.43 | 1.38 |
| 24 | 4 | 617 | BCR | C17-C18 | 2.26 | 1.41 | 1.35 |
| 24 | 6 | 618 | BCR | C19-C18 | -2.26 | 1.41 | 1.46 |
| 24 | 2 | 618 | BCR | C10-C9 | 2.26 | 1.41 | 1.35 |
| 30 | 4 | 615 | LUT | C12-C13 | -2.26 | 1.41 | 1.46 |
| 24 | 4 | 617 | BCR | C21-C22 | 2.26 | 1.41 | 1.35 |
| 30 | a | 615 | LUT | C32-C33 | -2.26 | 1.41 | 1.46 |
| 21 | 4 | 613 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 24 | F | 303 | BCR | C14-C13 | 2.26 | 1.41 | 1.35 |
| 30 | 9 | 614 | LUT | C14-C13 | 2.26 | 1.41 | 1.35 |
| 21 | L | 304 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 30 | c | 615 | LUT | C14-C13 | 2.25 | 1.41 | 1.35 |
| 30 | 5 | 615 | LUT | C14-C13 | 2.25 | 1.41 | 1.35 |
| 30 | 9 | 615 | LUT | C30-C29 | 2.25 | 1.41 | 1.35 |
| 30 | 3 | 416 | LUT | C14-C13 | 2.25 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 7 | 401 | CLA | MG-NB | -2.25 | 2.01 | 2.05 |
| 21 | A | 815 | CLA | CHC-C1C | 2.25 | 1.43 | 1.38 |
| 21 | 6 | 612 | CLA | CHC-C1C | 2.25 | 1.43 | 1.38 |
| 24 | B | 842 | BCR | C10-C9 | 2.25 | 1.41 | 1.35 |
| 21 | B | 808 | CLA | MG-NB | -2.25 | 2.01 | 2.05 |
| 21 | A | 829 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | B | 813 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | 7 | 403 | CLA | CHC-C1C | 2.25 | 1.43 | 1.38 |
| 30 | b | 316 | LUT | C30-C29 | 2.25 | 1.41 | 1.35 |
| 30 | a | 615 | LUT | C12-C13 | -2.25 | 1.41 | 1.46 |
| 31 | 5 | 616 | XAT | C8-C9 | -2.25 | 1.41 | 1.46 |
| 21 | a | 604 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | A | 828 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | 7 | 411 | CLA | CHC-C1C | 2.25 | 1.43 | 1.38 |
| 24 | A | 846 | BCR | C14-C13 | 2.25 | 1.41 | 1.35 |
| 21 | B | 828 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | 9 | 604 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | c | 602 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 24 | 3 | 419 | BCR | C10-C9 | 2.25 | 1.41 | 1.35 |
| 31 | c | 617 | XAT | C14-C13 | 2.25 | 1.41 | 1.35 |
| 30 | 8 | 614 | LUT | C32-C33 | -2.25 | 1.41 | 1.46 |
| 21 | B | 808 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | 8 | 609 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 21 | c | 612 | CLA | CHC-C1C | 2.25 | 1.43 | 1.38 |
| 21 | A | 811 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 24 | 3 | 418 | BCR | C21-C22 | 2.25 | 1.41 | 1.35 |
| 30 | 9 | 615 | LUT | C34-C33 | 2.25 | 1.41 | 1.35 |
| 30 | a | 616 | LUT | C28-C29 | -2.25 | 1.41 | 1.46 |
| 21 | 6 | 604 | CLA | CHC-C1C | 2.25 | 1.43 | 1.38 |
| 24 | G | 205 | BCR | C14-C13 | 2.25 | 1.41 | 1.35 |
| 21 | 1 | 316 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | A | 831 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 24 | 4 | 617 | BCR | C10-C9 | 2.24 | 1.41 | 1.35 |
| 24 | J | 103 | BCR | C12-C13 | -2.24 | 1.41 | 1.46 |
| 21 | B | 830 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 21 | 9 | 613 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 24 | F | 303 | BCR | C19-C18 | -2.24 | 1.41 | 1.46 |
| 21 | B | 817 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 21 | 1 | 304 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 24 | L | 306 | BCR | C17-C18 | 2.24 | 1.41 | 1.35 |
| 21 | 2 | 613 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | K | 202 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 831 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 21 | F | 302 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | 2 | 603 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 32 | c | 618 | NEX | C12-C13 | -2.24 | 1.41 | 1.46 |
| 21 | 3 | 405 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 21 | B | 802 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | 8 | 610 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 31 | 5 | 616 | XAT | C10-C9 | 2.24 | 1.41 | 1.35 |
| 21 | B | 818 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 21 | O | 203 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 21 | 1 | 306 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 32 | b | 318 | NEX | C14-C13 | 2.24 | 1.41 | 1.35 |
| 24 | 3 | 419 | BCR | C12-C13 | -2.24 | 1.41 | 1.46 |
| 30 | 7 | 415 | LUT | C34-C33 | 2.24 | 1.41 | 1.35 |
| 21 | A | 821 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 21 | 5 | 603 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 21 | G | 204 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | B | 807 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 21 | A | 829 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | 6 | 609 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 21 | 7 | 408 | CLA | CHC-C1C | 2.24 | 1.43 | 1.38 |
| 31 | a | 618 | XAT | C10-C9 | 2.24 | 1.41 | 1.35 |
| 30 | 6 | 616 | LUT | C12-C13 | -2.24 | 1.41 | 1.46 |
| 24 | I | 101 | BCR | C21-C22 | 2.23 | 1.41 | 1.35 |
| 21 | B | 805 | CLA | MG-NB | -2.23 | 2.01 | 2.05 |
| 24 | B | 845 | BCR | C14-C13 | 2.23 | 1.41 | 1.35 |
| 30 | c | 616 | LUT | C34-C33 | 2.23 | 1.41 | 1.35 |
| 21 | 4 | 609 | CLA | C4D-CHA | 2.23 | 1.46 | 1.38 |
| 21 | b | 305 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | A | 808 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 21 | B | 812 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 21 | B | 840 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 21 | 5 | 608 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | a | 603 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | a | 611 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 24 | 7 | 418 | BCR | C12-C13 | -2.23 | 1.41 | 1.46 |
| 24 | B | 842 | BCR | C17-C18 | 2.23 | 1.41 | 1.35 |
| 21 | 3 | 406 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | A | 808 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 24 | G | 201 | BCR | C21-C22 | 2.23 | 1.41 | 1.35 |
| 21 | A | 810 | CLA | MG-NB | -2.23 | 2.01 | 2.05 |
| 21 | 1 | 303 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | c | 616 | LUT | C30-C29 | 2.23 | 1.41 | 1.35 |
| 21 | 2 | 611 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | 7 | 404 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 24 | J | 101 | BCR | C17-C18 | 2.23 | 1.41 | 1.35 |
| 21 | F | 305 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 24 | I | 101 | BCR | C12-C13 | -2.23 | 1.41 | 1.46 |
| 21 | B | 825 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 21 | B | 820 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | B | 831 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 31 | c | 617 | XAT | C10-C9 | 2.23 | 1.41 | 1.35 |
| 21 | 4 | 611 | CLA | CHC-C1C | 2.23 | 1.43 | 1.38 |
| 21 | B | 832 | CLA | CMB-C2B | -2.23 | 1.46 | 1.50 |
| 21 | A | 819 | CLA | MG-NB | -2.23 | 2.01 | 2.05 |
| 21 | 9 | 610 | CLA | MG-NB | -2.23 | 2.01 | 2.05 |
| 31 | 1 | 318 | XAT | C14-C13 | 2.23 | 1.41 | 1.35 |
| 21 | B | 811 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 21 | A | 806 | CLA | CHC-C1C | 2.23 | 1.42 | 1.38 |
| 21 | G | 202 | CLA | CHC-C1C | 2.23 | 1.42 | 1.38 |
| 24 | B | 845 | BCR | C10-C9 | 2.23 | 1.40 | 1.35 |
| 21 | A | 828 | CLA | MG-NB | -2.23 | 2.01 | 2.05 |
| 31 | 8 | 615 | XAT | C12-C13 | -2.23 | 1.41 | 1.46 |
| 30 | 9 | 615 | LUT | C14-C13 | 2.23 | 1.40 | 1.35 |
| 21 | 2 | 604 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 30 | 7 | 415 | LUT | C32-C33 | -2.23 | 1.41 | 1.46 |
| 31 | 3 | 417 | XAT | C34-C33 | 2.23 | 1.40 | 1.35 |
| 21 | F | 304 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | c | 610 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | B | 824 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | 1 | 314 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | A | 814 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 21 | 3 | 404 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | A | 812 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | 1 | 313 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | c | 614 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | A | 810 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 24 | A | 846 | BCR | C17-C18 | 2.22 | 1.40 | 1.35 |
| 21 | B | 818 | CLA | CMB-C2B | -2.22 | 1.46 | 1.50 |
| 21 | 1 | 303 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | A | 815 | CLA | MG-NB | -2.22 | 2.01 | 2.05 |
| 21 | B | 834 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 21 | 3 | 408 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | A | 842 | CLA | CMB-C2B | -2.22 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 838 | CLA | MG-NB | -2.22 | 2.01 | 2.05 |
| 21 | 1 | 310 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | B | 822 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 21 | 3 | 402 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | B | 821 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 21 | B | 822 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 30 | b | 317 | LUT | C14-C13 | 2.22 | 1.40 | 1.35 |
| 21 | A | 818 | CLA | MG-NB | -2.22 | 2.01 | 2.05 |
| 21 | A | 811 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 30 | 8 | 614 | LUT | C28-C29 | -2.22 | 1.41 | 1.46 |
| 21 | A | 804 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | 4 | 613 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | c | 603 | CLA | CHC-C1C | 2.22 | 1.42 | 1.38 |
| 21 | A | 832 | CLA | MG-NB | -2.22 | 2.01 | 2.05 |
| 21 | A | 806 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 21 | B | 823 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 31 | a | 618 | XAT | C28-C29 | -2.22 | 1.41 | 1.46 |
| 30 | c | 615 | LUT | C10-C9 | 2.21 | 1.40 | 1.35 |
| 31 | c | 617 | XAT | C34-C33 | 2.21 | 1.40 | 1.35 |
| 21 | 6 | 603 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 21 | c | 613 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 21 | B | 819 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 31 | 5 | 616 | XAT | C34-C33 | 2.21 | 1.40 | 1.35 |
| 24 | L | 306 | BCR | C19-C18 | -2.21 | 1.41 | 1.46 |
| 24 | 6 | 618 | BCR | C12-C13 | -2.21 | 1.41 | 1.46 |
| 30 | 5 | 615 | LUT | C28-C29 | -2.21 | 1.41 | 1.46 |
| 30 | b | 317 | LUT | C30-C29 | 2.21 | 1.40 | 1.35 |
| 21 | B | 814 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 29 | 5 | 601 | CHL | CBD-CGD | -2.21 | 1.49 | 1.52 |
| 21 | 5 | 612 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 31 | 7 | 416 | XAT | C28-C29 | -2.21 | 1.41 | 1.46 |
| 21 | A | 827 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 24 | O | 205 | BCR | C12-C13 | -2.21 | 1.41 | 1.46 |
| 21 | 3 | 414 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 24 | 3 | 418 | BCR | C10-C9 | 2.21 | 1.40 | 1.35 |
| 21 | A | 825 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 24 | G | 205 | BCR | C21-C22 | 2.21 | 1.40 | 1.35 |
| 21 | 1 | 311 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 21 | 4 | 610 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 30 | b | 316 | LUT | C12-C13 | -2.21 | 1.41 | 1.46 |
| 31 | c | 617 | XAT | C30-C29 | 2.21 | 1.40 | 1.35 |
| 21 | A | 827 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 803 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 24 | J | 103 | BCR | C19-C18 | -2.21 | 1.41 | 1.46 |
| 21 | O | 201 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 21 | c | 602 | CLA | CHC-C1C | 2.21 | 1.42 | 1.38 |
| 30 | 9 | 614 | LUT | C10-C9 | 2.21 | 1.40 | 1.35 |
| 24 | 2 | 618 | BCR | C19-C18 | -2.21 | 1.41 | 1.46 |
| 24 | G | 201 | BCR | C14-C13 | 2.20 | 1.40 | 1.35 |
| 21 | A | 838 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 32 | 9 | 617 | NEX | C12-C13 | -2.20 | 1.41 | 1.46 |
| 21 | B | 829 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 21 | L | 302 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 21 | A | 820 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 21 | 8 | 608 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 24 | L | 301 | BCR | C21-C22 | 2.20 | 1.40 | 1.35 |
| 21 | B | 806 | CLA | MG-NB | -2.20 | 2.01 | 2.05 |
| 21 | 9 | 604 | CLA | MG-NB | -2.20 | 2.01 | 2.05 |
| 21 | a | 614 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 30 | c | 616 | LUT | C10-C9 | 2.20 | 1.40 | 1.35 |
| 21 | B | 826 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 32 | 9 | 617 | NEX | C30-C29 | 2.20 | 1.40 | 1.35 |
| 24 | 7 | 417 | BCR | C19-C18 | -2.20 | 1.41 | 1.46 |
| 21 | A | 807 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 21 | A | 842 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 21 | A | 812 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 21 | G | 203 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 24 | A | 849 | BCR | C21-C22 | 2.20 | 1.40 | 1.35 |
| 24 | G | 201 | BCR | C17-C18 | 2.20 | 1.40 | 1.35 |
| 21 | 9 | 604 | CLA | CMB-C2B | -2.20 | 1.46 | 1.50 |
| 21 | 9 | 611 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 21 | J | 102 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 21 | 1 | 306 | CLA | MG-NB | -2.20 | 2.01 | 2.05 |
| 21 | 4 | 609 | CLA | C3D-C4D | -2.20 | 1.39 | 1.44 |
| 21 | 4 | 604 | CLA | CHC-C1C | 2.20 | 1.42 | 1.38 |
| 21 | B | 816 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 21 | 6 | 613 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 24 | B | 842 | BCR | C21-C22 | 2.20 | 1.40 | 1.35 |
| 21 | A | 840 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 24 | 3 | 419 | BCR | C19-C18 | -2.19 | 1.41 | 1.46 |
| 21 | 1 | 315 | CLA | CHC-C1C | 2.19 | 1.42 | 1.38 |
| 24 | A | 849 | BCR | C17-C18 | 2.19 | 1.40 | 1.35 |
| 21 | B | 813 | CLA | MG-NB | -2.19 | 2.01 | 2.05 |
| 24 | 2 | 618 | BCR | C17-C18 | 2.19 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 839 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 31 | 1 | 318 | XAT | C10-C9 | 2.19 | 1.40 | 1.35 |
| 21 | A | 820 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 21 | H | 201 | CLA | CMB-C2B | -2.19 | 1.46 | 1.50 |
| 21 | B | 821 | CLA | CHC-C1C | 2.19 | 1.42 | 1.38 |
| 21 | B | 817 | CLA | MG-NB | -2.19 | 2.01 | 2.05 |
| 21 | B | 805 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 21 | B | 814 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 21 | B | 832 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 30 | 8 | 614 | LUT | C10-C9 | 2.19 | 1.40 | 1.35 |
| 21 | A | 807 | CLA | MG-NB | -2.19 | 2.01 | 2.05 |
| 21 | A | 819 | CLA | CHC-C1C | 2.19 | 1.42 | 1.38 |
| 30 | 6 | 616 | LUT | C28-C29 | -2.19 | 1.41 | 1.46 |
| 21 | 2 | 610 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 21 | B | 835 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 21 | b | 304 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 21 | A | 824 | CLA | CHC-C1C | 2.19 | 1.42 | 1.38 |
| 21 | B | 812 | CLA | MG-NB | -2.19 | 2.01 | 2.05 |
| 24 | L | 305 | BCR | C17-C18 | 2.19 | 1.40 | 1.35 |
| 21 | G | 204 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 21 | b | 304 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 21 | A | 842 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 32 | c | 618 | NEX | C32-C33 | -2.19 | 1.41 | 1.46 |
| 24 | 3 | 418 | BCR | C17-C18 | 2.19 | 1.40 | 1.35 |
| 21 | c | 602 | CLA | MG-NB | -2.19 | 2.01 | 2.05 |
| 21 | A | 801 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | 1 | 304 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 21 | A | 821 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 31 | 1 | 318 | XAT | C34-C33 | 2.18 | 1.40 | 1.35 |
| 31 | 3 | 417 | XAT | C30-C29 | 2.18 | 1.40 | 1.35 |
| 21 | B | 836 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 21 | H | 201 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 21 | B | 823 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 21 | 2 | 610 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 21 | B | 834 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | B | 812 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 21 | b | 304 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 21 | 5 | 609 | CLA | CMB-C2B | -2.18 | 1.46 | 1.50 |
| 21 | A | 825 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 30 | 9 | 614 | LUT | C30-C29 | 2.18 | 1.40 | 1.35 |
| 24 | A | 850 | BCR | C14-C13 | 2.18 | 1.40 | 1.35 |
| 24 | L | 305 | BCR | C14-C13 | 2.18 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 813 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | B | 836 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | c | 602 | CLA | CMB-C2B | -2.18 | 1.46 | 1.50 |
| 21 | 7 | 407 | CLA | CHD-C1D | 2.18 | 1.42 | 1.38 |
| 21 | 5 | 605 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | A | 819 | CLA | CMB-C2B | -2.18 | 1.46 | 1.50 |
| 21 | B | 816 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 21 | 3 | 413 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | B | 839 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 21 | B | 806 | CLA | C3B-C4B | 2.18 | 1.49 | 1.42 |
| 21 | A | 808 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 24 | A | 846 | BCR | C10-C9 | 2.18 | 1.40 | 1.35 |
| 21 | B | 840 | CLA | MG-NB | -2.18 | 2.01 | 2.05 |
| 21 | 4 | 611 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 21 | A | 825 | CLA | CHC-C1C | 2.18 | 1.42 | 1.38 |
| 21 | A | 837 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 21 | A | 804 | CLA | C3B-C4B | 2.17 | 1.49 | 1.42 |
| 21 | 9 | 604 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 24 | 7 | 418 | BCR | C19-C18 | -2.17 | 1.41 | 1.46 |
| 21 | 3 | 401 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 21 | B | 810 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 21 | 4 | 601 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 24 | A | 850 | BCR | C10-C9 | 2.17 | 1.40 | 1.35 |
| 21 | A | 823 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 21 | B | 821 | CLA | CMB-C2B | -2.17 | 1.46 | 1.50 |
| 24 | 3 | 418 | BCR | C14-C13 | 2.17 | 1.40 | 1.35 |
| 31 | 3 | 417 | XAT | C14-C13 | 2.17 | 1.40 | 1.35 |
| 21 | A | 828 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 30 | b | 317 | LUT | C34-C33 | 2.17 | 1.40 | 1.35 |
| 31 | 9 | 616 | XAT | C28-C29 | -2.17 | 1.41 | 1.46 |
| 21 | 1 | 311 | CLA | MG-NB | -2.17 | 2.01 | 2.05 |
| 21 | B | 829 | CLA | CMB-C2B | -2.17 | 1.46 | 1.50 |
| 24 | O | 205 | BCR | C19-C18 | -2.17 | 1.41 | 1.46 |
| 21 | B | 818 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 21 | B | 834 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 31 | 1 | 318 | XAT | C30-C29 | 2.17 | 1.40 | 1.35 |
| 21 | L | 304 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 31 | 5 | 616 | XAT | C14-C13 | 2.17 | 1.40 | 1.35 |
| 21 | A | 812 | CLA | CMB-C2B | -2.17 | 1.46 | 1.50 |
| 31 | 8 | 615 | XAT | C28-C29 | -2.17 | 1.41 | 1.46 |
| 21 | 4 | 601 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 21 | A | 804 | CLA | MG-NB | -2.17 | 2.01 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 9 | 604 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 21 | B | 830 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 21 | 3 | 410 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 21 | B | 838 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 21 | 5 | 604 | CLA | CHC-C1C | 2.17 | 1.42 | 1.38 |
| 21 | A | 833 | CLA | CMB-C2B | -2.17 | 1.46 | 1.50 |
| 21 | B | 827 | CLA | CMB-C2B | -2.17 | 1.46 | 1.50 |
| 21 | A | 820 | CLA | MG-NB | -2.17 | 2.01 | 2.05 |
| 21 | A | 829 | CLA | MG-NB | -2.17 | 2.01 | 2.05 |
| 21 | 3 | 404 | CLA | MG-NB | -2.17 | 2.01 | 2.05 |
| 21 | A | 828 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | B | 818 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 21 | 9 | 612 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | c | 611 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | F | 304 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | K | 203 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 24 | A | 847 | BCR | C17-C18 | 2.16 | 1.40 | 1.35 |
| 31 | 2 | 617 | XAT | C14-C13 | 2.16 | 1.40 | 1.35 |
| 21 | 2 | 613 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 30 | 6 | 616 | LUT | C32-C33 | -2.16 | 1.41 | 1.46 |
| 21 | 9 | 604 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 21 | B | 819 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 21 | B | 821 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | 3 | 408 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | A | 801 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 24 | 8 | 616 | BCR | C12-C13 | -2.16 | 1.41 | 1.46 |
| 21 | 8 | 618 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | 5 | 602 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | L | 304 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 24 | B | 845 | BCR | C17-C18 | 2.16 | 1.40 | 1.35 |
| 21 | B | 828 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | L | 304 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 21 | A | 840 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | 6 | 603 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | A | 816 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | H | 201 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 31 | 4 | 616 | XAT | C10-C9 | 2.16 | 1.40 | 1.35 |
| 21 | G | 204 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 21 | B | 809 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | 4 | 612 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | L | 303 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | B | 808 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 9 | 603 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | K | 202 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | A | 824 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | A | 839 | CLA | CMB-C2B | -2.16 | 1.46 | 1.50 |
| 21 | B | 827 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | 5 | 603 | CLA | MG-NB | -2.16 | 2.01 | 2.05 |
| 21 | B | 822 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | B | 832 | CLA | CHC-C1C | 2.16 | 1.42 | 1.38 |
| 21 | A | 834 | CLA | C3B-C4B | 2.15 | 1.49 | 1.42 |
| 21 | A | 821 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 24 | A | 847 | BCR | C14-C13 | 2.15 | 1.40 | 1.35 |
| 24 | L | 305 | BCR | C10-C9 | 2.15 | 1.40 | 1.35 |
| 21 | A | 816 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | B | 835 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | O | 202 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | O | 203 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | A | 810 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | K | 204 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 24 | G | 205 | BCR | C10-C9 | 2.15 | 1.40 | 1.35 |
| 21 | A | 825 | CLA | C3B-C4B | 2.15 | 1.49 | 1.42 |
| 21 | 4 | 603 | CLA | CMB-C2B | -2.15 | 1.46 | 1.50 |
| 31 | 8 | 615 | XAT | C32-C33 | -2.15 | 1.41 | 1.46 |
| 21 | 4 | 601 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | 9 | 612 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | A | 813 | CLA | C3B-C4B | 2.15 | 1.49 | 1.42 |
| 24 | L | 305 | BCR | C21-C22 | 2.15 | 1.40 | 1.35 |
| 21 | A | 842 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 21 | 9 | 602 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | c | 613 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | A | 835 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | c | 613 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | B | 822 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | K | 202 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | B | 833 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | 9 | 602 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 21 | B | 813 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | 3 | 405 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | B | 830 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | A | 811 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | A | 842 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | A | 802 | CLA | CMB-C2B | -2.15 | 1.46 | 1.50 |
| 21 | A | 831 | CLA | CMB-C2B | -2.15 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 312 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | 3 | 413 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | A | 822 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | B | 825 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 21 | O | 203 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | A | 852 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | b | 313 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | 2 | 603 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | 7 | 403 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | 9 | 602 | CLA | CMB-C2B | -2.15 | 1.46 | 1.50 |
| 21 | a | 602 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 21 | B | 834 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | B | 837 | CLA | MG-NB | -2.15 | 2.01 | 2.05 |
| 21 | B | 827 | CLA | C3B-C4B | 2.15 | 1.49 | 1.42 |
| 24 | A | 847 | BCR | C21-C22 | 2.15 | 1.40 | 1.35 |
| 21 | A | 822 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 24 | A | 854 | BCR | C17-C18 | 2.15 | 1.40 | 1.35 |
| 31 | 2 | 617 | XAT | C10-C9 | 2.15 | 1.40 | 1.35 |
| 21 | 7 | 402 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 21 | B | 840 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 30 | 9 | 615 | LUT | C10-C9 | 2.15 | 1.40 | 1.35 |
| 21 | B | 835 | CLA | CHC-C1C | 2.15 | 1.42 | 1.38 |
| 24 | B | 845 | BCR | C21-C22 | 2.15 | 1.40 | 1.35 |
| 21 | B | 818 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | A | 842 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | A | 809 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | 4 | 602 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 31 | 4 | 616 | XAT | C30-C29 | 2.14 | 1.40 | 1.35 |
| 24 | 7 | 417 | BCR | C12-C13 | -2.14 | 1.41 | 1.46 |
| 31 | 4 | 616 | XAT | C14-C13 | 2.14 | 1.40 | 1.35 |
| 21 | B | 826 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | B | 838 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | B | 840 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | F | 305 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | B | 826 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | B | 828 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | a | 610 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | 5 | 610 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | B | 809 | CLA | CMB-C2B | -2.14 | 1.46 | 1.50 |
| 21 | 2 | 610 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 21 | B | 808 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | 3 | 412 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 414 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 31 | 2 | 617 | XAT | C34-C33 | 2.14 | 1.40 | 1.35 |
| 21 | 5 | 609 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | 8 | 604 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | c | 610 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 24 | G | 201 | BCR | C10-C9 | 2.14 | 1.40 | 1.35 |
| 24 | J | 101 | BCR | C10-C9 | 2.14 | 1.40 | 1.35 |
| 21 | B | 829 | CLA | C3B-C4B | 2.14 | 1.49 | 1.42 |
| 21 | 3 | 402 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 21 | O | 204 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 21 | 9 | 603 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | 1 | 314 | CLA | CMB-C2B | -2.14 | 1.46 | 1.50 |
| 21 | 2 | 603 | CLA | CMB-C2B | -2.14 | 1.46 | 1.50 |
| 21 | 7 | 413 | CLA | CBD-CAD | 2.14 | 1.56 | 1.51 |
| 21 | O | 201 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | 4 | 603 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 21 | A | 839 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | A | 809 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 21 | A | 803 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | 4 | 610 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | B | 811 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | A | 803 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | B | 825 | CLA | CHC-C1C | 2.14 | 1.42 | 1.38 |
| 21 | K | 203 | CLA | MG-NB | -2.14 | 2.01 | 2.05 |
| 21 | 3 | 401 | CLA | C3B-C4B | 2.14 | 1.49 | 1.42 |
| 21 | L | 302 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 21 | B | 817 | CLA | CMB-C2B | -2.14 | 1.46 | 1.50 |
| 21 | B | 824 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 3 | 415 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | A | 812 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 21 | 4 | 613 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 21 | 9 | 613 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 24 | L | 301 | BCR | C14-C13 | 2.13 | 1.40 | 1.35 |
| 21 | 9 | 613 | CLA | CHC-C1C | 2.13 | 1.42 | 1.38 |
| 21 | 1 | 313 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 24 | A | 850 | BCR | C17-C18 | 2.13 | 1.40 | 1.35 |
| 21 | K | 203 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 30 | 7 | 415 | LUT | C14-C13 | 2.13 | 1.40 | 1.35 |
| 21 | 3 | 405 | CLA | C3B-C4B | 2.13 | 1.49 | 1.42 |
| 21 | L | 303 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 21 | 4 | 601 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 30 | b | 317 | LUT | C10-C9 | 2.13 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 812 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 9 | 610 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | c | 602 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 32 | c | 618 | NEX | C28-C29 | -2.13 | 1.41 | 1.46 |
| 21 | 3 | 412 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 6 | 609 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | 5 | 603 | CLA | CHC-C1C | 2.13 | 1.42 | 1.38 |
| 21 | A | 806 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 4 | 612 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | 4 | 608 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 21 | 4 | 608 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 24 | M | 101 | BCR | C19-C18 | -2.13 | 1.41 | 1.46 |
| 21 | A | 804 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | A | 820 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | 9 | 611 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | A | 831 | CLA | CHC-C1C | 2.13 | 1.42 | 1.38 |
| 21 | B | 837 | CLA | CHC-C1C | 2.13 | 1.42 | 1.38 |
| 21 | 2 | 609 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 21 | A | 817 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | B | 815 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | B | 817 | CLA | CHC-C1C | 2.13 | 1.42 | 1.38 |
| 21 | A | 818 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | 2 | 612 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 3 | 410 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | 3 | 414 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | c | 614 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 31 | 5 | 616 | XAT | C30-C29 | 2.13 | 1.40 | 1.35 |
| 21 | B | 816 | CLA | CHC-C1C | 2.13 | 1.42 | 1.38 |
| 24 | A | 849 | BCR | C14-C13 | 2.13 | 1.40 | 1.35 |
| 21 | A | 802 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 21 | A | 806 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 21 | B | 836 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | a | 613 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 21 | B | 826 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 1 | 310 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 21 | B | 819 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | K | 203 | CLA | CMB-C2B | -2.13 | 1.46 | 1.50 |
| 21 | 4 | 604 | CLA | MG-NB | -2.13 | 2.01 | 2.05 |
| 24 | L | 301 | BCR | C17-C18 | 2.12 | 1.40 | 1.35 |
| 21 | 3 | 401 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | B | 825 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | c | 603 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 805 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | c | 612 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | B | 824 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 24 | 8 | 616 | BCR | C19-C18 | -2.12 | 1.41 | 1.46 |
| 21 | A | 830 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 21 | A | 841 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | b | 313 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | J | 102 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 3 | 406 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | A | 807 | CLA | CHC-C1C | 2.12 | 1.42 | 1.38 |
| 21 | 3 | 403 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | A | 841 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 7 | 401 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | B | 830 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | B | 804 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | F | 302 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | B | 823 | CLA | CHC-C1C | 2.12 | 1.42 | 1.38 |
| 21 | 3 | 411 | CLA | CHC-C1C | 2.12 | 1.42 | 1.38 |
| 21 | 7 | 402 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | c | 604 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 1 | 303 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | 6 | 608 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | 3 | 406 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | 3 | 411 | CLA | CMB-C2B | -2.12 | 1.46 | 1.50 |
| 21 | B | 838 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | A | 811 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | B | 823 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | 3 | 401 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | A | 803 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | B | 810 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 4 | 610 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | b | 303 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | B | 827 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | A | 810 | CLA | C3B-C4B | 2.12 | 1.48 | 1.42 |
| 21 | F | 305 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 1 | 304 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 1 | 312 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 21 | 3 | 403 | CLA | MG-NB | -2.12 | 2.01 | 2.05 |
| 21 | B | 806 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | F | 302 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 21 | K | 201 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | 3 | 406 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 805 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 24 | A | 854 | BCR | C10-C9 | 2.11 | 1.40 | 1.35 |
| 21 | B | 819 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 21 | c | 603 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | A | 808 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | A | 834 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 21 | B | 820 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 31 | 4 | 616 | XAT | C34-C33 | 2.11 | 1.40 | 1.35 |
| 21 | A | 833 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 21 | J | 102 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 31 | 2 | 617 | XAT | C30-C29 | 2.11 | 1.40 | 1.35 |
| 21 | A | 836 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | 7 | 401 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | A | 838 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 21 | 5 | 610 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | 1 | 313 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | B | 807 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 21 | A | 802 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | A | 803 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 21 | B | 804 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | 4 | 613 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 21 | 9 | 610 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | B | 814 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 21 | B | 832 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 21 | 1 | 303 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | c | 614 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 24 | F | 303 | BCR | C10-C9 | 2.11 | 1.40 | 1.35 |
| 21 | B | 825 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | 1 | 304 | CLA | CHC-C1C | 2.11 | 1.42 | 1.38 |
| 21 | A | 821 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | A | 813 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | A | 834 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | O | 201 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 21 | B | 833 | CLA | CMB-C2B | -2.11 | 1.46 | 1.50 |
| 21 | O | 201 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | 4 | 602 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | B | 837 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | B | 807 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | K | 204 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 21 | 5 | 609 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 21 | A | 815 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 8 | 608 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 802 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | K | 202 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 1 | 310 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 1 | 305 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | 3 | 405 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | A | 828 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 5 | 603 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 8 | 604 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | F | 305 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | A | 814 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |
| 21 | K | 203 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |
| 21 | O | 202 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | c | 602 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 21 | 2 | 608 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | b | 313 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | B | 809 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | 3 | 414 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 5 | 603 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 9 | 611 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | A | 841 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |
| 21 | A | 810 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 3 | 415 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | 8 | 609 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |
| 24 | A | 848 | BCR | C14-C13 | 2.10 | 1.40 | 1.35 |
| 21 | A | 824 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | A | 832 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 1 | 310 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 3 | 411 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | c | 611 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | B | 810 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | c | 604 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | B | 809 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |
| 21 | O | 201 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 7 | 402 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 8 | 608 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | A | 839 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | B | 823 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 2 | 604 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 4 | 612 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | b | 303 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | 1 | 316 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 2 | 612 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 309 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 21 | 1 | 308 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | K | 201 | CLA | CHC-C1C | 2.10 | 1.42 | 1.38 |
| 21 | B | 836 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | 1 | 315 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | A | 817 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | B | 819 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 2 | 611 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 5 | 605 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | A | 834 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 2 | 603 | CLA | MG-NB | -2.10 | 2.01 | 2.05 |
| 21 | A | 838 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 3 | 412 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | A | 807 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | B | 805 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | 2 | 612 | CLA | CMB-C2B | -2.10 | 1.46 | 1.50 |
| 21 | b | 305 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 21 | 8 | 609 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 21 | A | 837 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | B | 810 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | 2 | 613 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | B | 828 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 24 | F | 301 | BCR | C21-C22 | 2.09 | 1.40 | 1.35 |
| 24 | K | 205 | BCR | C30-C25 | -2.09 | 1.51 | 1.53 |
| 21 | A | 805 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | 3 | 409 | CLA | MG-ND | -2.09 | 2.01 | 2.05 |
| 21 | A | 840 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | B | 831 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | F | 304 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | a | 610 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | 3 | 403 | CLA | CHC-C1C | 2.09 | 1.42 | 1.38 |
| 21 | A | 840 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | F | 302 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | B | 822 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | 9 | 612 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | b | 305 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | 9 | 611 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 24 | L | 301 | BCR | C10-C9 | 2.09 | 1.40 | 1.35 |
| 21 | B | 837 | CLA | C3B-C4B | 2.09 | 1.48 | 1.42 |
| 21 | 4 | 609 | CLA | MG-ND | -2.09 | 2.01 | 2.05 |
| 21 | L | 302 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 31 | 8 | 615 | XAT | C8-C9 | -2.09 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 831 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 24 | A | 854 | BCR | C14-C13 | 2.09 | 1.40 | 1.35 |
| 21 | A | 816 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | O | 203 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | 1 | 311 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | A | 833 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | 1 | 308 | CLA | CHC-C1C | 2.09 | 1.42 | 1.38 |
| 21 | 7 | 414 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | c | 611 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | B | 812 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 31 | 9 | 616 | XAT | C8-C9 | -2.09 | 1.41 | 1.46 |
| 21 | B | 833 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | b | 311 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | A | 826 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | 1 | 308 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | B | 806 | CLA | CHC-C1C | 2.09 | 1.42 | 1.38 |
| 21 | 8 | 603 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | a | 604 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 21 | 8 | 603 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | B | 816 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 21 | B | 836 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | 1 | 314 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | 2 | 613 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | 3 | 410 | CLA | MG-NB | -2.09 | 2.01 | 2.05 |
| 31 | 3 | 417 | XAT | C10-C9 | 2.09 | 1.40 | 1.35 |
| 21 | B | 838 | CLA | CMB-C2B | -2.09 | 1.46 | 1.50 |
| 21 | G | 202 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 21 | 6 | 613 | CLA | MG-NB | -2.08 | 2.01 | 2.05 |
| 24 | A | 848 | BCR | C21-C22 | 2.08 | 1.40 | 1.35 |
| 24 | A | 854 | BCR | C21-C22 | 2.08 | 1.40 | 1.35 |
| 21 | L | 302 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | 8 | 618 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 817 | CLA | C3B-C4B | 2.08 | 1.48 | 1.42 |
| 21 | B | 825 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | b | 314 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 21 | K | 201 | CLA | MG-NB | -2.08 | 2.01 | 2.05 |
| 21 | 3 | 403 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | 7 | 404 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 805 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | B | 803 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | 9 | 603 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | H | 201 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 611 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 840 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | 1 | 315 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | A | 817 | CLA | MG-NB | -2.08 | 2.01 | 2.05 |
| 24 | F | 301 | BCR | C17-C18 | 2.08 | 1.40 | 1.35 |
| 21 | 2 | 604 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 813 | CLA | CHC-C1C | 2.08 | 1.42 | 1.38 |
| 21 | B | 811 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 21 | A | 823 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | B | 832 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | a | 604 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | 1 | 312 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | b | 315 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | 1 | 305 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | 7 | 404 | CLA | MG-NB | -2.08 | 2.01 | 2.05 |
| 21 | A | 812 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 814 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 822 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | 4 | 613 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | A | 826 | CLA | MG-NB | -2.08 | 2.01 | 2.05 |
| 21 | A | 825 | CLA | CMB-C2B | -2.08 | 1.46 | 1.50 |
| 21 | B | 811 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 21 | B | 802 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | B | 817 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 21 | b | 314 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | a | 614 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | B | 801 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | B | 817 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | J | 102 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | B | 811 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | A | 839 | CLA | CHC-C1C | 2.07 | 1.42 | 1.38 |
| 21 | a | 603 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | A | 830 | CLA | CHC-C1C | 2.07 | 1.42 | 1.38 |
| 21 | A | 836 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | 6 | 609 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | A | 823 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 21 | B | 826 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | K | 204 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | 3 | 404 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | 1 | 315 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | b | 304 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 24 | A | 849 | BCR | C10-C9 | 2.07 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 408 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | 3 | 412 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | 6 | 609 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | b | 305 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | A | 852 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 21 | B | 815 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | 3 | 405 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | 8 | 608 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | A | 827 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | G | 203 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | 1 | 316 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 21 | 3 | 411 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | A | 834 | CLA | CHC-C1C | 2.07 | 1.42 | 1.38 |
| 21 | c | 614 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | b | 313 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | 2 | 608 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | B | 807 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 21 | 8 | 611 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | A | 806 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | A | 811 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | A | 813 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | G | 203 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | 4 | 604 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 24 | M | 101 | BCR | C12-C13 | -2.07 | 1.41 | 1.46 |
| 21 | a | 603 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | B | 814 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | A | 819 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | 8 | 610 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | b | 311 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | c | 611 | CLA | CMB-C2B | -2.07 | 1.46 | 1.50 |
| 21 | 2 | 611 | CLA | MG-NB | -2.07 | 2.01 | 2.05 |
| 21 | B | 815 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 21 | 3 | 413 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 21 | a | 614 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 21 | A | 821 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | B | 830 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | A | 836 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | B | 824 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | K | 204 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | 1 | 313 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | 6 | 610 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | A | 807 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 304 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | A | 837 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | B | 839 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | B | 820 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | 7 | 403 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | F | 305 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | L | 304 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | 1 | 306 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 21 | 8 | 618 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 21 | O | 202 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | A | 841 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 1 | 308 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 24 | A | 850 | BCR | C21-C22 | 2.06 | 1.40 | 1.35 |
| 21 | B | 818 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 21 | A | 813 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 1 | 314 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 4 | 603 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 5 | 602 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 2 | 610 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | 9 | 613 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | c | 604 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 21 | 1 | 303 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | 3 | 402 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | A | 852 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 7 | 413 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 5 | 612 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | B | 819 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 21 | 7 | 405 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 3 | 405 | CLA | CHC-C1C | 2.06 | 1.42 | 1.38 |
| 21 | 1 | 305 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 21 | 5 | 605 | CLA | CMB-C2B | -2.06 | 1.46 | 1.50 |
| 21 | b | 314 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 1 | 316 | CLA | MG-NB | -2.06 | 2.01 | 2.05 |
| 21 | 7 | 414 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 21 | B | 803 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 21 | A | 805 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | A | 809 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | B | 814 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | B | 828 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | 6 | 610 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | 5 | 613 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | B | 806 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 8 | 602 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | 7 | 411 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | A | 814 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | B | 808 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | F | 305 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | a | 614 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | A | 841 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | A | 814 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | A | 833 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | 7 | 405 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | a | 602 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | B | 803 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | 3 | 411 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | A | 831 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | A | 827 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | 5 | 607 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | 5 | 612 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 29 | 2 | 606 | CHL | CBD-CGD | -2.05 | 1.49 | 1.52 |
| 21 | A | 832 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | 2 | 608 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | a | 612 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | 4 | 611 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | 5 | 608 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | B | 832 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | B | 840 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | 5 | 604 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | 8 | 604 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | a | 613 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | b | 311 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | A | 816 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | A | 819 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | B | 806 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | B | 834 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | K | 201 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | A | 823 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | 7 | 403 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | b | 313 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | B | 831 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 21 | K | 202 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | 1 | 311 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | 5 | 611 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | 1 | 312 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 9 | 613 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 21 | c | 610 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | 8 | 610 | CLA | MG-NB | -2.05 | 2.01 | 2.05 |
| 21 | A | 852 | CLA | CMB-C2B | -2.05 | 1.46 | 1.50 |
| 21 | a | 611 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 21 | 1 | 306 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | c | 612 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 4 | 602 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 7 | 412 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | 1 | 309 | CLA | CHC-C1C | 2.04 | 1.42 | 1.38 |
| 21 | 5 | 614 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | b | 315 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | O | 203 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | A | 806 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 21 | A | 829 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | L | 303 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 3 | 412 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | a | 613 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 31 | 9 | 616 | XAT | C32-C33 | -2.04 | 1.41 | 1.46 |
| 21 | 8 | 612 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | 3 | 402 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 21 | 3 | 413 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 6 | 608 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 8 | 611 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | 6 | 604 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 21 | 3 | 415 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 6 | 610 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | A | 808 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | B | 840 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 5 | 608 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | B | 805 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | B | 814 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | L | 303 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | c | 613 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 3 | 401 | CLA | CHC-C1C | 2.04 | 1.42 | 1.38 |
| 21 | 4 | 611 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 31 | 9 | 616 | XAT | C12-C13 | -2.04 | 1.41 | 1.46 |
| 21 | 8 | 611 | CLA | CMB-C2B | -2.04 | 1.46 | 1.50 |
| 21 | 2 | 610 | CLA | CHC-C1C | 2.04 | 1.42 | 1.38 |
| 21 | 3 | 410 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | c | 610 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | B | 803 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 2 | 611 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | c | 614 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | 5 | 605 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 21 | A | 840 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | O | 201 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 24 | F | 301 | BCR | C10-C9 | 2.04 | 1.40 | 1.35 |
| 21 | B | 835 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 21 | 5 | 608 | CLA | MG-NB | -2.04 | 2.01 | 2.05 |
| 21 | 4 | 608 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 5 | 607 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | B | 827 | CLA | CHC-C1C | 2.03 | 1.42 | 1.38 |
| 21 | A | 822 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | B | 837 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 7 | 410 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | c | 603 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | a | 602 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | 3 | 413 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | b | 304 | CLA | CHC-C1C | 2.03 | 1.42 | 1.38 |
| 21 | A | 815 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | A | 831 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | H | 201 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | b | 303 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 8 | 601 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | A | 804 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 6 | 608 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | a | 613 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | 8 | 603 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | b | 303 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | 7 | 409 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | a | 612 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | a | 612 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 3 | 414 | CLA | CBD-CAD | 2.03 | 1.56 | 1.51 |
| 21 | A | 815 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | A | 827 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | G | 204 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | a | 611 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | B | 829 | CLA | CHC-C1C | 2.03 | 1.42 | 1.38 |
| 21 | c | 603 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 24 | A | 847 | BCR | C10-C9 | 2.03 | 1.40 | 1.35 |
| 21 | B | 801 | CLA | C3B-C2B | 2.03 | 1.48 | 1.41 |
| 21 | 2 | 603 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | 7 | 405 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 7 | 408 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | B | 809 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | 6 | 611 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | 7 | 411 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 2 | 609 | CLA | CHC-C1C | 2.03 | 1.42 | 1.38 |
| 21 | 6 | 611 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | A | 816 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | G | 202 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | a | 610 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | A | 808 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 1 | 316 | CLA | CMB-C2B | -2.03 | 1.46 | 1.50 |
| 21 | 8 | 612 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 21 | 7 | 413 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | b | 312 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | 5 | 612 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 21 | 5 | 613 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 24 | F | 301 | BCR | C14-C13 | 2.03 | 1.40 | 1.35 |
| 21 | 5 | 614 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | A | 826 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | A | 836 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | B | 804 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | A | 820 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 6 | 612 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 21 | 6 | 613 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | 5 | 610 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 24 | A | 848 | BCR | C10-C9 | 2.02 | 1.40 | 1.35 |
| 21 | A | 833 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 7 | 412 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | A | 822 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | c | 612 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | A | 838 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | 8 | 602 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 21 | c | 612 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | A | 824 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | 3 | 408 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 8 | 601 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | A | 827 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | B | 835 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | 9 | 610 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 7 | 407 | CLA | C3D-C2D | 2.02 | 1.44 | 1.39 |
| 21 | 7 | 408 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 31 | 6 | 617 | XAT | C12-C13 | -2.02 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | b | 314 | CLA | CMB-C2B | -2.02 | 1.46 | 1.50 |
| 21 | A | 805 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | A | 835 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 7 | 410 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | 4 | 603 | CLA | CHC-C1C | 2.02 | 1.42 | 1.38 |
| 31 | 6 | 617 | XAT | C8-C9 | -2.02 | 1.41 | 1.46 |
| 21 | G | 203 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | A | 824 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | K | 204 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 4 | 603 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 21 | 7 | 411 | CLA | MG-NB | -2.02 | 2.01 | 2.05 |
| 21 | c | 613 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | A | 832 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | G | 204 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 21 | B | 815 | CLA | MG-NB | -2.01 | 2.01 | 2.05 |
| 21 | J | 102 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | A | 817 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | A | 821 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | A | 829 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | O | 203 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | 2 | 608 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | 1 | 312 | CLA | MG-NB | -2.01 | 2.01 | 2.05 |
| 21 | 4 | 604 | CLA | CMB-C2B | -2.01 | 1.46 | 1.50 |
| 21 | 5 | 614 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 21 | 7 | 409 | CLA | CMB-C2B | -2.01 | 1.46 | 1.50 |
| 21 | 6 | 604 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 21 | 7 | 409 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 21 | 8 | 610 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | G | 202 | CLA | MG-NB | -2.01 | 2.01 | 2.05 |
| 21 | 5 | 604 | CLA | MG-NB | -2.01 | 2.01 | 2.05 |
| 29 | b | 309 | CHL | CBD-CGD | -2.01 | 1.50 | 1.52 |
| 21 | b | 315 | CLA | MG-NB | -2.01 | 2.01 | 2.05 |
| 21 | A | 807 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | c | 604 | CLA | CMB-C2B | -2.01 | 1.46 | 1.50 |
| 21 | 6 | 612 | CLA | CMB-C2B | -2.01 | 1.46 | 1.50 |
| 21 | 6 | 604 | CLA | CMB-C2B | -2.01 | 1.46 | 1.50 |
| 21 | B | 839 | CLA | CHC-C1C | 2.01 | 1.42 | 1.38 |
| 21 | B | 827 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | 1 | 303 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | A | 817 | CLA | CHC-C1C | 2.01 | 1.42 | 1.38 |
| 21 | A | 826 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 21 | 6 | 611 | CLA | CMB-C2B | -2.01 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 828 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | A | 813 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 5 | 604 | CLA | CMB-C2B | -2.00 | 1.46 | 1.50 |
| 21 | A | 804 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 1 | 311 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 4 | 611 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 5 | 611 | CLA | CMB-C2B | -2.00 | 1.46 | 1.50 |
| 24 | A | 848 | BCR | C17-C18 | 2.00 | 1.40 | 1.35 |
| 21 | B | 834 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 1 | 308 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 3 | 403 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 21 | 4 | 610 | CLA | CMB-C2B | -2.00 | 1.46 | 1.50 |
| 21 | 5 | 602 | CLA | CMB-C2B | -2.00 | 1.46 | 1.50 |

All (2790) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 7 | 407 | CLA | CAC-C3C-C4C | 16.77 | 146.62 | 124.79 |
| 29 | a | 601 | CHL | C4D-ND-C1D | 10.89 | 113.49 | 105.22 |
| 29 | 9 | 601 | CHL | C4D-ND-C1D | 10.87 | 113.47 | 105.22 |
| 29 | c | 609 | CHL | C4D-ND-C1D | 10.83 | 113.44 | 105.22 |
| 29 | a | 609 | CHL | C4D-ND-C1D | 10.80 | 113.41 | 105.22 |
| 29 | a | 605 | CHL | C4D-ND-C1D | 10.78 | 113.40 | 105.22 |
| 21 | 7 | 407 | CLA | C1D-ND-C4D | -10.78 | 98.75 | 106.31 |
| 29 | 7 | 406 | CHL | C4D-ND-C1D | 10.70 | 113.34 | 105.22 |
| 29 | c | 607 | CHL | C4D-ND-C1D | 10.64 | 113.29 | 105.22 |
| 29 | b | 302 | CHL | C4D-ND-C1D | 10.61 | 113.27 | 105.22 |
| 29 | c | 605 | CHL | C4D-ND-C1D | 10.60 | 113.27 | 105.22 |
| 29 | a | 606 | CHL | C1B-CHB-C4A | -10.55 | 114.53 | 121.32 |
| 29 | 8 | 606 | CHL | C4D-ND-C1D | 10.48 | 113.17 | 105.22 |
| 29 | 6 | 607 | CHL | C4D-ND-C1D | 10.38 | 113.10 | 105.22 |
| 29 | 9 | 607 | CHL | C4D-ND-C1D | 10.38 | 113.10 | 105.22 |
| 29 | c | 608 | CHL | C4D-ND-C1D | 10.37 | 113.09 | 105.22 |
| 29 | 6 | 601 | CHL | C4D-ND-C1D | 10.33 | 113.06 | 105.22 |
| 29 | b | 308 | CHL | C4D-ND-C1D | 10.14 | 112.92 | 105.22 |
| 29 | 6 | 614 | CHL | C4D-ND-C1D | 10.11 | 112.89 | 105.22 |
| 29 | b | 310 | CHL | C4D-ND-C1D | 10.11 | 112.89 | 105.22 |
| 29 | 9 | 609 | CHL | C4D-ND-C1D | 10.09 | 112.88 | 105.22 |
| 29 | 5 | 606 | CHL | C4D-ND-C1D | 10.08 | 112.87 | 105.22 |
| 29 | 6 | 601 | CHL | O2D-CGD-CBD | 10.08 | 122.02 | 110.95 |
| 29 | 1 | 302 | CHL | C4D-ND-C1D | 10.07 | 112.86 | 105.22 |
| 29 | b | 306 | CHL | C4D-ND-C1D | 10.06 | 112.86 | 105.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 9 | 605 | CHL | C4D-ND-C1D | 10.05 | 112.84 | 105.22 |
| 29 | 8 | 613 | CHL | C4D-ND-C1D | 9.99 | 112.80 | 105.22 |
| 29 | c | 601 | CHL | C4D-ND-C1D | 9.99 | 112.80 | 105.22 |
| 29 | c | 606 | CHL | C4D-ND-C1D | 9.97 | 112.79 | 105.22 |
| 29 | a | 607 | CHL | C4D-ND-C1D | 9.95 | 112.77 | 105.22 |
| 29 | 1 | 302 | CHL | O2D-CGD-CBD | 9.93 | 121.86 | 110.95 |
| 29 | 2 | 607 | CHL | C4D-ND-C1D | 9.93 | 112.75 | 105.22 |
| 29 | 2 | 605 | CHL | C4D-ND-C1D | 9.92 | 112.75 | 105.22 |
| 29 | 8 | 607 | CHL | C4D-ND-C1D | 9.92 | 112.75 | 105.22 |
| 29 | 9 | 608 | CHL | C4D-ND-C1D | 9.91 | 112.74 | 105.22 |
| 29 | a | 606 | CHL | C4D-ND-C1D | 9.90 | 112.73 | 105.22 |
| 29 | 1 | 307 | CHL | C4D-ND-C1D | 9.89 | 112.72 | 105.22 |
| 29 | 2 | 614 | CHL | C4D-ND-C1D | 9.87 | 112.71 | 105.22 |
| 29 | 6 | 602 | CHL | C4D-ND-C1D | 9.86 | 112.70 | 105.22 |
| 29 | 9 | 606 | CHL | C4D-ND-C1D | 9.83 | 112.68 | 105.22 |
| 29 | 4 | 606 | CHL | C4D-ND-C1D | 9.82 | 112.67 | 105.22 |
| 29 | 4 | 614 | CHL | C4D-ND-C1D | 9.75 | 112.62 | 105.22 |
| 29 | b | 307 | CHL | C4D-ND-C1D | 9.75 | 112.61 | 105.22 |
| 29 | a | 601 | CHL | O2D-CGD-CBD | 9.72 | 121.63 | 110.95 |
| 29 | 6 | 606 | CHL | C4D-ND-C1D | 9.72 | 112.60 | 105.22 |
| 29 | 2 | 601 | CHL | C4D-ND-C1D | 9.71 | 112.59 | 105.22 |
| 29 | b | 309 | CHL | C4D-ND-C1D | 9.71 | 112.59 | 105.22 |
| 29 | 3 | 407 | CHL | C4D-ND-C1D | 9.68 | 112.56 | 105.22 |
| 29 | a | 608 | CHL | C4D-ND-C1D | 9.65 | 112.54 | 105.22 |
| 29 | 5 | 601 | CHL | C4D-ND-C1D | 9.63 | 112.53 | 105.22 |
| 29 | a | 609 | CHL | C1B-CHB-C4A | -9.63 | 115.13 | 121.32 |
| 29 | b | 302 | CHL | C1B-CHB-C4A | -9.62 | 115.13 | 121.32 |
| 29 | 4 | 605 | CHL | C4D-ND-C1D | 9.61 | 112.52 | 105.22 |
| 29 | 2 | 606 | CHL | C4D-ND-C1D | 9.60 | 112.51 | 105.22 |
| 29 | 2 | 602 | CHL | C4D-ND-C1D | 9.59 | 112.49 | 105.22 |
| 29 | 4 | 607 | CHL | C4D-ND-C1D | 9.58 | 112.49 | 105.22 |
| 29 | 6 | 605 | CHL | C4D-ND-C1D | 9.53 | 112.45 | 105.22 |
| 29 | 8 | 605 | CHL | C4D-ND-C1D | 9.41 | 112.36 | 105.22 |
| 21 | B | 801 | CLA | C1D-ND-C4D | -9.39 | 99.72 | 106.31 |
| 29 | a | 605 | CHL | C1B-CHB-C4A | -9.33 | 115.32 | 121.32 |
| 29 | a | 606 | CHL | O2D-CGD-CBD | 9.33 | 121.19 | 110.95 |
| 29 | a | 607 | CHL | O2D-CGD-CBD | 9.25 | 121.11 | 110.95 |
| 29 | a | 601 | CHL | C1B-CHB-C4A | -9.23 | 115.39 | 121.32 |
| 21 | 7 | 407 | CLA | CAC-C3C-C2C | -9.17 | 110.71 | 127.56 |
| 29 | b | 307 | CHL | C1C-C2C-CMC | 9.14 | 143.28 | 126.80 |
| 29 | 2 | 606 | CHL | O2D-CGD-CBD | 9.08 | 120.93 | 110.95 |
| 29 | 2 | 601 | CHL | O2D-CGD-CBD | 9.06 | 120.90 | 110.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 5 | 601 | CHL | O2D-CGD-CBD | 8.98 | 120.82 | 110.95 |
| 29 | 1 | 307 | CHL | O2D-CGD-CBD | 8.97 | 120.80 | 110.95 |
| 24 | B | 843 | BCR | C24-C23-C22 | -8.97 | 112.97 | 126.23 |
| 29 | c | 609 | CHL | C1C-C2C-CMC | 8.96 | 142.96 | 126.80 |
| 29 | 4 | 605 | CHL | O2D-CGD-CBD | 8.86 | 120.68 | 110.95 |
| 29 | 6 | 602 | CHL | O2D-CGD-CBD | 8.84 | 120.66 | 110.95 |
| 29 | 9 | 605 | CHL | O2D-CGD-CBD | 8.73 | 120.54 | 110.95 |
| 29 | c | 607 | CHL | O2D-CGD-CBD | 8.73 | 120.54 | 110.95 |
| 29 | c | 605 | CHL | C1B-CHB-C4A | -8.71 | 115.72 | 121.32 |
| 29 | 2 | 605 | CHL | C1C-C2C-CMC | 8.71 | 142.50 | 126.80 |
| 29 | 4 | 607 | CHL | C1C-C2C-CMC | 8.68 | 142.45 | 126.80 |
| 29 | 2 | 605 | CHL | O2D-CGD-CBD | 8.64 | 120.44 | 110.95 |
| 29 | 9 | 606 | CHL | O2D-CGD-CBD | 8.55 | 120.34 | 110.95 |
| 29 | 8 | 605 | CHL | O2D-CGD-CBD | 8.53 | 120.32 | 110.95 |
| 29 | 6 | 605 | CHL | O2D-CGD-CBD | 8.52 | 120.31 | 110.95 |
| 29 | 4 | 606 | CHL | O2D-CGD-CBD | 8.52 | 120.30 | 110.95 |
| 29 | 9 | 601 | CHL | C1B-CHB-C4A | -8.50 | 115.86 | 121.32 |
| 29 | 6 | 601 | CHL | CMC-C2C-C1C | 8.47 | 139.98 | 124.73 |
| 29 | 8 | 606 | CHL | C1B-CHB-C4A | -8.45 | 115.89 | 121.32 |
| 29 | b | 307 | CHL | O2D-CGD-CBD | 8.45 | 120.23 | 110.95 |
| 29 | 5 | 606 | CHL | O2D-CGD-CBD | 8.38 | 120.16 | 110.95 |
| 29 | b | 308 | CHL | O2D-CGD-CBD | 8.37 | 120.14 | 110.95 |
| 29 | 2 | 602 | CHL | O2D-CGD-CBD | 8.36 | 120.13 | 110.95 |
| 29 | 7 | 406 | CHL | CMC-C2C-C1C | 8.33 | 139.72 | 124.73 |
| 29 | 8 | 606 | CHL | O2D-CGD-CBD | 8.33 | 120.10 | 110.95 |
| 29 | 6 | 606 | CHL | O2D-CGD-CBD | 8.32 | 120.09 | 110.95 |
| 29 | a | 609 | CHL | O2D-CGD-CBD | 8.31 | 120.08 | 110.95 |
| 29 | 9 | 606 | CHL | C1C-C2C-CMC | 8.31 | 141.78 | 126.80 |
| 29 | c | 608 | CHL | O2D-CGD-CBD | 8.31 | 120.08 | 110.95 |
| 24 | B | 843 | BCR | C16-C17-C18 | -8.29 | 115.65 | 127.28 |
| 29 | 4 | 605 | CHL | C1C-C2C-CMC | 8.28 | 141.73 | 126.80 |
| 29 | 4 | 614 | CHL | O2D-CGD-CBD | 8.26 | 120.03 | 110.95 |
| 29 | b | 302 | CHL | O2D-CGD-CBD | 8.26 | 120.02 | 110.95 |
| 29 | b | 306 | CHL | O2D-CGD-CBD | 8.24 | 120.00 | 110.95 |
| 29 | 8 | 613 | CHL | O2D-CGD-CBD | 8.20 | 119.95 | 110.95 |
| 24 | J | 101 | BCR | C15-C16-C17 | 8.18 | 140.25 | 123.52 |
| 29 | 6 | 605 | CHL | CHA-C1A-C2A | -8.17 | 114.14 | 133.31 |
| 29 | b | 307 | CHL | CHA-C1A-C2A | -8.16 | 114.14 | 133.31 |
| 24 | 7 | 418 | BCR | C15-C16-C17 | 8.14 | 140.18 | 123.52 |
| 29 | 4 | 605 | CHL | CHA-C1A-C2A | -8.13 | 114.21 | 133.31 |
| 29 | 2 | 601 | CHL | CHA-C1A-C2A | -8.13 | 114.21 | 133.31 |
| 29 | c | 606 | CHL | O2D-CGD-CBD | 8.12 | 119.87 | 110.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 9 | 607 | CHL | O2D-CGD-CBD | 8.11 | 119.86 | 110.95 |
| 29 | 8 | 605 | CHL | CHA-C1A-C2A | -8.11 | 114.27 | 133.31 |
| 24 | A | 850 | BCR | C15-C16-C17 | 8.11 | 140.10 | 123.52 |
| 29 | 8 | 613 | CHL | C1C-C2C-CMC | 8.09 | 141.38 | 126.80 |
| 29 | 2 | 602 | CHL | C1C-C2C-CMC | 8.09 | 141.38 | 126.80 |
| 29 | c | 601 | CHL | O2D-CGD-CBD | 8.02 | 119.76 | 110.95 |
| 29 | 8 | 607 | CHL | C1C-C2C-CMC | 8.02 | 141.26 | 126.80 |
| 29 | 2 | 607 | CHL | CHA-C1A-C2A | -8.02 | 114.48 | 133.31 |
| 29 | 2 | 614 | CHL | CHA-C1A-C2A | -8.01 | 114.49 | 133.31 |
| 29 | a | 608 | CHL | CHA-C1A-C2A | -8.01 | 114.49 | 133.31 |
| 29 | 9 | 608 | CHL | CHA-C1A-C2A | -8.01 | 114.50 | 133.31 |
| 29 | a | 607 | CHL | CHA-C1A-C2A | -8.00 | 114.52 | 133.31 |
| 29 | 2 | 606 | CHL | CHA-C1A-C2A | -8.00 | 114.53 | 133.31 |
| 29 | 1 | 307 | CHL | CHA-C1A-C2A | -7.98 | 114.57 | 133.31 |
| 29 | 6 | 614 | CHL | O2D-CGD-CBD | 7.98 | 119.71 | 110.95 |
| 29 | 9 | 609 | CHL | CHA-C1A-C2A | -7.95 | 114.64 | 133.31 |
| 29 | b | 309 | CHL | CHA-C1A-C2A | -7.95 | 114.65 | 133.31 |
| 29 | a | 608 | CHL | C1C-C2C-CMC | 7.94 | 141.12 | 126.80 |
| 29 | 2 | 614 | CHL | O2D-CGD-CBD | 7.93 | 119.66 | 110.95 |
| 29 | 5 | 601 | CHL | CHA-C1A-C2A | -7.92 | 114.71 | 133.31 |
| 29 | 2 | 605 | CHL | CHA-C1A-C2A | -7.91 | 114.73 | 133.31 |
| 29 | 2 | 602 | CHL | CHA-C1A-C2A | -7.91 | 114.73 | 133.31 |
| 29 | 4 | 606 | CHL | CHA-C1A-C2A | -7.91 | 114.73 | 133.31 |
| 29 | 6 | 606 | CHL | CHA-C1A-C2A | -7.90 | 114.76 | 133.31 |
| 29 | b | 310 | CHL | CHA-C1A-C2A | -7.88 | 114.81 | 133.31 |
| 29 | 4 | 607 | CHL | CHA-C1A-C2A | -7.87 | 114.82 | 133.31 |
| 29 | b | 309 | CHL | O2D-CGD-CBD | 7.86 | 119.58 | 110.95 |
| 29 | 6 | 606 | CHL | C1C-C2C-CMC | 7.85 | 140.95 | 126.80 |
| 29 | 9 | 608 | CHL | O2D-CGD-CBD | 7.85 | 119.57 | 110.95 |
| 29 | 9 | 606 | CHL | CHA-C1A-C2A | -7.83 | 114.92 | 133.31 |
| 29 | 1 | 302 | CHL | CHA-C1A-C2A | -7.81 | 114.98 | 133.31 |
| 29 | c | 601 | CHL | CHA-C1A-C2A | -7.81 | 114.98 | 133.31 |
| 29 | 6 | 602 | CHL | C1C-C2C-CMC | 7.79 | 140.84 | 126.80 |
| 29 | 6 | 602 | CHL | CHA-C1A-C2A | -7.79 | 115.02 | 133.31 |
| 29 | b | 306 | CHL | CHA-C1A-C2A | -7.79 | 115.02 | 133.31 |
| 29 | c | 606 | CHL | C1C-C2C-CMC | 7.78 | 140.83 | 126.80 |
| 29 | 9 | 605 | CHL | CHA-C1A-C2A | -7.78 | 115.04 | 133.31 |
| 29 | c | 606 | CHL | C1B-CHB-C4A | -7.76 | 116.33 | 121.32 |
| 29 | 8 | 607 | CHL | CHA-C1A-C2A | -7.76 | 115.10 | 133.31 |
| 29 | 7 | 406 | CHL | C1B-CHB-C4A | -7.73 | 116.35 | 121.32 |
| 21 | B | 811 | CLA | C4A-NA-C1A | 7.71 | 110.20 | 106.68 |
| 29 | 4 | 607 | CHL | O2D-CGD-CBD | 7.71 | 119.42 | 110.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 607 | CHL | O2D-CGD-CBD | 7.71 | 119.42 | 110.95 |
| 29 | 9 | 609 | CHL | O2D-CGD-CBD | 7.70 | 119.41 | 110.95 |
| 29 | 2 | 607 | CHL | C1C-C2C-CMC | 7.68 | 140.65 | 126.80 |
| 29 | b | 306 | CHL | C1C-C2C-CMC | 7.67 | 140.63 | 126.80 |
| 29 | 6 | 614 | CHL | CHA-C1A-C2A | -7.66 | 115.32 | 133.31 |
| 29 | a | 608 | CHL | O2D-CGD-CBD | 7.66 | 119.36 | 110.95 |
| 29 | 2 | 614 | CHL | C1C-C2C-CMC | 7.65 | 140.59 | 126.80 |
| 29 | 5 | 601 | CHL | C1C-C2C-CMC | 7.63 | 140.56 | 126.80 |
| 29 | b | 308 | CHL | CHA-C1A-C2A | -7.62 | 115.41 | 133.31 |
| 29 | c | 606 | CHL | CHA-C1A-C2A | -7.60 | 115.45 | 133.31 |
| 29 | 6 | 607 | CHL | CHA-C1A-C2A | -7.60 | 115.46 | 133.31 |
| 29 | 1 | 307 | CHL | C1C-C2C-CMC | 7.58 | 140.46 | 126.80 |
| 29 | 2 | 606 | CHL | C1C-C2C-CMC | 7.58 | 140.46 | 126.80 |
| 29 | 6 | 605 | CHL | C1C-C2C-CMC | 7.57 | 140.45 | 126.80 |
| 29 | 5 | 606 | CHL | C1B-CHB-C4A | -7.56 | 116.46 | 121.32 |
| 29 | 6 | 607 | CHL | O2D-CGD-CBD | 7.44 | 119.13 | 110.95 |
| 29 | 5 | 606 | CHL | CHA-C1A-C2A | -7.44 | 115.84 | 133.31 |
| 29 | 5 | 606 | CHL | C1C-C2C-CMC | 7.42 | 140.18 | 126.80 |
| 29 | 9 | 605 | CHL | C1C-C2C-CMC | 7.41 | 140.15 | 126.80 |
| 21 | B | 829 | CLA | C4A-NA-C1A | 7.39 | 110.05 | 106.68 |
| 29 | 6 | 601 | CHL | CHA-C1A-C2A | -7.38 | 115.98 | 133.31 |
| 29 | c | 608 | CHL | CHA-C1A-C2A | -7.37 | 116.02 | 133.31 |
| 29 | 9 | 607 | CHL | CHA-C1A-C2A | -7.36 | 116.02 | 133.31 |
| 29 | 2 | 601 | CHL | C1C-C2C-CMC | 7.35 | 140.04 | 126.80 |
| 29 | a | 609 | CHL | CHA-C1A-C2A | -7.34 | 116.08 | 133.31 |
| 29 | c | 608 | CHL | C1B-CHB-C4A | -7.33 | 116.61 | 121.32 |
| 29 | 6 | 607 | CHL | C1C-C2C-CMC | 7.31 | 139.98 | 126.80 |
| 21 | G | 202 | CLA | C4A-NA-C1A | 7.30 | 110.01 | 106.68 |
| 29 | 6 | 601 | CHL | C1B-CHB-C4A | -7.30 | 116.63 | 121.32 |
| 29 | c | 607 | CHL | CHA-C1A-C2A | -7.29 | 116.19 | 133.31 |
| 29 | b | 302 | CHL | C1C-C2C-CMC | 7.24 | 139.84 | 126.80 |
| 29 | c | 607 | CHL | C1C-C2C-CMC | 7.23 | 139.83 | 126.80 |
| 29 | 8 | 606 | CHL | CHA-C1A-C2A | -7.23 | 116.34 | 133.31 |
| 29 | 1 | 302 | CHL | C1C-C2C-CMC | 7.21 | 139.81 | 126.80 |
| 29 | c | 609 | CHL | C1B-CHB-C4A | -7.21 | 116.69 | 121.32 |
| 29 | 6 | 614 | CHL | C1C-C2C-CMC | 7.20 | 139.78 | 126.80 |
| 29 | c | 605 | CHL | CHA-C1A-C2A | -7.20 | 116.41 | 133.31 |
| 29 | b | 308 | CHL | C1B-CHB-C4A | -7.15 | 116.72 | 121.32 |
| 29 | 9 | 607 | CHL | C1B-CHB-C4A | -7.14 | 116.73 | 121.32 |
| 21 | A | 841 | CLA | C4A-NA-C1A | 7.14 | 109.94 | 106.68 |
| 21 | 3 | 405 | CLA | C4A-NA-C1A | 7.12 | 109.93 | 106.68 |
| 21 | A | 817 | CLA | C4A-NA-C1A | 7.09 | 109.92 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 823 | CLA | C4A-NA-C1A | 7.09 | 109.91 | 106.68 |
| 29 | a | 607 | CHL | C1C-C2C-CMC | 7.08 | 139.57 | 126.80 |
| 29 | b | 309 | CHL | C1C-C2C-CMC | 7.08 | 139.56 | 126.80 |
| 29 | 8 | 605 | CHL | C1C-C2C-CMC | 7.07 | 139.55 | 126.80 |
| 21 | B | 836 | CLA | C4A-NA-C1A | 7.07 | 109.91 | 106.68 |
| 29 | 9 | 608 | CHL | C1C-C2C-CMC | 7.06 | 139.52 | 126.80 |
| 29 | c | 605 | CHL | C1C-C2C-CMC | 7.05 | 139.51 | 126.80 |
| 21 | A | 801 | CLA | C1D-ND-C4D | -7.05 | 101.36 | 106.31 |
| 21 | B | 802 | CLA | C4A-NA-C1A | 7.05 | 109.89 | 106.68 |
| 29 | 8 | 606 | CHL | C1C-C2C-CMC | 7.05 | 139.50 | 126.80 |
| 21 | 6 | 612 | CLA | C4A-NA-C1A | 7.04 | 109.89 | 106.68 |
| 29 | b | 310 | CHL | C1C-C2C-CMC | 7.02 | 139.45 | 126.80 |
| 29 | a | 605 | CHL | C1C-C2C-CMC | 7.01 | 139.43 | 126.80 |
| 21 | B | 821 | CLA | C4A-NA-C1A | 7.01 | 109.88 | 106.68 |
| 29 | 9 | 601 | CHL | O2D-CGD-CBD | 7.00 | 118.64 | 110.95 |
| 21 | A | 827 | CLA | C4A-NA-C1A | 6.99 | 109.87 | 106.68 |
| 29 | 9 | 601 | CHL | C1C-C2C-CMC | 6.98 | 139.38 | 126.80 |
| 29 | 8 | 607 | CHL | O2D-CGD-CBD | 6.97 | 118.60 | 110.95 |
| 21 | 3 | 401 | CLA | C4A-NA-C1A | 6.97 | 109.86 | 106.68 |
| 21 | B | 804 | CLA | C4A-NA-C1A | 6.95 | 109.85 | 106.68 |
| 29 | 9 | 601 | CHL | CHA-C1A-C2A | -6.94 | 117.00 | 133.31 |
| 21 | A | 839 | CLA | C4A-NA-C1A | 6.92 | 109.84 | 106.68 |
| 29 | c | 601 | CHL | C1C-C2C-CMC | 6.90 | 139.23 | 126.80 |
| 29 | 9 | 609 | CHL | C1C-C2C-CMC | 6.89 | 139.22 | 126.80 |
| 29 | 4 | 614 | CHL | C1C-C2C-CMC | 6.88 | 139.21 | 126.80 |
| 21 | A | 806 | CLA | C4A-NA-C1A | 6.87 | 109.81 | 106.68 |
| 21 | L | 302 | CLA | C4A-NA-C1A | 6.86 | 109.81 | 106.68 |
| 21 | A | 804 | CLA | C4A-NA-C1A | 6.86 | 109.81 | 106.68 |
| 21 | c | 613 | CLA | C4A-NA-C1A | 6.85 | 109.81 | 106.68 |
| 21 | A | 813 | CLA | C4A-NA-C1A | 6.84 | 109.80 | 106.68 |
| 21 | A | 838 | CLA | C4A-NA-C1A | 6.83 | 109.80 | 106.68 |
| 29 | a | 609 | CHL | C1C-C2C-CMC | 6.81 | 139.07 | 126.80 |
| 21 | B | 814 | CLA | C4A-NA-C1A | 6.81 | 109.78 | 106.68 |
| 29 | b | 308 | CHL | C1C-C2C-CMC | 6.80 | 139.06 | 126.80 |
| 21 | B | 837 | CLA | C4A-NA-C1A | 6.80 | 109.78 | 106.68 |
| 21 | 9 | 603 | CLA | C4A-NA-C1A | 6.79 | 109.78 | 106.68 |
| 21 | 9 | 604 | CLA | C4A-NA-C1A | 6.78 | 109.77 | 106.68 |
| 21 | 9 | 613 | CLA | C4A-NA-C1A | 6.78 | 109.77 | 106.68 |
| 29 | 6 | 607 | CHL | C1B-CHB-C4A | -6.77 | 116.97 | 121.32 |
| 29 | c | 609 | CHL | CHA-C1A-C2A | -6.76 | 117.43 | 133.31 |
| 21 | 5 | 612 | CLA | C4A-NA-C1A | 6.76 | 109.76 | 106.68 |
| 29 | 8 | 613 | CHL | C1B-CHB-C4A | -6.75 | 116.98 | 121.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 834 | CLA | C4A-NA-C1A | 6.75 | 109.76 | 106.68 |
| 21 | 7 | 401 | CLA | C4A-NA-C1A | 6.73 | 109.75 | 106.68 |
| 21 | 7 | 408 | CLA | C4A-NA-C1A | 6.73 | 109.75 | 106.68 |
| 29 | 6 | 614 | CHL | C1B-CHB-C4A | -6.72 | 117.00 | 121.32 |
| 29 | b | 302 | CHL | CHA-C1A-C2A | -6.71 | 117.54 | 133.31 |
| 21 | A | 840 | CLA | C4A-NA-C1A | 6.71 | 109.74 | 106.68 |
| 21 | 7 | 407 | CLA | C4A-NA-C1A | 6.71 | 109.74 | 106.68 |
| 21 | A | 822 | CLA | C4A-NA-C1A | 6.71 | 109.74 | 106.68 |
| 21 | A | 810 | CLA | C4A-NA-C1A | 6.70 | 109.74 | 106.68 |
| 21 | K | 204 | CLA | C4A-NA-C1A | 6.70 | 109.74 | 106.68 |
| 21 | 1 | 309 | CLA | C4A-NA-C1A | 6.70 | 109.74 | 106.68 |
| 21 | 6 | 611 | CLA | C4A-NA-C1A | 6.70 | 109.73 | 106.68 |
| 21 | b | 304 | CLA | C4A-NA-C1A | 6.69 | 109.73 | 106.68 |
| 21 | K | 201 | CLA | C4A-NA-C1A | 6.68 | 109.73 | 106.68 |
| 21 | B | 803 | CLA | C4A-NA-C1A | 6.67 | 109.72 | 106.68 |
| 21 | 1 | 309 | CLA | O2D-CGD-CBD | 6.67 | 122.88 | 111.23 |
| 29 | a | 605 | CHL | CHA-C1A-C2A | -6.66 | 117.67 | 133.31 |
| 21 | O | 201 | CLA | C4A-NA-C1A | 6.65 | 109.71 | 106.68 |
| 21 | B | 805 | CLA | C4A-NA-C1A | 6.64 | 109.71 | 106.68 |
| 21 | 1 | 308 | CLA | C4A-NA-C1A | 6.64 | 109.71 | 106.68 |
| 21 | 3 | 409 | CLA | C4A-NA-C1A | 6.64 | 109.71 | 106.68 |
| 29 | a | 606 | CHL | CHA-C1A-C2A | -6.64 | 117.72 | 133.31 |
| 21 | B | 806 | CLA | C4A-NA-C1A | 6.64 | 109.71 | 106.68 |
| 21 | 7 | 404 | CLA | C4A-NA-C1A | 6.64 | 109.71 | 106.68 |
| 21 | G | 204 | CLA | C4A-NA-C1A | 6.62 | 109.70 | 106.68 |
| 21 | A | 831 | CLA | C4A-NA-C1A | 6.62 | 109.70 | 106.68 |
| 21 | 8 | 609 | CLA | C4A-NA-C1A | 6.62 | 109.70 | 106.68 |
| 29 | 4 | 606 | CHL | C1C-C2C-CMC | 6.62 | 138.73 | 126.80 |
| 29 | a | 601 | CHL | CHA-C1A-C2A | -6.60 | 117.81 | 133.31 |
| 21 | A | 830 | CLA | C4A-NA-C1A | 6.60 | 109.69 | 106.68 |
| 21 | 5 | 604 | CLA | C4A-NA-C1A | 6.60 | 109.69 | 106.68 |
| 21 | a | 613 | CLA | C4A-NA-C1A | 6.60 | 109.69 | 106.68 |
| 21 | 2 | 609 | CLA | C4A-NA-C1A | 6.59 | 109.68 | 106.68 |
| 24 | 3 | 419 | BCR | C15-C16-C17 | 6.59 | 137.00 | 123.52 |
| 21 | B | 840 | CLA | C4A-NA-C1A | 6.58 | 109.68 | 106.68 |
| 21 | 7 | 405 | CLA | C4A-NA-C1A | 6.58 | 109.68 | 106.68 |
| 21 | 6 | 609 | CLA | C4A-NA-C1A | 6.57 | 109.68 | 106.68 |
| 21 | A | 820 | CLA | C4A-NA-C1A | 6.57 | 109.67 | 106.68 |
| 21 | 4 | 609 | CLA | C4A-NA-C1A | 6.56 | 109.67 | 106.68 |
| 21 | 3 | 406 | CLA | C4A-NA-C1A | 6.55 | 109.67 | 106.68 |
| 21 | 5 | 610 | CLA | C4A-NA-C1A | 6.55 | 109.67 | 106.68 |
| 21 | b | 305 | CLA | C4A-NA-C1A | 6.54 | 109.66 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 607 | CLA | C4A-NA-C1A | 6.54 | 109.66 | 106.68 |
| 21 | 5 | 614 | CLA | C4A-NA-C1A | 6.54 | 109.66 | 106.68 |
| 24 | J | 104 | BCR | C7-C8-C9 | -6.54 | 116.57 | 126.23 |
| 21 | 1 | 316 | CLA | C4A-NA-C1A | 6.53 | 109.66 | 106.68 |
| 21 | c | 604 | CLA | C4A-NA-C1A | 6.53 | 109.66 | 106.68 |
| 21 | B | 822 | CLA | C4A-NA-C1A | 6.52 | 109.66 | 106.68 |
| 21 | 7 | 409 | CLA | C4A-NA-C1A | 6.52 | 109.66 | 106.68 |
| 21 | 8 | 610 | CLA | C4A-NA-C1A | 6.52 | 109.66 | 106.68 |
| 21 | 8 | 612 | CLA | C4A-NA-C1A | 6.51 | 109.65 | 106.68 |
| 21 | B | 826 | CLA | C4A-NA-C1A | 6.51 | 109.65 | 106.68 |
| 21 | 5 | 611 | CLA | C4A-NA-C1A | 6.51 | 109.65 | 106.68 |
| 21 | a | 611 | CLA | C4A-NA-C1A | 6.51 | 109.65 | 106.68 |
| 21 | B | 839 | CLA | C4A-NA-C1A | 6.51 | 109.65 | 106.68 |
| 21 | H | 201 | CLA | C4A-NA-C1A | 6.50 | 109.65 | 106.68 |
| 21 | 2 | 604 | CLA | C4A-NA-C1A | 6.50 | 109.65 | 106.68 |
| 21 | 2 | 612 | CLA | C4A-NA-C1A | 6.49 | 109.64 | 106.68 |
| 21 | 3 | 404 | CLA | C4A-NA-C1A | 6.49 | 109.64 | 106.68 |
| 21 | 4 | 611 | CLA | C4A-NA-C1A | 6.49 | 109.64 | 106.68 |
| 21 | a | 604 | CLA | C4A-NA-C1A | 6.49 | 109.64 | 106.68 |
| 21 | 2 | 610 | CLA | C4A-NA-C1A | 6.49 | 109.64 | 106.68 |
| 21 | 1 | 310 | CLA | C4A-NA-C1A | 6.49 | 109.64 | 106.68 |
| 21 | 6 | 603 | CLA | C4A-NA-C1A | 6.48 | 109.64 | 106.68 |
| 21 | 7 | 410 | CLA | C4A-NA-C1A | 6.48 | 109.64 | 106.68 |
| 21 | B | 825 | CLA | C4A-NA-C1A | 6.47 | 109.63 | 106.68 |
| 21 | c | 611 | CLA | C4A-NA-C1A | 6.47 | 109.63 | 106.68 |
| 21 | A | 808 | CLA | C4A-NA-C1A | 6.47 | 109.63 | 106.68 |
| 21 | L | 304 | CLA | C4A-NA-C1A | 6.47 | 109.63 | 106.68 |
| 21 | K | 203 | CLA | C4A-NA-C1A | 6.47 | 109.63 | 106.68 |
| 21 | L | 303 | CLA | C4A-NA-C1A | 6.46 | 109.63 | 106.68 |
| 21 | B | 824 | CLA | C4A-NA-C1A | 6.46 | 109.63 | 106.68 |
| 29 | 2 | 605 | CHL | C1B-CHB-C4A | -6.46 | 117.17 | 121.32 |
| 21 | 8 | 601 | CLA | C4A-NA-C1A | 6.46 | 109.62 | 106.68 |
| 21 | 3 | 410 | CLA | C4A-NA-C1A | 6.45 | 109.62 | 106.68 |
| 21 | 3 | 414 | CLA | C4A-NA-C1A | 6.45 | 109.62 | 106.68 |
| 21 | 4 | 612 | CLA | C4A-NA-C1A | 6.45 | 109.62 | 106.68 |
| 21 | 5 | 609 | CLA | C4A-NA-C1A | 6.45 | 109.62 | 106.68 |
| 21 | A | 825 | CLA | C4A-NA-C1A | 6.45 | 109.62 | 106.68 |
| 21 | A | 842 | CLA | C4A-NA-C1A | 6.45 | 109.62 | 106.68 |
| 21 | B | 838 | CLA | C4A-NA-C1A | 6.44 | 109.62 | 106.68 |
| 21 | 1 | 313 | CLA | C4A-NA-C1A | 6.44 | 109.62 | 106.68 |
| 21 | 1 | 315 | CLA | C4A-NA-C1A | 6.44 | 109.62 | 106.68 |
| 21 | 7 | 411 | CLA | C4A-NA-C1A | 6.44 | 109.62 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | a | 612 | CLA | C4A-NA-C1A | 6.44 | 109.62 | 106.68 |
| 21 | A | 807 | CLA | C4A-NA-C1A | 6.43 | 109.61 | 106.68 |
| 21 | 6 | 604 | CLA | C4A-NA-C1A | 6.43 | 109.61 | 106.68 |
| 21 | 4 | 603 | CLA | C4A-NA-C1A | 6.42 | 109.61 | 106.68 |
| 24 | J | 104 | BCR | C16-C17-C18 | -6.42 | 118.27 | 127.28 |
| 21 | F | 302 | CLA | C4A-NA-C1A | 6.42 | 109.61 | 106.68 |
| 21 | F | 305 | CLA | C4A-NA-C1A | 6.42 | 109.61 | 106.68 |
| 21 | 6 | 610 | CLA | C4A-NA-C1A | 6.41 | 109.61 | 106.68 |
| 21 | a | 610 | CLA | C4A-NA-C1A | 6.41 | 109.60 | 106.68 |
| 21 | A | 818 | CLA | C4A-NA-C1A | 6.40 | 109.60 | 106.68 |
| 29 | c | 608 | CHL | C1C-C2C-CMC | 6.40 | 138.34 | 126.80 |
| 21 | A | 816 | CLA | C4A-NA-C1A | 6.40 | 109.60 | 106.68 |
| 21 | A | 823 | CLA | C4A-NA-C1A | 6.40 | 109.60 | 106.68 |
| 29 | a | 601 | CHL | C1C-C2C-CMC | 6.39 | 138.33 | 126.80 |
| 21 | A | 826 | CLA | C4A-NA-C1A | 6.39 | 109.59 | 106.68 |
| 21 | O | 203 | CLA | C4A-NA-C1A | 6.39 | 109.59 | 106.68 |
| 21 | A | 814 | CLA | C4A-NA-C1A | 6.39 | 109.59 | 106.68 |
| 21 | 1 | 305 | CLA | C4A-NA-C1A | 6.39 | 109.59 | 106.68 |
| 21 | 7 | 403 | CLA | C4A-NA-C1A | 6.38 | 109.59 | 106.68 |
| 21 | 9 | 611 | CLA | C4A-NA-C1A | 6.38 | 109.59 | 106.68 |
| 21 | a | 602 | CLA | C4A-NA-C1A | 6.38 | 109.59 | 106.68 |
| 29 | a | 606 | CHL | C1C-C2C-CMC | 6.38 | 138.29 | 126.80 |
| 21 | 5 | 613 | CLA | C4A-NA-C1A | 6.37 | 109.59 | 106.68 |
| 21 | B | 813 | CLA | C4A-NA-C1A | 6.37 | 109.58 | 106.68 |
| 29 | b | 310 | CHL | C1B-CHB-C4A | -6.37 | 117.23 | 121.32 |
| 21 | J | 102 | CLA | C4A-NA-C1A | 6.36 | 109.58 | 106.68 |
| 21 | 4 | 601 | CLA | C4A-NA-C1A | 6.36 | 109.58 | 106.68 |
| 21 | 8 | 608 | CLA | C4A-NA-C1A | 6.36 | 109.58 | 106.68 |
| 21 | 8 | 603 | CLA | C4A-NA-C1A | 6.36 | 109.58 | 106.68 |
| 24 | L | 306 | BCR | C15-C16-C17 | 6.36 | 136.53 | 123.52 |
| 21 | 4 | 610 | CLA | C4A-NA-C1A | 6.35 | 109.58 | 106.68 |
| 21 | A | 833 | CLA | C4A-NA-C1A | 6.35 | 109.58 | 106.68 |
| 21 | 1 | 312 | CLA | C4A-NA-C1A | 6.35 | 109.58 | 106.68 |
| 21 | 4 | 613 | CLA | C4A-NA-C1A | 6.35 | 109.58 | 106.68 |
| 21 | 3 | 402 | CLA | C4A-NA-C1A | 6.35 | 109.57 | 106.68 |
| 21 | 8 | 604 | CLA | C4A-NA-C1A | 6.35 | 109.57 | 106.68 |
| 21 | 3 | 412 | CLA | C4A-NA-C1A | 6.34 | 109.57 | 106.68 |
| 21 | 8 | 618 | CLA | C4A-NA-C1A | 6.34 | 109.57 | 106.68 |
| 21 | 4 | 604 | CLA | C4A-NA-C1A | 6.34 | 109.57 | 106.68 |
| 21 | B | 809 | CLA | C4A-NA-C1A | 6.33 | 109.57 | 106.68 |
| 21 | B | 801 | CLA | CMD-C2D-C1D | 6.33 | 135.88 | 124.73 |
| 21 | 1 | 303 | CLA | C4A-NA-C1A | 6.33 | 109.57 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 607 | CHL | C1B-CHB-C4A | -6.32 | 117.25 | 121.32 |
| 21 | A | 811 | CLA | C4A-NA-C1A | 6.32 | 109.56 | 106.68 |
| 21 | B | 815 | CLA | C4A-NA-C1A | 6.32 | 109.56 | 106.68 |
| 21 | 2 | 613 | CLA | C4A-NA-C1A | 6.32 | 109.56 | 106.68 |
| 21 | A | 815 | CLA | C4A-NA-C1A | 6.31 | 109.56 | 106.68 |
| 21 | 7 | 414 | CLA | C4A-NA-C1A | 6.31 | 109.56 | 106.68 |
| 21 | B | 810 | CLA | C4A-NA-C1A | 6.30 | 109.55 | 106.68 |
| 29 | 6 | 602 | CHL | C1B-CHB-C4A | -6.29 | 117.27 | 121.32 |
| 21 | 1 | 311 | CLA | C4A-NA-C1A | 6.28 | 109.55 | 106.68 |
| 21 | 4 | 608 | CLA | C4A-NA-C1A | 6.28 | 109.55 | 106.68 |
| 21 | A | 821 | CLA | C4A-NA-C1A | 6.28 | 109.54 | 106.68 |
| 21 | c | 612 | CLA | C4A-NA-C1A | 6.27 | 109.54 | 106.68 |
| 21 | B | 817 | CLA | C4A-NA-C1A | 6.27 | 109.54 | 106.68 |
| 21 | 5 | 608 | CLA | C4A-NA-C1A | 6.26 | 109.53 | 106.68 |
| 21 | B | 816 | CLA | C4A-NA-C1A | 6.26 | 109.53 | 106.68 |
| 21 | B | 820 | CLA | C4A-NA-C1A | 6.26 | 109.53 | 106.68 |
| 21 | 7 | 413 | CLA | C4A-NA-C1A | 6.26 | 109.53 | 106.68 |
| 21 | B | 808 | CLA | C4A-NA-C1A | 6.25 | 109.53 | 106.68 |
| 21 | 6 | 613 | CLA | C4A-NA-C1A | 6.25 | 109.53 | 106.68 |
| 21 | A | 809 | CLA | C4A-NA-C1A | 6.24 | 109.53 | 106.68 |
| 21 | 1 | 306 | CLA | C4A-NA-C1A | 6.23 | 109.52 | 106.68 |
| 21 | 3 | 411 | CLA | C4A-NA-C1A | 6.23 | 109.52 | 106.68 |
| 21 | b | 314 | CLA | C4A-NA-C1A | 6.23 | 109.52 | 106.68 |
| 21 | 4 | 602 | CLA | C4A-NA-C1A | 6.23 | 109.52 | 106.68 |
| 21 | B | 819 | CLA | C4A-NA-C1A | 6.23 | 109.52 | 106.68 |
| 21 | A | 834 | CLA | C4A-NA-C1A | 6.22 | 109.52 | 106.68 |
| 21 | K | 202 | CLA | C4A-NA-C1A | 6.21 | 109.51 | 106.68 |
| 21 | A | 802 | CLA | C4A-NA-C1A | 6.21 | 109.51 | 106.68 |
| 21 | c | 610 | CLA | C4A-NA-C1A | 6.20 | 109.51 | 106.68 |
| 21 | 7 | 412 | CLA | C4A-NA-C1A | 6.20 | 109.51 | 106.68 |
| 21 | B | 818 | CLA | C4A-NA-C1A | 6.19 | 109.50 | 106.68 |
| 21 | O | 204 | CLA | C4A-NA-C1A | 6.18 | 109.50 | 106.68 |
| 21 | A | 824 | CLA | C4A-NA-C1A | 6.18 | 109.50 | 106.68 |
| 21 | G | 203 | CLA | C4A-NA-C1A | 6.17 | 109.50 | 106.68 |
| 21 | b | 312 | CLA | C4A-NA-C1A | 6.17 | 109.49 | 106.68 |
| 21 | 9 | 612 | CLA | C4A-NA-C1A | 6.17 | 109.49 | 106.68 |
| 21 | 5 | 602 | CLA | C4A-NA-C1A | 6.16 | 109.49 | 106.68 |
| 21 | 9 | 602 | CLA | C4A-NA-C1A | 6.16 | 109.49 | 106.68 |
| 21 | B | 812 | CLA | C4A-NA-C1A | 6.15 | 109.49 | 106.68 |
| 21 | B | 833 | CLA | C4A-NA-C1A | 6.15 | 109.49 | 106.68 |
| 21 | A | 836 | CLA | C4A-NA-C1A | 6.15 | 109.48 | 106.68 |
| 21 | B | 807 | CLA | C4A-NA-C1A | 6.14 | 109.48 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 827 | CLA | C4A-NA-C1A | 6.14 | 109.48 | 106.68 |
| 21 | 3 | 413 | CLA | C4A-NA-C1A | 6.14 | 109.48 | 106.68 |
| 24 | F | 301 | BCR | C15-C16-C17 | 6.14 | 136.08 | 123.52 |
| 29 | 9 | 607 | CHL | C1C-C2C-CMC | 6.14 | 137.87 | 126.80 |
| 21 | A | 830 | CLA | O2D-CGD-CBD | 6.12 | 121.93 | 111.23 |
| 21 | 6 | 608 | CLA | C4A-NA-C1A | 6.12 | 109.47 | 106.68 |
| 21 | O | 202 | CLA | C4A-NA-C1A | 6.12 | 109.47 | 106.68 |
| 21 | 3 | 408 | CLA | C4A-NA-C1A | 6.11 | 109.47 | 106.68 |
| 29 | 3 | 407 | CHL | CBC-CAC-C3C | -6.10 | 104.13 | 112.87 |
| 21 | 8 | 611 | CLA | C4A-NA-C1A | 6.09 | 109.46 | 106.68 |
| 21 | 5 | 605 | CLA | C4A-NA-C1A | 6.09 | 109.46 | 106.68 |
| 21 | b | 303 | CLA | C4A-NA-C1A | 6.09 | 109.46 | 106.68 |
| 29 | 8 | 605 | CHL | C1B-CHB-C4A | -6.09 | 117.41 | 121.32 |
| 21 | A | 832 | CLA | C4A-NA-C1A | 6.09 | 109.46 | 106.68 |
| 21 | a | 614 | CLA | C4A-NA-C1A | 6.09 | 109.46 | 106.68 |
| 21 | 7 | 402 | CLA | C4A-NA-C1A | 6.08 | 109.45 | 106.68 |
| 21 | 1 | 304 | CLA | C4A-NA-C1A | 6.08 | 109.45 | 106.68 |
| 21 | 8 | 602 | CLA | C4A-NA-C1A | 6.08 | 109.45 | 106.68 |
| 21 | A | 805 | CLA | C4A-NA-C1A | 6.07 | 109.45 | 106.68 |
| 24 | A | 846 | BCR | C15-C16-C17 | 6.07 | 135.93 | 123.52 |
| 21 | b | 313 | CLA | C4A-NA-C1A | 6.05 | 109.44 | 106.68 |
| 21 | a | 603 | CLA | C4A-NA-C1A | 6.04 | 109.44 | 106.68 |
| 21 | 9 | 610 | CLA | C4A-NA-C1A | 6.03 | 109.43 | 106.68 |
| 21 | b | 315 | CLA | C4A-NA-C1A | 6.02 | 109.43 | 106.68 |
| 21 | A | 801 | CLA | C4A-NA-C1A | 6.02 | 109.43 | 106.68 |
| 21 | 4 | 609 | CLA | CMD-C2D-C1D | 6.01 | 135.31 | 124.73 |
| 29 | 8 | 607 | CHL | C1B-CHB-C4A | -6.00 | 117.47 | 121.32 |
| 21 | b | 311 | CLA | C4A-NA-C1A | 5.99 | 109.41 | 106.68 |
| 29 | b | 309 | CHL | C1B-CHB-C4A | -5.99 | 117.47 | 121.32 |
| 29 | 1 | 302 | CHL | C1B-CHB-C4A | -5.98 | 117.48 | 121.32 |
| 21 | 2 | 611 | CLA | C4A-NA-C1A | 5.96 | 109.40 | 106.68 |
| 29 | 9 | 605 | CHL | C1B-CHB-C4A | -5.95 | 117.49 | 121.32 |
| 21 | c | 602 | CLA | C4A-NA-C1A | 5.95 | 109.39 | 106.68 |
| 21 | F | 304 | CLA | C4A-NA-C1A | 5.95 | 109.39 | 106.68 |
| 21 | B | 832 | CLA | C4A-NA-C1A | 5.94 | 109.39 | 106.68 |
| 31 | 9 | 616 | XAT | C28-C29-C30 | 5.94 | 128.35 | 119.01 |
| 21 | A | 835 | CLA | C4A-NA-C1A | 5.94 | 109.39 | 106.68 |
| 29 | 6 | 606 | CHL | C1B-CHB-C4A | -5.93 | 117.51 | 121.32 |
| 21 | A | 812 | CLA | C4A-NA-C1A | 5.92 | 109.38 | 106.68 |
| 21 | B | 801 | CLA | CHD-C4C-C3C | -5.92 | 116.14 | 124.77 |
| 21 | B | 801 | CLA | C2D-C1D-ND | 5.91 | 115.97 | 110.13 |
| 21 | A | 819 | CLA | C4A-NA-C1A | 5.90 | 109.37 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 803 | CLA | C4A-NA-C1A | 5.89 | 109.37 | 106.68 |
| 29 | a | 605 | CHL | C1A-CHA-C4D | -5.86 | 109.21 | 118.98 |
| 21 | B | 828 | CLA | C4A-NA-C1A | 5.85 | 109.35 | 106.68 |
| 21 | 5 | 603 | CLA | C4A-NA-C1A | 5.84 | 109.34 | 106.68 |
| 21 | 3 | 403 | CLA | C4A-NA-C1A | 5.83 | 109.34 | 106.68 |
| 21 | B | 830 | CLA | C4A-NA-C1A | 5.81 | 109.33 | 106.68 |
| 29 | 9 | 601 | CHL | C1A-CHA-C4D | -5.76 | 109.36 | 118.98 |
| 21 | B | 835 | CLA | C4A-NA-C1A | 5.75 | 109.30 | 106.68 |
| 29 | b | 306 | CHL | C1B-CHB-C4A | -5.74 | 117.63 | 121.32 |
| 29 | b | 302 | CHL | C1A-CHA-C4D | -5.73 | 109.43 | 118.98 |
| 21 | 2 | 608 | CLA | C4A-NA-C1A | 5.71 | 109.28 | 106.68 |
| 21 | c | 614 | CLA | C4A-NA-C1A | 5.70 | 109.28 | 106.68 |
| 21 | A | 830 | CLA | CMD-C2D-C1D | 5.69 | 134.75 | 124.73 |
| 21 | 3 | 409 | CLA | CMD-C2D-C1D | 5.69 | 134.75 | 124.73 |
| 21 | 2 | 609 | CLA | CMD-C2D-C1D | 5.69 | 134.75 | 124.73 |
| 21 | 1 | 314 | CLA | C4A-NA-C1A | 5.68 | 109.27 | 106.68 |
| 29 | 9 | 606 | CHL | C1B-CHB-C4A | -5.68 | 117.67 | 121.32 |
| 21 | B | 831 | CLA | C4A-NA-C1A | 5.65 | 109.26 | 106.68 |
| 21 | 8 | 609 | CLA | O2D-CGD-CBD | 5.64 | 121.09 | 111.23 |
| 29 | 5 | 606 | CHL | C1A-CHA-C4D | -5.63 | 109.58 | 118.98 |
| 29 | 6 | 601 | CHL | C1A-CHA-C4D | -5.63 | 109.58 | 118.98 |
| 24 | M | 101 | BCR | C15-C16-C17 | 5.63 | 135.03 | 123.52 |
| 21 | 8 | 609 | CLA | CMD-C2D-C1D | 5.63 | 134.63 | 124.73 |
| 21 | A | 852 | CLA | C4A-NA-C1A | 5.61 | 109.24 | 106.68 |
| 29 | 1 | 302 | CHL | C1A-CHA-C4D | -5.59 | 109.65 | 118.98 |
| 21 | 2 | 603 | CLA | C4A-NA-C1A | 5.55 | 109.21 | 106.68 |
| 29 | 7 | 406 | CHL | C1A-CHA-C4D | -5.53 | 109.76 | 118.98 |
| 29 | 9 | 609 | CHL | C1B-CHB-C4A | -5.52 | 117.77 | 121.32 |
| 29 | b | 307 | CHL | C1A-CHA-C4D | -5.52 | 109.77 | 118.98 |
| 29 | 4 | 607 | CHL | OBD-CAD-CBD | 5.52 | 133.92 | 125.82 |
| 29 | a | 601 | CHL | C1A-CHA-C4D | -5.52 | 109.78 | 118.98 |
| 29 | 2 | 607 | CHL | OBD-CAD-CBD | 5.51 | 133.91 | 125.82 |
| 29 | b | 308 | CHL | C1A-CHA-C4D | -5.50 | 109.81 | 118.98 |
| 29 | b | 307 | CHL | C1B-CHB-C4A | -5.49 | 117.79 | 121.32 |
| 29 | 2 | 614 | CHL | C1B-CHB-C4A | -5.49 | 117.79 | 121.32 |
| 21 | c | 603 | CLA | C4A-NA-C1A | 5.49 | 109.18 | 106.68 |
| 29 | 2 | 606 | CHL | C1A-CHA-C4D | -5.48 | 109.84 | 118.98 |
| 29 | 8 | 606 | CHL | C1A-CHA-C4D | -5.48 | 109.84 | 118.98 |
| 29 | 6 | 606 | CHL | C1A-CHA-C4D | -5.48 | 109.84 | 118.98 |
| 21 | 4 | 609 | CLA | C1D-ND-C4D | -5.46 | 102.48 | 106.31 |
| 29 | 4 | 606 | CHL | C1B-CHB-C4A | -5.46 | 117.81 | 121.32 |
| 24 | K | 205 | BCR | C20-C21-C22 | -5.46 | 119.62 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | b | 306 | CHL | C1A-CHA-C4D | -5.46 | 109.88 | 118.98 |
| 29 | 9 | 606 | CHL | C1A-CHA-C4D | -5.45 | 109.89 | 118.98 |
| 29 | c | 606 | CHL | C1A-CHA-C4D | -5.45 | 109.89 | 118.98 |
| 21 | 7 | 407 | CLA | CMC-C2C-C1C | -5.45 | 116.52 | 125.03 |
| 29 | b | 309 | CHL | C1A-CHA-C4D | -5.45 | 109.89 | 118.98 |
| 29 | 2 | 605 | CHL | C1A-CHA-C4D | -5.44 | 109.90 | 118.98 |
| 29 | 9 | 605 | CHL | C1A-CHA-C4D | -5.44 | 109.91 | 118.98 |
| 29 | 6 | 602 | CHL | C1A-CHA-C4D | -5.43 | 109.92 | 118.98 |
| 29 | 1 | 307 | CHL | C1A-CHA-C4D | -5.42 | 109.93 | 118.98 |
| 29 | 5 | 601 | CHL | C1B-CHB-C4A | -5.42 | 117.84 | 121.32 |
| 29 | 9 | 609 | CHL | C1A-CHA-C4D | -5.42 | 109.94 | 118.98 |
| 29 | 2 | 607 | CHL | C1B-CHB-C4A | -5.41 | 117.84 | 121.32 |
| 29 | 9 | 608 | CHL | C1B-CHB-C4A | -5.41 | 117.84 | 121.32 |
| 29 | c | 607 | CHL | C1A-CHA-C4D | -5.40 | 109.97 | 118.98 |
| 24 | G | 205 | BCR | C15-C16-C17 | 5.40 | 134.56 | 123.52 |
| 29 | 6 | 614 | CHL | C1A-CHA-C4D | -5.39 | 109.98 | 118.98 |
| 29 | c | 605 | CHL | C1A-CHA-C4D | -5.39 | 109.99 | 118.98 |
| 29 | 3 | 407 | CHL | C1A-CHA-C4D | -5.39 | 110.00 | 118.98 |
| 29 | b | 310 | CHL | C1A-CHA-C4D | -5.38 | 110.00 | 118.98 |
| 29 | c | 601 | CHL | C1B-CHB-C4A | -5.38 | 117.86 | 121.32 |
| 29 | 6 | 607 | CHL | C1A-CHA-C4D | -5.38 | 110.01 | 118.98 |
| 29 | 4 | 607 | CHL | C1A-CHA-C4D | -5.38 | 110.01 | 118.98 |
| 29 | 4 | 606 | CHL | C1A-CHA-C4D | -5.38 | 110.01 | 118.98 |
| 29 | a | 608 | CHL | C1A-CHA-C4D | -5.38 | 110.01 | 118.98 |
| 29 | c | 601 | CHL | C1A-CHA-C4D | -5.37 | 110.03 | 118.98 |
| 29 | a | 607 | CHL | C1B-CHB-C4A | -5.36 | 117.87 | 121.32 |
| 29 | 4 | 614 | CHL | C1A-CHA-C4D | -5.36 | 110.03 | 118.98 |
| 29 | a | 609 | CHL | C1A-CHA-C4D | -5.36 | 110.03 | 118.98 |
| 29 | 6 | 605 | CHL | C1B-CHB-C4A | -5.36 | 117.87 | 121.32 |
| 21 | A | 829 | CLA | C4A-NA-C1A | 5.36 | 109.12 | 106.68 |
| 24 | B | 846 | BCR | C16-C17-C18 | -5.35 | 119.77 | 127.28 |
| 21 | B | 801 | CLA | C4A-NA-C1A | -5.35 | 104.24 | 106.68 |
| 29 | 2 | 602 | CHL | C1A-CHA-C4D | -5.35 | 110.06 | 118.98 |
| 29 | 3 | 407 | CHL | C1B-CHB-C4A | -5.35 | 117.88 | 121.32 |
| 29 | c | 608 | CHL | C1A-CHA-C4D | -5.35 | 110.06 | 118.98 |
| 29 | 2 | 601 | CHL | C1A-CHA-C4D | -5.34 | 110.06 | 118.98 |
| 29 | 8 | 613 | CHL | C1A-CHA-C4D | -5.34 | 110.08 | 118.98 |
| 29 | a | 606 | CHL | C1A-CHA-C4D | -5.32 | 110.10 | 118.98 |
| 29 | 9 | 608 | CHL | C1A-CHA-C4D | -5.32 | 110.10 | 118.98 |
| 21 | A | 801 | CLA | CMD-C2D-C1D | 5.32 | 134.10 | 124.73 |
| 29 | c | 609 | CHL | C1A-CHA-C4D | -5.32 | 110.11 | 118.98 |
| 29 | 2 | 607 | CHL | C1A-CHA-C4D | -5.31 | 110.12 | 118.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 6 | 605 | CHL | C1A-CHA-C4D | -5.31 | 110.12 | 118.98 |
| 29 | 4 | 605 | CHL | C1A-CHA-C4D | -5.31 | 110.13 | 118.98 |
| 29 | 1 | 307 | CHL | C1B-CHB-C4A | -5.31 | 117.91 | 121.32 |
| 29 | 8 | 605 | CHL | C1A-CHA-C4D | -5.30 | 110.13 | 118.98 |
| 29 | 2 | 606 | CHL | C1B-CHB-C4A | -5.30 | 117.91 | 121.32 |
| 29 | 9 | 607 | CHL | C1A-CHA-C4D | -5.27 | 110.18 | 118.98 |
| 29 | a | 607 | CHL | C1A-CHA-C4D | -5.27 | 110.19 | 118.98 |
| 24 | A | 849 | BCR | C15-C16-C17 | 5.25 | 134.26 | 123.52 |
| 24 | 6 | 618 | BCR | C15-C16-C17 | -5.24 | 112.79 | 123.52 |
| 29 | 2 | 602 | CHL | C1B-CHB-C4A | -5.23 | 117.96 | 121.32 |
| 29 | 5 | 601 | CHL | C1A-CHA-C4D | -5.23 | 110.26 | 118.98 |
| 29 | 8 | 607 | CHL | C1A-CHA-C4D | -5.23 | 110.26 | 118.98 |
| 21 | 3 | 409 | CLA | C1-C2-C3 | -5.22 | 117.64 | 126.20 |
| 29 | 4 | 607 | CHL | C1B-CHB-C4A | -5.17 | 118.00 | 121.32 |
| 21 | A | 828 | CLA | C4A-NA-C1A | 5.16 | 109.03 | 106.68 |
| 30 | 2 | 616 | LUT | C35-C15-C14 | 5.14 | 134.04 | 123.52 |
| 31 | a | 618 | XAT | C35-C15-C14 | 5.14 | 134.04 | 123.52 |
| 21 | 3 | 415 | CLA | C4A-NA-C1A | 5.14 | 109.02 | 106.68 |
| 21 | B | 801 | CLA | C2B-C1B-NB | 5.13 | 115.65 | 110.33 |
| 29 | 4 | 614 | CHL | C1B-CHB-C4A | -5.12 | 118.03 | 121.32 |
| 29 | 2 | 614 | CHL | C1A-CHA-C4D | -5.08 | 110.51 | 118.98 |
| 30 | 7 | 415 | LUT | C35-C15-C14 | 5.04 | 133.84 | 123.52 |
| 29 | a | 608 | CHL | C1B-CHB-C4A | -5.04 | 118.08 | 121.32 |
| 29 | c | 601 | CHL | OBD-CAD-CBD | 5.02 | 133.20 | 125.82 |
| 29 | 9 | 608 | CHL | OBD-CAD-CBD | 5.01 | 133.17 | 125.82 |
| 29 | b | 309 | CHL | OBD-CAD-CBD | 5.01 | 133.17 | 125.82 |
| 21 | B | 801 | CLA | C3B-C2B-C1B | -5.00 | 101.27 | 107.17 |
| 24 | K | 205 | BCR | C16-C17-C18 | -5.00 | 120.27 | 127.28 |
| 29 | a | 608 | CHL | OBD-CAD-CBD | 4.99 | 133.15 | 125.82 |
| 29 | 5 | 606 | CHL | OBD-CAD-CBD | 4.99 | 133.14 | 125.82 |
| 24 | G | 201 | BCR | C15-C16-C17 | 4.97 | 133.69 | 123.52 |
| 29 | 8 | 607 | CHL | OBD-CAD-CBD | 4.95 | 133.09 | 125.82 |
| 29 | 6 | 601 | CHL | OBD-CAD-CBD | 4.93 | 133.06 | 125.82 |
| 29 | 2 | 607 | CHL | OBD-CAD-C3D | -4.90 | 120.25 | 127.89 |
| 31 | 6 | 617 | XAT | C15-C35-C34 | 4.90 | 133.54 | 123.52 |
| 29 | 9 | 601 | CHL | OBD-CAD-CBD | 4.87 | 132.97 | 125.82 |
| 29 | c | 608 | CHL | OBD-CAD-CBD | 4.87 | 132.97 | 125.82 |
| 30 | 6 | 616 | LUT | C35-C15-C14 | 4.87 | 133.48 | 123.52 |
| 24 | J | 104 | BCR | C24-C23-C22 | -4.85 | 119.06 | 126.23 |
| 29 | 4 | 605 | CHL | C1B-CHB-C4A | -4.84 | 118.21 | 121.32 |
| 29 | 8 | 613 | CHL | OBD-CAD-CBD | 4.83 | 132.91 | 125.82 |
| 21 | A | 837 | CLA | C4A-NA-C1A | 4.83 | 108.88 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 6 | 601 | CHL | CMC-C2C-C3C | -4.83 | 116.69 | 126.76 |
| 24 | B | 844 | BCR | C3-C4-C5 | -4.83 | 105.45 | 114.06 |
| 29 | a | 605 | CHL | OBD-CAD-CBD | 4.82 | 132.90 | 125.82 |
| 29 | b | 302 | CHL | OBD-CAD-CBD | 4.82 | 132.90 | 125.82 |
| 21 | 4 | 609 | CLA | O2D-CGD-CBD | 4.82 | 119.65 | 111.23 |
| 29 | 2 | 601 | CHL | C1B-CHB-C4A | -4.81 | 118.23 | 121.32 |
| 30 | 4 | 615 | LUT | C15-C35-C34 | 4.79 | 133.32 | 123.52 |
| 29 | 4 | 607 | CHL | OBD-CAD-C3D | -4.78 | 120.43 | 127.89 |
| 31 | 8 | 615 | XAT | C35-C15-C14 | 4.78 | 133.29 | 123.52 |
| 24 | B | 844 | BCR | C20-C21-C22 | -4.77 | 120.58 | 127.28 |
| 29 | 6 | 607 | CHL | OBD-CAD-CBD | 4.76 | 132.81 | 125.82 |
| 30 | 3 | 416 | LUT | C15-C35-C34 | 4.76 | 133.26 | 123.52 |
| 29 | 8 | 606 | CHL | OBD-CAD-CBD | 4.76 | 132.81 | 125.82 |
| 21 | 7 | 407 | CLA | C3B-C4B-NB | 4.75 | 114.77 | 110.53 |
| 29 | 6 | 602 | CHL | OBD-CAD-CBD | 4.73 | 132.77 | 125.82 |
| 29 | c | 607 | CHL | OBD-CAD-CBD | 4.70 | 132.72 | 125.82 |
| 21 | 3 | 409 | CLA | C3B-C4B-NB | 4.70 | 114.72 | 110.53 |
| 21 | 7 | 407 | CLA | C4D-C3D-CAD | 4.69 | 113.20 | 108.11 |
| 29 | 8 | 605 | CHL | OBD-CAD-CBD | 4.69 | 132.70 | 125.82 |
| 29 | b | 307 | CHL | OBD-CAD-CBD | 4.66 | 132.67 | 125.82 |
| 29 | 6 | 606 | CHL | OBD-CAD-CBD | 4.65 | 132.65 | 125.82 |
| 29 | 9 | 601 | CHL | C1A-CHA-CBD | 4.65 | 144.26 | 132.36 |
| 29 | b | 310 | CHL | OBD-CAD-CBD | 4.65 | 132.64 | 125.82 |
| 29 | 9 | 607 | CHL | OBD-CAD-CBD | 4.61 | 132.59 | 125.82 |
| 21 | 4 | 609 | CLA | C3B-C4B-NB | 4.61 | 114.64 | 110.53 |
| 24 | B | 846 | BCR | C3-C4-C5 | -4.61 | 105.84 | 114.06 |
| 29 | 2 | 606 | CHL | OBD-CAD-CBD | 4.61 | 132.58 | 125.82 |
| 29 | c | 606 | CHL | OBD-CAD-CBD | 4.61 | 132.58 | 125.82 |
| 29 | 2 | 601 | CHL | OBD-CAD-CBD | 4.60 | 132.58 | 125.82 |
| 24 | B | 843 | BCR | C15-C14-C13 | -4.60 | 120.83 | 127.28 |
| 31 | 9 | 616 | XAT | C30-C31-C32 | 4.58 | 136.47 | 123.20 |
| 29 | a | 605 | CHL | C1A-CHA-CBD | 4.58 | 144.08 | 132.36 |
| 29 | 4 | 614 | CHL | OBD-CAD-CBD | 4.57 | 132.53 | 125.82 |
| 21 | 2 | 609 | CLA | O2D-CGD-CBD | 4.57 | 119.22 | 111.23 |
| 29 | 9 | 605 | CHL | OBD-CAD-CBD | 4.55 | 132.50 | 125.82 |
| 29 | 4 | 606 | CHL | OBD-CAD-CBD | 4.55 | 132.50 | 125.82 |
| 29 | 2 | 602 | CHL | OBD-CAD-CBD | 4.52 | 132.46 | 125.82 |
| 30 | a | 615 | LUT | C27-C28-C29 | 4.52 | 136.05 | 126.32 |
| 30 | 1 | 317 | LUT | C15-C35-C34 | 4.51 | 132.75 | 123.52 |
| 29 | 2 | 614 | CHL | OBD-CAD-CBD | 4.50 | 132.43 | 125.82 |
| 29 | b | 308 | CHL | OBD-CAD-CBD | 4.50 | 132.43 | 125.82 |
| 29 | b | 306 | CHL | OBD-CAD-CBD | 4.50 | 132.42 | 125.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | K | 205 | BCR | C7-C8-C9 | -4.50 | 119.58 | 126.23 |
| 21 | B | 801 | CLA | C2C-C1C-NC | 4.49 | 114.70 | 109.98 |
| 21 | B | 801 | CLA | C3D-C2D-C1D | -4.49 | 99.71 | 105.83 |
| 24 | K | 205 | BCR | C3-C4-C5 | -4.49 | 106.05 | 114.06 |
| 30 | 4 | 615 | LUT | C35-C15-C14 | 4.46 | 132.65 | 123.52 |
| 29 | 9 | 608 | CHL | OBD-CAD-C3D | -4.46 | 120.94 | 127.89 |
| 21 | B | 801 | CLA | C3D-C4D-ND | 4.46 | 117.23 | 109.99 |
| 29 | 1 | 302 | CHL | OBD-CAD-CBD | 4.46 | 132.36 | 125.82 |
| 30 | 1 | 317 | LUT | C35-C15-C14 | 4.45 | 132.63 | 123.52 |
| 30 | 3 | 416 | LUT | C10-C11-C12 | 4.45 | 136.10 | 123.20 |
| 29 | 1 | 307 | CHL | OBD-CAD-CBD | 4.45 | 132.35 | 125.82 |
| 31 | 9 | 616 | XAT | C35-C15-C14 | 4.44 | 132.61 | 123.52 |
| 29 | c | 601 | CHL | OBD-CAD-C3D | -4.44 | 120.97 | 127.89 |
| 29 | 7 | 406 | CHL | OBD-CAD-CBD | 4.44 | 132.34 | 125.82 |
| 29 | 5 | 606 | CHL | OBD-CAD-C3D | -4.43 | 120.98 | 127.89 |
| 29 | b | 302 | CHL | C1A-CHA-CBD | 4.43 | 143.70 | 132.36 |
| 21 | 3 | 409 | CLA | O2D-CGD-CBD | 4.42 | 118.96 | 111.23 |
| 29 | 9 | 609 | CHL | OBD-CAD-CBD | 4.42 | 132.31 | 125.82 |
| 29 | 8 | 613 | CHL | OBD-CAD-C3D | -4.41 | 121.01 | 127.89 |
| 24 | B | 844 | BCR | C11-C10-C9 | -4.41 | 121.09 | 127.28 |
| 29 | a | 609 | CHL | OBD-CAD-CBD | 4.41 | 132.30 | 125.82 |
| 21 | 1 | 309 | CLA | CMD-C2D-C1D | 4.40 | 132.48 | 124.73 |
| 29 | 6 | 614 | CHL | OBD-CAD-CBD | 4.38 | 132.25 | 125.82 |
| 29 | 6 | 605 | CHL | OBD-CAD-CBD | 4.37 | 132.23 | 125.82 |
| 30 | a | 616 | LUT | C35-C15-C14 | 4.35 | 132.42 | 123.52 |
| 29 | a | 601 | CHL | OBD-CAD-CBD | 4.35 | 132.21 | 125.82 |
| 29 | a | 601 | CHL | C1A-CHA-CBD | 4.35 | 143.50 | 132.36 |
| 29 | 2 | 605 | CHL | OBD-CAD-CBD | 4.34 | 132.20 | 125.82 |
| 21 | B | 801 | CLA | CHD-C1D-ND | -4.34 | 118.70 | 124.80 |
| 31 | 9 | 616 | XAT | C39-C29-C30 | -4.33 | 115.80 | 122.82 |
| 24 | J | 101 | BCR | C21-C20-C19 | 4.33 | 135.74 | 123.20 |
| 29 | a | 608 | CHL | OBD-CAD-C3D | -4.31 | 121.16 | 127.89 |
| 29 | b | 309 | CHL | OBD-CAD-C3D | -4.31 | 121.17 | 127.89 |
| 29 | 6 | 601 | CHL | OBD-CAD-C3D | -4.31 | 121.17 | 127.89 |
| 29 | 6 | 601 | CHL | C1A-CHA-CBD | 4.30 | 143.38 | 132.36 |
| 31 | 9 | 616 | XAT | C8-C9-C10 | 4.30 | 125.77 | 119.01 |
| 29 | c | 607 | CHL | OBD-CAD-C3D | -4.30 | 121.19 | 127.89 |
| 29 | b | 310 | CHL | OBD-CAD-C3D | -4.29 | 121.20 | 127.89 |
| 29 | a | 609 | CHL | CMD-C2D-C3D | -4.28 | 116.12 | 124.68 |
| 29 | 6 | 602 | CHL | OBD-CAD-C3D | -4.28 | 121.22 | 127.89 |
| 29 | a | 607 | CHL | OBD-CAD-CBD | 4.27 | 132.09 | 125.82 |
| 29 | 5 | 601 | CHL | OBD-CAD-CBD | 4.27 | 132.09 | 125.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | c | 617 | XAT | C35-C15-C14 | 4.27 | 132.25 | 123.52 |
| 29 | c | 608 | CHL | OBD-CAD-C3D | -4.25 | 121.26 | 127.89 |
| 31 | 9 | 616 | XAT | C32-C33-C34 | 4.25 | 125.69 | 119.01 |
| 21 | 2 | 609 | CLA | C1-C2-C3 | -4.25 | 119.24 | 126.20 |
| 29 | 8 | 607 | CHL | OBD-CAD-C3D | -4.24 | 121.28 | 127.89 |
| 32 | c | 618 | NEX | C15-C35-C34 | 4.24 | 132.19 | 123.52 |
| 29 | 8 | 606 | CHL | OBD-CAD-C3D | -4.23 | 121.29 | 127.89 |
| 30 | 8 | 614 | LUT | C15-C35-C34 | 4.23 | 132.17 | 123.52 |
| 31 | 9 | 616 | XAT | C27-C28-C29 | 4.21 | 132.07 | 125.53 |
| 29 | b | 307 | CHL | OBD-CAD-C3D | -4.21 | 121.33 | 127.89 |
| 21 | A | 801 | CLA | CHD-C1D-ND | -4.21 | 118.88 | 124.80 |
| 30 | 8 | 614 | LUT | C35-C15-C14 | 4.20 | 132.11 | 123.52 |
| 29 | 2 | 606 | CHL | OBD-CAD-C3D | -4.19 | 121.36 | 127.89 |
| 29 | 5 | 606 | CHL | C1A-CHA-CBD | 4.18 | 143.06 | 132.36 |
| 29 | 2 | 602 | CHL | OBD-CAD-C3D | -4.18 | 121.38 | 127.89 |
| 29 | b | 302 | CHL | OBD-CAD-C3D | -4.17 | 121.39 | 127.89 |
| 29 | a | 605 | CHL | OBD-CAD-C3D | -4.16 | 121.41 | 127.89 |
| 27 | B | 847 | DGD | O2G-C1B-C2B | 4.15 | 120.46 | 111.48 |
| 29 | 2 | 602 | CHL | C1-C2-C3 | -4.15 | 119.40 | 126.20 |
| 29 | a | 606 | CHL | OBD-CAD-CBD | 4.14 | 131.90 | 125.82 |
| 29 | 9 | 601 | CHL | OBD-CAD-C3D | -4.14 | 121.44 | 127.89 |
| 29 | c | 608 | CHL | C1A-CHA-CBD | 4.12 | 142.90 | 132.36 |
| 29 | 1 | 302 | CHL | OBD-CAD-C3D | -4.12 | 121.47 | 127.89 |
| 29 | 9 | 605 | CHL | OBD-CAD-C3D | -4.12 | 121.47 | 127.89 |
| 29 | b | 308 | CHL | C1A-CHA-CBD | 4.11 | 142.89 | 132.36 |
| 29 | a | 606 | CHL | CMD-C2D-C3D | -4.11 | 116.47 | 124.68 |
| 29 | 9 | 606 | CHL | OBD-CAD-CBD | 4.11 | 131.85 | 125.82 |
| 24 | 3 | 419 | BCR | C8-C9-C10 | 4.10 | 125.46 | 119.01 |
| 29 | 4 | 605 | CHL | OBD-CAD-CBD | 4.09 | 131.83 | 125.82 |
| 24 | M | 101 | BCR | C16-C15-C14 | 4.09 | 131.89 | 123.52 |
| 29 | 4 | 606 | CHL | OBD-CAD-C3D | -4.09 | 121.52 | 127.89 |
| 29 | 9 | 609 | CHL | CMD-C2D-C3D | -4.09 | 116.52 | 124.68 |
| 30 | a | 615 | LUT | C26-C27-C28 | 4.09 | 130.94 | 124.58 |
| 24 | B | 845 | BCR | C15-C16-C17 | -4.08 | 115.17 | 123.52 |
| 29 | 8 | 606 | CHL | C1A-CHA-CBD | 4.08 | 142.80 | 132.36 |
| 24 | B | 843 | BCR | C28-C27-C26 | -4.07 | 106.79 | 114.06 |
| 29 | c | 606 | CHL | C1A-CHA-CBD | 4.07 | 142.78 | 132.36 |
| 29 | b | 306 | CHL | OBD-CAD-C3D | -4.07 | 121.54 | 127.89 |
| 24 | 7 | 418 | BCR | C16-C15-C14 | 4.07 | 131.84 | 123.52 |
| 29 | 2 | 606 | CHL | C1A-CHA-CBD | 4.07 | 142.78 | 132.36 |
| 29 | 1 | 302 | CHL | C1A-CHA-CBD | 4.06 | 142.76 | 132.36 |
| 29 | a | 606 | CHL | C1A-CHA-CBD | 4.06 | 142.75 | 132.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 6 | 602 | CHL | C1A-CHA-CBD | 4.06 | 142.75 | 132.36 |
| 29 | 6 | 606 | CHL | C1A-CHA-CBD | 4.06 | 142.75 | 132.36 |
| 31 | 3 | 417 | XAT | C15-C35-C34 | 4.05 | 131.81 | 123.52 |
| 29 | 2 | 601 | CHL | OBD-CAD-C3D | -4.05 | 121.58 | 127.89 |
| 29 | 8 | 605 | CHL | OBD-CAD-C3D | -4.04 | 121.58 | 127.89 |
| 29 | 9 | 607 | CHL | C1A-CHA-CBD | 4.04 | 142.70 | 132.36 |
| 29 | 9 | 606 | CHL | C1A-CHA-CBD | 4.04 | 142.70 | 132.36 |
| 29 | b | 309 | CHL | C1A-CHA-CBD | 4.03 | 142.68 | 132.36 |
| 29 | 7 | 406 | CHL | C1A-CHA-CBD | 4.03 | 142.67 | 132.36 |
| 24 | O | 205 | BCR | C15-C16-C17 | 4.03 | 131.76 | 123.52 |
| 29 | 6 | 607 | CHL | OBD-CAD-C3D | -4.02 | 121.61 | 127.89 |
| 29 | c | 609 | CHL | C1A-CHA-CBD | 4.02 | 142.65 | 132.36 |
| 29 | 7 | 406 | CHL | OBD-CAD-C3D | -4.01 | 121.63 | 127.89 |
| 29 | 6 | 607 | CHL | CMD-C2D-C3D | -4.01 | 116.67 | 124.68 |
| 29 | c | 606 | CHL | OBD-CAD-C3D | -4.01 | 121.64 | 127.89 |
| 30 | 5 | 615 | LUT | C35-C15-C14 | 4.01 | 131.72 | 123.52 |
| 29 | 9 | 607 | CHL | OBD-CAD-C3D | -4.00 | 121.65 | 127.89 |
| 32 | b | 318 | NEX | C15-C35-C34 | 4.00 | 131.70 | 123.52 |
| 29 | a | 608 | CHL | C1A-CHA-CBD | 4.00 | 142.60 | 132.36 |
| 24 | J | 104 | BCR | C11-C12-C13 | -3.99 | 115.41 | 126.36 |
| 29 | 9 | 609 | CHL | C1A-CHA-CBD | 3.99 | 142.59 | 132.36 |
| 29 | 6 | 607 | CHL | C1A-CHA-CBD | 3.99 | 142.58 | 132.36 |
| 29 | 7 | 406 | CHL | CMD-C2D-C3D | -3.99 | 116.71 | 124.68 |
| 29 | 4 | 607 | CHL | C1A-CHA-CBD | 3.99 | 142.58 | 132.36 |
| 31 | 6 | 617 | XAT | C8-C9-C10 | 3.99 | 125.28 | 119.01 |
| 29 | c | 605 | CHL | OBD-CAD-C3D | -3.99 | 121.68 | 127.89 |
| 29 | 3 | 407 | CHL | C3D-CAD-CBD | 3.98 | 112.85 | 107.61 |
| 29 | 2 | 614 | CHL | OBD-CAD-C3D | -3.98 | 121.68 | 127.89 |
| 29 | 4 | 614 | CHL | OBD-CAD-C3D | -3.98 | 121.69 | 127.89 |
| 29 | 8 | 607 | CHL | CMD-C2D-C3D | -3.97 | 116.74 | 124.68 |
| 29 | 1 | 307 | CHL | OBD-CAD-C3D | -3.97 | 121.69 | 127.89 |
| 29 | c | 601 | CHL | C1A-CHA-CBD | 3.97 | 142.53 | 132.36 |
| 24 | J | 104 | BCR | C38-C26-C25 | -3.97 | 120.15 | 124.48 |
| 21 | 7 | 407 | CLA | C3D-C2D-C1D | -3.97 | 100.41 | 105.83 |
| 29 | c | 605 | CHL | CMD-C2D-C3D | -3.97 | 116.75 | 124.68 |
| 29 | a | 606 | CHL | OBD-CAD-C3D | -3.97 | 121.70 | 127.89 |
| 24 | B | 844 | BCR | C7-C8-C9 | -3.96 | 120.38 | 126.23 |
| 21 | 7 | 407 | CLA | C3D-C4D-ND | 3.96 | 116.42 | 109.99 |
| 24 | O | 205 | BCR | C16-C15-C14 | 3.96 | 131.61 | 123.52 |
| 21 | 4 | 609 | CLA | CMD-C2D-C3D | -3.95 | 118.62 | 127.69 |
| 24 | 3 | 419 | BCR | C16-C15-C14 | 3.95 | 131.61 | 123.52 |
| 30 | b | 316 | LUT | C15-C35-C34 | 3.95 | 131.60 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 4 | 614 | CHL | C1A-CHA-CBD | 3.95 | 142.47 | 132.36 |
| 29 | 6 | 606 | CHL | OBD-CAD-C3D | -3.94 | 121.74 | 127.89 |
| 29 | 1 | 307 | CHL | CMD-C2D-C3D | -3.94 | 116.81 | 124.68 |
| 29 | 6 | 605 | CHL | CMD-C2D-C3D | -3.94 | 116.81 | 124.68 |
| 29 | b | 306 | CHL | C1A-CHA-CBD | 3.94 | 142.44 | 132.36 |
| 29 | b | 308 | CHL | OBD-CAD-C3D | -3.94 | 121.75 | 127.89 |
| 29 | a | 609 | CHL | OBD-CAD-C3D | -3.93 | 121.76 | 127.89 |
| 29 | 6 | 614 | CHL | CMD-C2D-C3D | -3.93 | 116.83 | 124.68 |
| 29 | 6 | 614 | CHL | OBD-CAD-C3D | -3.93 | 121.77 | 127.89 |
| 29 | 9 | 605 | CHL | C1A-CHA-CBD | 3.93 | 142.41 | 132.36 |
| 29 | c | 607 | CHL | C1A-CHA-CBD | 3.92 | 142.41 | 132.36 |
| 30 | 5 | 615 | LUT | C10-C11-C12 | 3.92 | 134.57 | 123.20 |
| 24 | B | 844 | BCR | C15-C14-C13 | -3.92 | 121.78 | 127.28 |
| 29 | 2 | 605 | CHL | C1A-CHA-CBD | 3.92 | 142.39 | 132.36 |
| 29 | 1 | 307 | CHL | C1A-CHA-CBD | 3.91 | 142.38 | 132.36 |
| 24 | B | 844 | BCR | C28-C27-C26 | -3.91 | 107.08 | 114.06 |
| 29 | 9 | 608 | CHL | C1A-CHA-CBD | 3.91 | 142.37 | 132.36 |
| 29 | 6 | 601 | CHL | CMD-C2D-C3D | -3.90 | 116.88 | 124.68 |
| 29 | b | 307 | CHL | C1A-CHA-CBD | 3.90 | 142.35 | 132.36 |
| 32 | 9 | 617 | NEX | C35-C15-C14 | 3.90 | 131.50 | 123.52 |
| 31 | 6 | 617 | XAT | C19-C9-C10 | -3.90 | 116.50 | 122.82 |
| 29 | 4 | 614 | CHL | CMD-C2D-C3D | -3.90 | 116.90 | 124.68 |
| 29 | 3 | 407 | CHL | CMD-C2D-C3D | -3.89 | 116.90 | 124.68 |
| 29 | 2 | 605 | CHL | CMD-C2D-C3D | -3.89 | 116.91 | 124.68 |
| 29 | 4 | 606 | CHL | C1A-CHA-CBD | 3.89 | 142.32 | 132.36 |
| 29 | 6 | 605 | CHL | OBD-CAD-C3D | -3.89 | 121.83 | 127.89 |
| 24 | J | 104 | BCR | C20-C21-C22 | -3.89 | 121.83 | 127.28 |
| 24 | J | 103 | BCR | C10-C11-C12 | 3.89 | 134.46 | 123.20 |
| 24 | 8 | 616 | BCR | C16-C15-C14 | 3.88 | 131.47 | 123.52 |
| 29 | 5 | 606 | CHL | CMD-C2D-C3D | -3.88 | 116.92 | 124.68 |
| 29 | c | 609 | CHL | OBD-CAD-CBD | 3.88 | 131.52 | 125.82 |
| 30 | a | 615 | LUT | C35-C15-C14 | 3.88 | 131.46 | 123.52 |
| 29 | 8 | 607 | CHL | C1A-CHA-CBD | 3.88 | 142.29 | 132.36 |
| 29 | 6 | 614 | CHL | C1A-CHA-CBD | 3.87 | 142.28 | 132.36 |
| 29 | 5 | 601 | CHL | C1A-CHA-CBD | 3.87 | 142.27 | 132.36 |
| 29 | c | 606 | CHL | CMD-C2D-C3D | -3.87 | 116.95 | 124.68 |
| 29 | b | 307 | CHL | CMD-C2D-C3D | -3.87 | 116.96 | 124.68 |
| 24 | 7 | 417 | BCR | C16-C15-C14 | 3.86 | 131.42 | 123.52 |
| 29 | 5 | 601 | CHL | CBC-CAC-C3C | -3.86 | 107.35 | 112.87 |
| 24 | J | 101 | BCR | C20-C21-C22 | 3.86 | 132.69 | 127.28 |
| 29 | a | 601 | CHL | CMD-C2D-C3D | -3.86 | 116.98 | 124.68 |
| 29 | 2 | 607 | CHL | C1A-CHA-CBD | 3.86 | 142.24 | 132.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 8 | 606 | CHL | CMD-C2D-C3D | -3.85 | 116.98 | 124.68 |
| 29 | b | 309 | CHL | CMD-C2D-C3D | -3.85 | 116.98 | 124.68 |
| 29 | a | 605 | CHL | CMD-C2D-C3D | -3.85 | 116.98 | 124.68 |
| 29 | 8 | 605 | CHL | C1A-CHA-CBD | 3.85 | 142.23 | 132.36 |
| 21 | B | 801 | CLA | C1D-CHD-C4C | -3.85 | 117.83 | 126.02 |
| 29 | c | 608 | CHL | CMD-C2D-C3D | -3.85 | 116.99 | 124.68 |
| 31 | 9 | 616 | XAT | C19-C9-C10 | -3.85 | 116.58 | 122.82 |
| 29 | 2 | 605 | CHL | OBD-CAD-C3D | -3.85 | 121.89 | 127.89 |
| 29 | 4 | 605 | CHL | C1A-CHA-CBD | 3.84 | 142.19 | 132.36 |
| 29 | 2 | 601 | CHL | CMD-C2D-C3D | -3.84 | 117.01 | 124.68 |
| 29 | 2 | 607 | CHL | CMD-C2D-C3D | -3.84 | 117.02 | 124.68 |
| 29 | 5 | 601 | CHL | CMD-C2D-C3D | -3.83 | 117.02 | 124.68 |
| 21 | K | 202 | CLA | CAA-C2A-C3A | -3.83 | 102.64 | 113.00 |
| 21 | B | 801 | CLA | C1C-C2C-C3C | -3.83 | 102.95 | 106.98 |
| 29 | 2 | 601 | CHL | C1A-CHA-CBD | 3.83 | 142.16 | 132.36 |
| 29 | 6 | 606 | CHL | CMD-C2D-C3D | -3.82 | 117.05 | 124.68 |
| 29 | c | 607 | CHL | CMD-C2D-C3D | -3.82 | 117.05 | 124.68 |
| 29 | a | 607 | CHL | C1A-CHA-CBD | 3.82 | 142.14 | 132.36 |
| 29 | 4 | 605 | CHL | CAB-C3B-C2B | -3.82 | 116.70 | 124.69 |
| 24 | L | 306 | BCR | C16-C15-C14 | 3.82 | 131.33 | 123.52 |
| 29 | 9 | 605 | CHL | CMD-C2D-C3D | -3.81 | 117.07 | 124.68 |
| 29 | a | 608 | CHL | CMD-C2D-C3D | -3.81 | 117.07 | 124.68 |
| 24 | 3 | 419 | BCR | C34-C9-C10 | -3.81 | 116.64 | 122.82 |
| 21 | A | 830 | CLA | C1-C2-C3 | -3.81 | 119.96 | 126.20 |
| 29 | 4 | 605 | CHL | CMD-C2D-C3D | -3.80 | 117.08 | 124.68 |
| 30 | a | 615 | LUT | C39-C29-C30 | -3.80 | 116.66 | 122.82 |
| 29 | 8 | 613 | CHL | C1A-CHA-CBD | 3.80 | 142.09 | 132.36 |
| 29 | b | 310 | CHL | C1A-CHA-CBD | 3.80 | 142.08 | 132.36 |
| 29 | b | 308 | CHL | CMD-C2D-C3D | -3.80 | 117.10 | 124.68 |
| 29 | 8 | 605 | CHL | CMD-C2D-C3D | -3.79 | 117.10 | 124.68 |
| 31 | 9 | 616 | XAT | C12-C13-C14 | 3.79 | 124.97 | 119.01 |
| 21 | B | 801 | CLA | O2D-CGD-CBD | 3.78 | 117.85 | 111.23 |
| 29 | 2 | 614 | CHL | CMD-C2D-C3D | -3.78 | 117.13 | 124.68 |
| 30 | 9 | 615 | LUT | C15-C35-C34 | 3.77 | 131.24 | 123.52 |
| 24 | J | 104 | BCR | C1-C6-C5 | -3.77 | 117.48 | 122.64 |
| 29 | a | 607 | CHL | OBD-CAD-C3D | -3.77 | 122.01 | 127.89 |
| 29 | b | 302 | CHL | CMD-C2D-C3D | -3.77 | 117.15 | 124.68 |
| 29 | b | 310 | CHL | CMD-C2D-C3D | -3.76 | 117.16 | 124.68 |
| 29 | 4 | 606 | CHL | CMD-C2D-C3D | -3.76 | 117.16 | 124.68 |
| 30 | 7 | 415 | LUT | C10-C11-C12 | 3.76 | 134.10 | 123.20 |
| 24 | B | 846 | BCR | C7-C8-C9 | -3.76 | 120.67 | 126.23 |
| 21 | B | 801 | CLA | C1-C2-C3 | -3.76 | 120.04 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 609 | CHL | OBD-CAD-C3D | -3.76 | 122.03 | 127.89 |
| 24 | J | 103 | BCR | C16-C15-C14 | 3.76 | 131.21 | 123.52 |
| 21 | 4 | 609 | CLA | C1-C2-C3 | -3.76 | 120.04 | 126.20 |
| 29 | 9 | 608 | CHL | CMD-C2D-C3D | -3.75 | 117.18 | 124.68 |
| 29 | a | 609 | CHL | C1A-CHA-CBD | 3.74 | 141.94 | 132.36 |
| 30 | 2 | 616 | LUT | C19-C9-C10 | -3.74 | 116.75 | 122.82 |
| 21 | F | 302 | CLA | O2D-CGD-O1D | -3.74 | 116.56 | 123.85 |
| 29 | a | 607 | CHL | CMD-C2D-C3D | -3.73 | 117.22 | 124.68 |
| 29 | 2 | 607 | CHL | C1-C2-C3 | -3.73 | 120.73 | 126.76 |
| 29 | 9 | 606 | CHL | CMD-C2D-C3D | -3.73 | 117.23 | 124.68 |
| 29 | 9 | 609 | CHL | OBD-CAD-C3D | -3.73 | 122.08 | 127.89 |
| 24 | L | 306 | BCR | C37-C22-C21 | -3.72 | 116.78 | 122.82 |
| 29 | b | 306 | CHL | CMD-C2D-C3D | -3.72 | 117.25 | 124.68 |
| 29 | 4 | 607 | CHL | CMD-C2D-C3D | -3.72 | 117.25 | 124.68 |
| 29 | 2 | 602 | CHL | C1A-CHA-CBD | 3.72 | 141.88 | 132.36 |
| 29 | a | 601 | CHL | OBD-CAD-C3D | -3.71 | 122.10 | 127.89 |
| 31 | 7 | 416 | XAT | C15-C35-C34 | 3.71 | 131.11 | 123.52 |
| 24 | A | 849 | BCR | C37-C22-C21 | -3.71 | 116.81 | 122.82 |
| 30 | b | 317 | LUT | C15-C35-C34 | 3.70 | 131.09 | 123.52 |
| 31 | 4 | 616 | XAT | C15-C35-C34 | 3.70 | 131.09 | 123.52 |
| 29 | 4 | 607 | CHL | C1-C2-C3 | -3.70 | 120.78 | 126.76 |
| 24 | O | 205 | BCR | C37-C22-C21 | -3.69 | 116.83 | 122.82 |
| 29 | 8 | 613 | CHL | CMD-C2D-C3D | -3.69 | 117.31 | 124.68 |
| 29 | c | 601 | CHL | CMD-C2D-C3D | -3.69 | 117.31 | 124.68 |
| 24 | B | 843 | BCR | C7-C8-C9 | -3.68 | 120.78 | 126.23 |
| 29 | 9 | 607 | CHL | CMD-C2D-C3D | -3.67 | 117.34 | 124.68 |
| 24 | M | 101 | BCR | C37-C22-C21 | -3.67 | 116.87 | 122.82 |
| 29 | 1 | 302 | CHL | CMD-C2D-C3D | -3.67 | 117.35 | 124.68 |
| 21 | 3 | 409 | CLA | CMD-C2D-C3D | -3.67 | 119.28 | 127.69 |
| 21 | A | 801 | CLA | C1-C2-C3 | -3.66 | 120.20 | 126.20 |
| 24 | 7 | 418 | BCR | C37-C22-C21 | -3.66 | 116.89 | 122.82 |
| 29 | 6 | 605 | CHL | C1A-CHA-CBD | 3.66 | 141.73 | 132.36 |
| 29 | 5 | 601 | CHL | OBD-CAD-C3D | -3.66 | 122.19 | 127.89 |
| 24 | 6 | 618 | BCR | C16-C15-C14 | 3.65 | 130.99 | 123.52 |
| 24 | M | 101 | BCR | C8-C9-C10 | 3.65 | 124.75 | 119.01 |
| 24 | 2 | 618 | BCR | C16-C15-C14 | 3.65 | 130.99 | 123.52 |
| 24 | J | 104 | BCR | C21-C20-C19 | -3.64 | 112.66 | 123.20 |
| 21 | A | 830 | CLA | CMD-C2D-C3D | -3.64 | 119.35 | 127.69 |
| 29 | 2 | 614 | CHL | C1A-CHA-CBD | 3.64 | 141.67 | 132.36 |
| 21 | 2 | 609 | CLA | CMD-C2D-C3D | -3.63 | 119.37 | 127.69 |
| 29 | 4 | 614 | CHL | CBC-CAC-C3C | -3.62 | 107.70 | 112.87 |
| 24 | 7 | 418 | BCR | C34-C9-C10 | -3.61 | 116.97 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 7 | 415 | LUT | C12-C13-C14 | 3.61 | 124.68 | 119.01 |
| 21 | 7 | 407 | CLA | CHD-C1D-ND | -3.61 | 119.72 | 124.80 |
| 31 | 1 | 318 | XAT | C15-C35-C34 | 3.60 | 130.88 | 123.52 |
| 21 | B | 801 | CLA | CMB-C2B-C1B | 3.59 | 130.89 | 125.42 |
| 24 | 7 | 417 | BCR | C34-C9-C10 | -3.59 | 117.00 | 122.82 |
| 31 | 5 | 616 | XAT | C35-C15-C14 | 3.59 | 130.86 | 123.52 |
| 31 | c | 617 | XAT | C39-C29-C30 | -3.59 | 117.00 | 122.82 |
| 29 | 2 | 602 | CHL | CMD-C2D-C3D | -3.59 | 117.52 | 124.68 |
| 21 | 8 | 609 | CLA | CMD-C2D-C3D | -3.59 | 119.46 | 127.69 |
| 30 | c | 615 | LUT | C35-C15-C14 | 3.58 | 130.85 | 123.52 |
| 29 | c | 605 | CHL | C1A-CHA-CBD | 3.58 | 142.60 | 131.97 |
| 24 | A | 854 | BCR | C37-C22-C21 | -3.58 | 117.02 | 122.82 |
| 21 | A | 831 | CLA | O2D-CGD-O1D | -3.57 | 116.89 | 123.85 |
| 31 | a | 618 | XAT | C19-C9-C10 | -3.57 | 117.03 | 122.82 |
| 24 | O | 205 | BCR | C34-C9-C10 | -3.57 | 117.03 | 122.82 |
| 29 | 8 | 613 | CHL | CBC-CAC-C3C | -3.57 | 107.77 | 112.87 |
| 30 | 6 | 616 | LUT | C19-C9-C10 | -3.56 | 117.04 | 122.82 |
| 29 | 3 | 407 | CHL | OBD-CAD-CBD | -3.56 | 120.60 | 125.82 |
| 29 | 2 | 606 | CHL | CMD-C2D-C3D | -3.56 | 117.58 | 124.68 |
| 31 | a | 618 | XAT | C39-C29-C30 | -3.55 | 117.06 | 122.82 |
| 29 | 9 | 606 | CHL | OBD-CAD-C3D | -3.55 | 122.35 | 127.89 |
| 24 | 3 | 419 | BCR | C37-C22-C21 | -3.55 | 117.07 | 122.82 |
| 24 | F | 303 | BCR | C37-C22-C21 | -3.55 | 117.07 | 122.82 |
| 31 | a | 618 | XAT | C12-C13-C14 | 3.54 | 124.58 | 119.01 |
| 29 | 4 | 605 | CHL | OBD-CAD-C3D | -3.54 | 122.37 | 127.89 |
| 30 | 5 | 615 | LUT | C11-C10-C9 | 3.54 | 132.24 | 127.28 |
| 29 | 8 | 605 | CHL | CAB-C3B-C2B | -3.53 | 117.30 | 124.69 |
| 30 | 9 | 614 | LUT | C15-C35-C34 | 3.53 | 130.75 | 123.52 |
| 24 | 6 | 618 | BCR | C34-C9-C10 | -3.53 | 117.09 | 122.82 |
| 24 | A | 850 | BCR | C34-C9-C10 | -3.53 | 117.09 | 122.82 |
| 24 | K | 205 | BCR | C24-C23-C22 | -3.53 | 121.01 | 126.23 |
| 24 | I | 101 | BCR | C34-C9-C10 | -3.53 | 117.10 | 122.82 |
| 31 | 8 | 615 | XAT | C19-C9-C10 | -3.53 | 117.10 | 122.82 |
| 21 | 1 | 309 | CLA | C1D-ND-C4D | -3.52 | 103.84 | 106.31 |
| 24 | M | 101 | BCR | C34-C9-C10 | -3.52 | 117.11 | 122.82 |
| 30 | 3 | 416 | LUT | C19-C9-C10 | -3.52 | 117.11 | 122.82 |
| 24 | A | 849 | BCR | C23-C22-C21 | 3.52 | 124.54 | 119.01 |
| 29 | 8 | 607 | CHL | C1-C2-C3 | -3.52 | 121.07 | 126.76 |
| 21 | B | 801 | CLA | C3C-C4C-NC | 3.51 | 114.93 | 110.43 |
| 30 | a | 615 | LUT | C39-C29-C28 | 3.50 | 123.44 | 118.09 |
| 24 | 3 | 418 | BCR | C34-C9-C10 | -3.50 | 117.14 | 122.82 |
| 21 | A | 835 | CLA | C3B-C4B-NB | -3.49 | 107.41 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 830 | CLA | O2D-CGD-O1D | -3.49 | 117.06 | 123.85 |
| 30 | 2 | 616 | LUT | C12-C13-C14 | 3.49 | 124.50 | 119.01 |
| 29 | c | 609 | CHL | CMD-C2D-C3D | -3.48 | 117.72 | 124.68 |
| 24 | B | 843 | BCR | C20-C21-C22 | -3.48 | 122.40 | 127.28 |
| 29 | 1 | 307 | CHL | C1-C2-C3 | -3.48 | 121.14 | 126.76 |
| 30 | 4 | 615 | LUT | C19-C9-C10 | -3.48 | 117.19 | 122.82 |
| 31 | 9 | 616 | XAT | C40-C33-C34 | -3.47 | 117.19 | 122.82 |
| 24 | 2 | 618 | BCR | C37-C22-C21 | -3.47 | 117.19 | 122.82 |
| 24 | 8 | 616 | BCR | C34-C9-C10 | -3.47 | 117.19 | 122.82 |
| 21 | 3 | 409 | CLA | C1D-ND-C4D | -3.47 | 103.88 | 106.31 |
| 29 | 9 | 601 | CHL | CMD-C2D-C3D | -3.47 | 117.75 | 124.68 |
| 30 | c | 616 | LUT | C35-C15-C14 | 3.47 | 130.62 | 123.52 |
| 29 | c | 608 | CHL | OMC-CMC-C2C | -3.46 | 119.10 | 125.12 |
| 24 | A | 848 | BCR | C37-C22-C21 | -3.46 | 117.20 | 122.82 |
| 24 | G | 201 | BCR | C34-C9-C10 | -3.46 | 117.20 | 122.82 |
| 24 | 6 | 618 | BCR | C37-C22-C21 | -3.46 | 117.20 | 122.82 |
| 30 | a | 616 | LUT | C19-C9-C10 | -3.46 | 117.21 | 122.82 |
| 24 | G | 205 | BCR | C37-C22-C21 | -3.46 | 117.21 | 122.82 |
| 24 | K | 205 | BCR | C15-C14-C13 | -3.46 | 122.42 | 127.28 |
| 24 | B | 846 | BCR | C15-C14-C13 | -3.46 | 122.43 | 127.28 |
| 32 | 9 | 617 | NEX | C39-C29-C30 | -3.46 | 117.21 | 122.82 |
| 24 | A | 846 | BCR | C37-C22-C21 | -3.45 | 117.22 | 122.82 |
| 30 | 6 | 616 | LUT | C12-C13-C14 | 3.45 | 124.44 | 119.01 |
| 31 | 8 | 615 | XAT | C39-C29-C30 | -3.45 | 117.23 | 122.82 |
| 24 | 7 | 417 | BCR | C37-C22-C21 | -3.45 | 117.23 | 122.82 |
| 24 | B | 843 | BCR | C33-C5-C6 | -3.45 | 120.72 | 124.48 |
| 24 | F | 301 | BCR | C37-C22-C21 | -3.44 | 117.23 | 122.82 |
| 24 | L | 306 | BCR | C34-C9-C10 | -3.44 | 117.24 | 122.82 |
| 30 | 1 | 317 | LUT | C19-C9-C10 | -3.44 | 117.24 | 122.82 |
| 31 | c | 617 | XAT | C19-C9-C10 | -3.44 | 117.25 | 122.82 |
| 30 | b | 316 | LUT | C19-C9-C10 | -3.43 | 117.26 | 122.82 |
| 24 | B | 846 | BCR | C24-C23-C22 | -3.43 | 121.16 | 126.23 |
| 21 | A | 809 | CLA | O2D-CGD-O1D | -3.42 | 117.19 | 123.85 |
| 32 | b | 318 | NEX | C39-C29-C30 | -3.42 | 117.27 | 122.82 |
| 24 | A | 850 | BCR | C37-C22-C21 | -3.42 | 117.28 | 122.82 |
| 24 | 3 | 418 | BCR | C37-C22-C21 | -3.41 | 117.29 | 122.82 |
| 31 | 2 | 617 | XAT | C39-C29-C30 | -3.41 | 117.29 | 122.82 |
| 31 | 5 | 616 | XAT | C19-C9-C10 | -3.41 | 117.29 | 122.82 |
| 24 | L | 305 | BCR | C34-C9-C10 | -3.41 | 117.29 | 122.82 |
| 24 | 2 | 618 | BCR | C34-C9-C10 | -3.41 | 117.30 | 122.82 |
| 32 | c | 618 | NEX | C39-C29-C30 | -3.41 | 117.30 | 122.82 |
| 30 | 5 | 615 | LUT | C39-C29-C30 | -3.40 | 117.31 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 8 | 605 | CHL | OMC-CMC-C2C | -3.40 | 119.22 | 125.12 |
| 24 | J | 101 | BCR | C16-C15-C14 | 3.40 | 130.47 | 123.52 |
| 30 | a | 615 | LUT | C19-C9-C10 | -3.40 | 117.31 | 122.82 |
| 24 | A | 847 | BCR | C34-C9-C10 | -3.40 | 117.31 | 122.82 |
| 21 | B | 823 | CLA | O2D-CGD-O1D | -3.40 | 117.24 | 123.85 |
| 24 | A | 848 | BCR | C34-C9-C10 | -3.39 | 117.32 | 122.82 |
| 24 | J | 103 | BCR | C37-C22-C21 | -3.39 | 117.32 | 122.82 |
| 24 | B | 845 | BCR | C34-C9-C10 | -3.39 | 117.32 | 122.82 |
| 30 | 8 | 614 | LUT | C19-C9-C10 | -3.39 | 117.32 | 122.82 |
| 21 | 7 | 407 | CLA | CMD-C2D-C3D | 3.39 | 135.46 | 127.69 |
| 21 | B | 807 | CLA | O2D-CGD-O1D | -3.39 | 117.25 | 123.85 |
| 31 | 7 | 416 | XAT | C39-C29-C30 | -3.39 | 117.33 | 122.82 |
| 24 | 4 | 617 | BCR | C37-C22-C21 | -3.39 | 117.33 | 122.82 |
| 24 | A | 850 | BCR | C16-C15-C14 | 3.38 | 130.44 | 123.52 |
| 24 | A | 854 | BCR | C34-C9-C10 | -3.38 | 117.34 | 122.82 |
| 31 | 5 | 616 | XAT | C39-C29-C30 | -3.38 | 117.34 | 122.82 |
| 24 | B | 842 | BCR | C34-C9-C10 | -3.38 | 117.34 | 122.82 |
| 24 | L | 305 | BCR | C37-C22-C21 | -3.38 | 117.34 | 122.82 |
| 31 | 1 | 318 | XAT | C39-C29-C30 | -3.38 | 117.34 | 122.82 |
| 29 | 2 | 606 | CHL | CBC-CAC-C3C | -3.38 | 108.04 | 112.87 |
| 24 | L | 301 | BCR | C34-C9-C10 | -3.38 | 117.34 | 122.82 |
| 24 | A | 846 | BCR | C34-C9-C10 | -3.38 | 117.34 | 122.82 |
| 29 | 4 | 614 | CHL | OMC-CMC-C2C | -3.38 | 119.26 | 125.12 |
| 29 | 1 | 302 | CHL | C1-C2-C3 | -3.37 | 121.30 | 126.76 |
| 30 | c | 616 | LUT | C15-C35-C34 | 3.37 | 130.42 | 123.52 |
| 24 | G | 201 | BCR | C37-C22-C21 | -3.37 | 117.36 | 122.82 |
| 24 | I | 101 | BCR | C16-C15-C14 | 3.36 | 130.40 | 123.52 |
| 24 | L | 301 | BCR | C16-C15-C14 | 3.36 | 130.39 | 123.52 |
| 31 | 9 | 616 | XAT | C10-C11-C12 | 3.36 | 132.93 | 123.20 |
| 24 | 8 | 616 | BCR | C37-C22-C21 | -3.36 | 117.38 | 122.82 |
| 24 | 7 | 418 | BCR | C23-C22-C21 | 3.35 | 124.28 | 119.01 |
| 24 | 7 | 418 | BCR | C19-C18-C17 | 3.35 | 124.28 | 119.01 |
| 24 | B | 843 | BCR | C3-C4-C5 | -3.35 | 108.08 | 114.06 |
| 31 | 4 | 616 | XAT | C39-C29-C30 | -3.35 | 117.39 | 122.82 |
| 24 | B | 845 | BCR | C37-C22-C21 | -3.35 | 117.39 | 122.82 |
| 29 | 3 | 407 | CHL | C4D-CHA-CBD | 3.35 | 112.34 | 108.97 |
| 30 | 9 | 615 | LUT | C39-C29-C30 | -3.34 | 117.40 | 122.82 |
| 30 | c | 615 | LUT | C19-C9-C10 | -3.34 | 117.40 | 122.82 |
| 30 | 1 | 317 | LUT | C39-C29-C30 | -3.34 | 117.40 | 122.82 |
| 30 | 7 | 415 | LUT | C11-C10-C9 | 3.34 | 131.96 | 127.28 |
| 24 | M | 101 | BCR | C12-C13-C14 | 3.34 | 124.26 | 119.01 |
| 21 | 9 | 602 | CLA | C1-C2-C3 | -3.33 | 120.73 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 4 | 615 | LUT | C39-C29-C30 | -3.33 | 117.42 | 122.82 |
| 24 | A | 849 | BCR | C16-C15-C14 | 3.33 | 130.33 | 123.52 |
| 30 | c | 616 | LUT | C39-C29-C30 | -3.33 | 117.42 | 122.82 |
| 31 | 9 | 616 | XAT | C15-C35-C34 | 3.33 | 130.32 | 123.52 |
| 21 | B | 801 | CLA | C3B-C4B-NB | 3.32 | 113.50 | 110.53 |
| 24 | I | 101 | BCR | C37-C22-C21 | -3.32 | 117.43 | 122.82 |
| 21 | A | 834 | CLA | O2D-CGD-O1D | -3.32 | 117.38 | 123.85 |
| 21 | A | 818 | CLA | C3B-C4B-NB | -3.32 | 107.57 | 110.53 |
| 24 | B | 844 | BCR | C16-C17-C18 | -3.32 | 122.63 | 127.28 |
| 31 | 6 | 617 | XAT | C39-C29-C30 | -3.32 | 117.44 | 122.82 |
| 24 | A | 847 | BCR | C37-C22-C21 | -3.31 | 117.45 | 122.82 |
| 30 | 7 | 415 | LUT | C26-C27-C28 | 3.31 | 129.72 | 124.58 |
| 24 | 4 | 617 | BCR | C34-C9-C10 | -3.31 | 117.46 | 122.82 |
| 30 | 9 | 614 | LUT | C39-C29-C30 | -3.30 | 117.46 | 122.82 |
| 30 | 8 | 614 | LUT | C39-C29-C30 | -3.30 | 117.47 | 122.82 |
| 30 | 2 | 616 | LUT | C8-C9-C10 | 3.30 | 124.20 | 119.01 |
| 24 | J | 101 | BCR | C34-C9-C10 | -3.30 | 117.47 | 122.82 |
| 24 | 7 | 418 | BCR | C12-C13-C14 | 3.30 | 124.19 | 119.01 |
| 21 | A | 839 | CLA | O2D-CGD-O1D | -3.29 | 117.44 | 123.85 |
| 24 | L | 306 | BCR | C23-C22-C21 | 3.29 | 124.18 | 119.01 |
| 21 | A | 807 | CLA | O2D-CGD-O1D | -3.29 | 117.45 | 123.85 |
| 24 | G | 205 | BCR | C34-C9-C10 | -3.29 | 117.49 | 122.82 |
| 31 | 9 | 616 | XAT | C20-C13-C14 | -3.29 | 117.49 | 122.82 |
| 24 | F | 301 | BCR | C34-C9-C10 | -3.28 | 117.50 | 122.82 |
| 24 | 4 | 617 | BCR | C16-C15-C14 | 3.28 | 130.24 | 123.52 |
| 21 | 4 | 609 | CLA | CHD-C1D-ND | -3.28 | 120.18 | 124.80 |
| 29 | 6 | 602 | CHL | OMC-CMC-C2C | -3.28 | 119.42 | 125.12 |
| 32 | b | 318 | NEX | C35-C15-C14 | 3.28 | 130.23 | 123.52 |
| 24 | B | 842 | BCR | C37-C22-C21 | -3.28 | 117.50 | 122.82 |
| 31 | 3 | 417 | XAT | C19-C9-C10 | -3.28 | 117.50 | 122.82 |
| 24 | 3 | 419 | BCR | C7-C8-C9 | 3.28 | 131.09 | 126.23 |
| 30 | b | 317 | LUT | C39-C29-C30 | -3.27 | 117.51 | 122.82 |
| 30 | c | 615 | LUT | C39-C29-C30 | -3.27 | 117.51 | 122.82 |
| 30 | c | 616 | LUT | C19-C9-C10 | -3.27 | 117.51 | 122.82 |
| 24 | J | 104 | BCR | C11-C10-C9 | -3.27 | 122.69 | 127.28 |
| 21 | A | 819 | CLA | O2D-CGD-O1D | -3.27 | 117.49 | 123.85 |
| 23 | 4 | 619 | LHG | O7-C7-C8 | 3.26 | 118.53 | 111.48 |
| 21 | 6 | 609 | CLA | O2D-CGD-O1D | -3.26 | 117.50 | 123.85 |
| 24 | 3 | 419 | BCR | C12-C13-C14 | 3.26 | 124.13 | 119.01 |
| 24 | L | 301 | BCR | C37-C22-C21 | -3.25 | 117.55 | 122.82 |
| 24 | A | 846 | BCR | C16-C15-C14 | 3.25 | 130.17 | 123.52 |
| 24 | M | 101 | BCR | C23-C22-C21 | 3.25 | 124.12 | 119.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 823 | CLA | O2D-CGD-O1D | -3.25 | 117.52 | 123.85 |
| 30 | b | 316 | LUT | C39-C29-C30 | -3.25 | 117.55 | 122.82 |
| 24 | B | 842 | BCR | C16-C15-C14 | 3.25 | 130.17 | 123.52 |
| 30 | b | 317 | LUT | C19-C9-C10 | -3.25 | 117.55 | 122.82 |
| 21 | K | 202 | CLA | O2D-CGD-O1D | -3.25 | 117.53 | 123.85 |
| 21 | A | 818 | CLA | O2D-CGD-O1D | -3.24 | 117.53 | 123.85 |
| 31 | 2 | 617 | XAT | C19-C9-C10 | -3.24 | 117.56 | 122.82 |
| 31 | 3 | 417 | XAT | C39-C29-C30 | -3.24 | 117.57 | 122.82 |
| 24 | M | 101 | BCR | C19-C18-C17 | 3.24 | 124.10 | 119.01 |
| 29 | 2 | 614 | CHL | OMC-CMC-C2C | -3.24 | 119.50 | 125.12 |
| 29 | a | 608 | CHL | CBC-CAC-C3C | -3.24 | 108.24 | 112.87 |
| 24 | 3 | 418 | BCR | C16-C15-C14 | 3.24 | 130.14 | 123.52 |
| 30 | 4 | 615 | LUT | C32-C33-C34 | 3.23 | 124.09 | 119.01 |
| 21 | L | 302 | CLA | O2D-CGD-O1D | -3.23 | 117.56 | 123.85 |
| 30 | 9 | 615 | LUT | C19-C9-C10 | -3.23 | 117.59 | 122.82 |
| 21 | 7 | 407 | CLA | CMC-C2C-C3C | 3.23 | 134.87 | 126.15 |
| 30 | 7 | 415 | LUT | C20-C13-C14 | -3.23 | 117.59 | 122.82 |
| 21 | A | 801 | CLA | CMD-C2D-C3D | -3.23 | 120.29 | 127.69 |
| 30 | 1 | 317 | LUT | C32-C33-C34 | 3.22 | 124.08 | 119.01 |
| 31 | 4 | 616 | XAT | C19-C9-C10 | -3.22 | 117.60 | 122.82 |
| 31 | 7 | 416 | XAT | C35-C15-C14 | 3.22 | 130.11 | 123.52 |
| 21 | A | 838 | CLA | O2D-CGD-O1D | -3.22 | 117.58 | 123.85 |
| 21 | B | 806 | CLA | O2D-CGD-O1D | -3.22 | 117.59 | 123.85 |
| 21 | B | 828 | CLA | O2D-CGD-O1D | -3.21 | 117.59 | 123.85 |
| 21 | B | 824 | CLA | O2D-CGD-O1D | -3.21 | 117.60 | 123.85 |
| 24 | L | 306 | BCR | C19-C18-C17 | 3.21 | 124.06 | 119.01 |
| 24 | 3 | 419 | BCR | C19-C18-C17 | 3.21 | 124.06 | 119.01 |
| 24 | A | 849 | BCR | C34-C9-C10 | -3.21 | 117.62 | 122.82 |
| 32 | 9 | 617 | NEX | C15-C35-C34 | 3.20 | 130.06 | 123.52 |
| 29 | c | 601 | CHL | OMC-CMC-C2C | -3.20 | 119.57 | 125.12 |
| 24 | K | 205 | BCR | C28-C27-C26 | -3.20 | 108.36 | 114.06 |
| 21 | 7 | 401 | CLA | C3B-C4B-NB | -3.19 | 107.68 | 110.53 |
| 24 | O | 205 | BCR | C23-C22-C21 | 3.19 | 124.03 | 119.01 |
| 21 | B | 814 | CLA | O2D-CGD-O1D | -3.19 | 117.64 | 123.85 |
| 31 | 2 | 617 | XAT | C35-C15-C14 | 3.19 | 130.05 | 123.52 |
| 21 | A | 825 | CLA | O2D-CGD-O1D | -3.19 | 117.64 | 123.85 |
| 32 | c | 618 | NEX | C32-C33-C34 | 3.19 | 124.02 | 119.01 |
| 29 | 2 | 607 | CHL | OMC-CMC-C2C | -3.19 | 119.59 | 125.12 |
| 21 | L | 303 | CLA | O2D-CGD-O1D | -3.18 | 117.65 | 123.85 |
| 21 | 2 | 608 | CLA | O2D-CGD-O1D | -3.18 | 117.65 | 123.85 |
| 30 | 9 | 614 | LUT | C19-C9-C10 | -3.18 | 117.66 | 122.82 |
| 21 | A | 813 | CLA | O2D-CGD-O1D | -3.18 | 117.66 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | F | 303 | BCR | C19-C18-C17 | 3.18 | 124.01 | 119.01 |
| 32 | c | 618 | NEX | C35-C15-C14 | 3.18 | 130.02 | 123.52 |
| 21 | A | 841 | CLA | O2D-CGD-O1D | -3.18 | 117.66 | 123.85 |
| 30 | 3 | 416 | LUT | C39-C29-C30 | -3.18 | 117.67 | 122.82 |
| 31 | 2 | 617 | XAT | C15-C35-C34 | 3.18 | 130.02 | 123.52 |
| 24 | O | 205 | BCR | C12-C13-C14 | 3.17 | 124.00 | 119.01 |
| 30 | 4 | 615 | LUT | C12-C13-C14 | 3.17 | 124.00 | 119.01 |
| 24 | O | 205 | BCR | C19-C18-C17 | 3.17 | 124.00 | 119.01 |
| 21 | B | 801 | CLA | O2A-CGA-CBA | 3.17 | 121.50 | 111.83 |
| 21 | A | 805 | CLA | O2D-CGD-O1D | -3.17 | 117.68 | 123.85 |
| 31 | 5 | 616 | XAT | C15-C35-C34 | 3.17 | 130.00 | 123.52 |
| 24 | F | 303 | BCR | C34-C9-C10 | -3.16 | 117.69 | 122.82 |
| 21 | A | 826 | CLA | O2D-CGD-O1D | -3.16 | 117.69 | 123.85 |
| 29 | 6 | 602 | CHL | CMD-C2D-C3D | -3.16 | 118.37 | 124.68 |
| 24 | K | 205 | BCR | C30-C25-C26 | -3.16 | 118.32 | 122.64 |
| 30 | 7 | 415 | LUT | C39-C29-C30 | -3.16 | 117.70 | 122.82 |
| 24 | A | 854 | BCR | C19-C18-C17 | 3.15 | 123.97 | 119.01 |
| 29 | 4 | 606 | CHL | OMC-CMC-C2C | -3.15 | 119.65 | 125.12 |
| 30 | a | 616 | LUT | C39-C29-C30 | -3.15 | 117.71 | 122.82 |
| 29 | a | 601 | CHL | O1D-CGD-CBD | -3.15 | 119.95 | 124.72 |
| 24 | B | 844 | BCR | C30-C25-C26 | -3.15 | 118.33 | 122.64 |
| 21 | 4 | 610 | CLA | O2D-CGD-O1D | -3.15 | 117.72 | 123.85 |
| 29 | 5 | 601 | CHL | OMC-CMC-C2C | -3.15 | 119.66 | 125.12 |
| 31 | 1 | 318 | XAT | C19-C9-C10 | -3.15 | 117.72 | 122.82 |
| 21 | B | 839 | CLA | O2D-CGD-O1D | -3.14 | 117.73 | 123.85 |
| 21 | B | 817 | CLA | O2D-CGD-O1D | -3.14 | 117.73 | 123.85 |
| 30 | 2 | 616 | LUT | C20-C13-C14 | -3.14 | 117.73 | 122.82 |
| 21 | B | 810 | CLA | O2D-CGD-O1D | -3.14 | 117.74 | 123.85 |
| 21 | B | 812 | CLA | C3B-C4B-NB | -3.14 | 107.73 | 110.53 |
| 29 | 6 | 605 | CHL | OMC-CMC-C2C | -3.14 | 119.67 | 125.12 |
| 24 | K | 205 | BCR | C11-C10-C9 | -3.14 | 122.88 | 127.28 |
| 21 | B | 802 | CLA | O2D-CGD-O1D | -3.13 | 117.75 | 123.85 |
| 21 | B | 825 | CLA | O2D-CGD-O1D | -3.13 | 117.75 | 123.85 |
| 21 | A | 808 | CLA | O2D-CGD-O1D | -3.13 | 117.76 | 123.85 |
| 24 | J | 104 | BCR | C15-C14-C13 | -3.13 | 122.89 | 127.28 |
| 24 | K | 205 | BCR | C33-C5-C6 | -3.13 | 121.07 | 124.48 |
| 21 | A | 817 | CLA | O2D-CGD-O1D | -3.13 | 117.76 | 123.85 |
| 21 | B | 821 | CLA | O2D-CGD-O1D | -3.12 | 117.77 | 123.85 |
| 21 | A | 824 | CLA | O2D-CGD-O1D | -3.12 | 117.77 | 123.85 |
| 31 | a | 618 | XAT | C20-C13-C14 | -3.12 | 117.76 | 122.82 |
| 21 | B | 833 | CLA | O2D-CGD-O1D | -3.12 | 117.77 | 123.85 |
| 21 | 7 | 401 | CLA | O2D-CGD-O1D | -3.12 | 117.78 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 803 | CLA | C3B-C4B-NB | -3.12 | 107.75 | 110.53 |
| 30 | 6 | 616 | LUT | C39-C29-C30 | -3.12 | 117.76 | 122.82 |
| 21 | A | 812 | CLA | O2D-CGD-O1D | -3.12 | 117.78 | 123.85 |
| 29 | 6 | 601 | CHL | O2D-CGD-O1D | -3.12 | 117.78 | 123.85 |
| 24 | 6 | 618 | BCR | C19-C18-C17 | 3.12 | 123.91 | 119.01 |
| 30 | 8 | 614 | LUT | C12-C13-C14 | 3.12 | 123.91 | 119.01 |
| 21 | B | 832 | CLA | O2D-CGD-O1D | -3.11 | 117.78 | 123.85 |
| 21 | H | 201 | CLA | C3B-C4B-NB | -3.11 | 107.75 | 110.53 |
| 29 | 3 | 407 | CHL | CAA-C2A-C3A | -3.11 | 109.09 | 116.23 |
| 21 | B | 816 | CLA | O2D-CGD-O1D | -3.11 | 117.79 | 123.85 |
| 21 | A | 828 | CLA | O2D-CGD-O1D | -3.11 | 117.79 | 123.85 |
| 21 | B | 836 | CLA | O2D-CGD-O1D | -3.11 | 117.80 | 123.85 |
| 31 | 7 | 416 | XAT | C7-C8-C9 | 3.11 | 130.35 | 125.53 |
| 21 | B | 838 | CLA | C3B-C4B-NB | -3.11 | 107.76 | 110.53 |
| 21 | 2 | 612 | CLA | O2D-CGD-O1D | -3.10 | 117.81 | 123.85 |
| 21 | B | 831 | CLA | O2D-CGD-O1D | -3.10 | 117.81 | 123.85 |
| 24 | L | 305 | BCR | C16-C15-C14 | 3.10 | 129.86 | 123.52 |
| 21 | 4 | 602 | CLA | C1-C2-C3 | -3.10 | 121.12 | 126.20 |
| 24 | 2 | 618 | BCR | C19-C18-C17 | 3.10 | 123.88 | 119.01 |
| 30 | 6 | 616 | LUT | C20-C13-C14 | -3.09 | 117.80 | 122.82 |
| 24 | B | 843 | BCR | C27-C26-C25 | -3.09 | 118.53 | 122.70 |
| 24 | M | 101 | BCR | C35-C13-C14 | -3.09 | 117.81 | 122.82 |
| 21 | 3 | 402 | CLA | O2D-CGD-O1D | -3.09 | 117.83 | 123.85 |
| 21 | B | 804 | CLA | O2D-CGD-O1D | -3.09 | 117.83 | 123.85 |
| 29 | 9 | 607 | CHL | OMC-CMC-C2C | -3.09 | 119.76 | 125.12 |
| 32 | b | 318 | NEX | C32-C33-C34 | 3.09 | 123.86 | 119.01 |
| 29 | b | 309 | CHL | OMC-CMC-C2C | -3.09 | 119.76 | 125.12 |
| 21 | B | 819 | CLA | O2D-CGD-O1D | -3.08 | 117.84 | 123.85 |
| 21 | 4 | 601 | CLA | O2D-CGD-O1D | -3.08 | 117.84 | 123.85 |
| 24 | J | 103 | BCR | C12-C13-C14 | 3.08 | 123.86 | 119.01 |
| 24 | J | 103 | BCR | C11-C10-C9 | 3.08 | 131.60 | 127.28 |
| 29 | 6 | 602 | CHL | C1-C2-C3 | -3.08 | 121.15 | 126.20 |
| 21 | A | 801 | CLA | O2D-CGD-O1D | -3.08 | 117.85 | 123.85 |
| 21 | A | 803 | CLA | O2D-CGD-O1D | -3.08 | 117.86 | 123.85 |
| 21 | 4 | 601 | CLA | C3B-C4B-NB | -3.08 | 107.78 | 110.53 |
| 24 | 2 | 618 | BCR | C36-C18-C17 | -3.08 | 117.83 | 122.82 |
| 29 | b | 308 | CHL | C1-C2-C3 | -3.07 | 121.16 | 126.20 |
| 31 | 7 | 416 | XAT | C19-C9-C10 | -3.07 | 117.84 | 122.82 |
| 21 | 6 | 611 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |
| 29 | b | 308 | CHL | OMC-CMC-C2C | -3.07 | 119.78 | 125.12 |
| 21 | A | 806 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |
| 21 | 2 | 611 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 820 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |
| 21 | B | 815 | CLA | C3B-C4B-NB | -3.07 | 107.79 | 110.53 |
| 21 | B | 812 | CLA | O2D-CGD-O1D | -3.07 | 117.88 | 123.85 |
| 21 | 1 | 306 | CLA | O2D-CGD-O1D | -3.07 | 117.88 | 123.85 |
| 24 | A | 854 | BCR | C16-C15-C14 | 3.07 | 129.79 | 123.52 |
| 21 | 2 | 610 | CLA | CBD-CHA-C1A | 3.07 | 132.01 | 127.38 |
| 21 | B | 833 | CLA | C3B-C4B-NB | -3.06 | 107.80 | 110.53 |
| 21 | 2 | 608 | CLA | C3B-C4B-NB | -3.06 | 107.80 | 110.53 |
| 24 | B | 846 | BCR | C16-C15-C14 | -3.06 | 117.25 | 123.52 |
| 21 | A | 833 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 21 | A | 815 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 21 | A | 822 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 29 | 1 | 302 | CHL | CBC-CAC-C3C | -3.06 | 108.49 | 112.87 |
| 21 | B | 826 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 21 | 2 | 613 | CLA | O2D-CGD-O1D | -3.06 | 117.90 | 123.85 |
| 30 | 2 | 616 | LUT | C39-C29-C30 | -3.06 | 117.86 | 122.82 |
| 21 | B | 840 | CLA | O2D-CGD-O1D | -3.05 | 117.90 | 123.85 |
| 21 | O | 201 | CLA | O2D-CGD-O1D | -3.05 | 117.90 | 123.85 |
| 21 | F | 302 | CLA | C3B-C4B-NB | -3.05 | 107.80 | 110.53 |
| 24 | 7 | 417 | BCR | C12-C13-C14 | 3.05 | 123.81 | 119.01 |
| 21 | 3 | 408 | CLA | O2D-CGD-O1D | -3.05 | 117.91 | 123.85 |
| 21 | B | 801 | CLA | CAA-C2A-C3A | -3.05 | 104.76 | 113.00 |
| 30 | 9 | 615 | LUT | C35-C15-C14 | 3.05 | 129.76 | 123.52 |
| 29 | 3 | 407 | CHL | O2D-CGD-CBD | 3.05 | 121.38 | 113.90 |
| 21 | 2 | 611 | CLA | CAA-C2A-C3A | -3.05 | 109.24 | 116.23 |
| 21 | 2 | 609 | CLA | C4-C3-C5 | 3.05 | 120.52 | 115.23 |
| 29 | 1 | 302 | CHL | O1D-CGD-CBD | -3.04 | 120.11 | 124.72 |
| 29 | 2 | 602 | CHL | OMC-CMC-C2C | -3.04 | 119.84 | 125.12 |
| 24 | 7 | 418 | BCR | C36-C18-C17 | -3.04 | 117.89 | 122.82 |
| 21 | B | 835 | CLA | O2D-CGD-O1D | -3.04 | 117.93 | 123.85 |
| 21 | 1 | 303 | CLA | O2D-CGD-O1D | -3.04 | 117.93 | 123.85 |
| 21 | A | 835 | CLA | O2D-CGD-O1D | -3.04 | 117.93 | 123.85 |
| 21 | K | 204 | CLA | O2D-CGD-O1D | -3.04 | 117.93 | 123.85 |
| 21 | 1 | 305 | CLA | O2D-CGD-O1D | -3.04 | 117.93 | 123.85 |
| 21 | A | 801 | CLA | C3B-C4B-NB | -3.04 | 107.82 | 110.53 |
| 21 | A | 820 | CLA | C3B-C4B-NB | -3.04 | 107.82 | 110.53 |
| 21 | 4 | 609 | CLA | C4D-CHA-C1A | 3.04 | 124.87 | 121.24 |
| 21 | 3 | 409 | CLA | C4B-C3B-C2B | -3.04 | 103.53 | 107.30 |
| 29 | 6 | 607 | CHL | C1-C2-C3 | -3.04 | 121.85 | 126.76 |
| 21 | 1 | 309 | CLA | C4D-CHA-C1A | 3.03 | 124.86 | 121.24 |
| 24 | A | 849 | BCR | C19-C18-C17 | 3.03 | 123.78 | 119.01 |
| 21 | B | 805 | CLA | O2D-CGD-O1D | -3.03 | 117.94 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | a | 605 | CHL | OMC-CMC-C2C | -3.03 | 119.86 | 125.12 |
| 21 | A | 842 | CLA | C3B-C4B-NB | -3.03 | 107.83 | 110.53 |
| 21 | B | 830 | CLA | O2D-CGD-O1D | -3.03 | 117.95 | 123.85 |
| 29 | a | 607 | CHL | O1D-CGD-CBD | -3.03 | 120.13 | 124.72 |
| 21 | b | 303 | CLA | C3B-C4B-NB | -3.03 | 107.83 | 110.53 |
| 21 | B | 801 | CLA | CHD-C4C-NC | 3.03 | 128.92 | 124.23 |
| 21 | c | 614 | CLA | O2D-CGD-O1D | -3.03 | 117.96 | 123.85 |
| 21 | K | 203 | CLA | O2D-CGD-O1D | -3.03 | 117.96 | 123.85 |
| 29 | 2 | 606 | CHL | OMC-CMC-C2C | -3.02 | 119.87 | 125.12 |
| 21 | A | 802 | CLA | C1-C2-C3 | -3.02 | 121.24 | 126.20 |
| 30 | b | 316 | LUT | C35-C15-C14 | 3.02 | 129.70 | 123.52 |
| 29 | 8 | 606 | CHL | OMC-CMC-C2C | -3.02 | 119.87 | 125.12 |
| 21 | A | 805 | CLA | C3B-C4B-NB | -3.02 | 107.83 | 110.53 |
| 21 | 6 | 608 | CLA | C3B-C4B-NB | -3.02 | 107.83 | 110.53 |
| 21 | 1 | 305 | CLA | C3B-C4B-NB | -3.02 | 107.83 | 110.53 |
| 21 | 5 | 602 | CLA | C3B-C4B-NB | -3.02 | 107.83 | 110.53 |
| 21 | a | 612 | CLA | C3B-C4B-NB | -3.02 | 107.83 | 110.53 |
| 21 | B | 816 | CLA | C3B-C4B-NB | -3.02 | 107.84 | 110.53 |
| 21 | 6 | 610 | CLA | CBD-CHA-C1A | 3.02 | 131.93 | 127.38 |
| 24 | G | 205 | BCR | C16-C15-C14 | 3.02 | 129.69 | 123.52 |
| 21 | 3 | 409 | CLA | C4D-CHA-C1A | 3.01 | 124.84 | 121.24 |
| 30 | a | 615 | LUT | C12-C13-C14 | 3.01 | 123.75 | 119.01 |
| 29 | 8 | 607 | CHL | OMC-CMC-C2C | -3.01 | 119.89 | 125.12 |
| 21 | a | 603 | CLA | CAA-C2A-C3A | -3.01 | 109.33 | 116.23 |
| 32 | c | 618 | NEX | C40-C33-C34 | -3.01 | 117.94 | 122.82 |
| 21 | B | 818 | CLA | C3B-C4B-NB | -3.01 | 107.84 | 110.53 |
| 29 | b | 302 | CHL | OMC-CMC-C2C | -3.01 | 119.90 | 125.12 |
| 21 | c | 604 | CLA | O2D-CGD-O1D | -3.01 | 118.00 | 123.85 |
| 21 | A | 801 | CLA | O2D-CGD-CBD | 3.00 | 116.48 | 111.23 |
| 21 | c | 611 | CLA | O2D-CGD-O1D | -3.00 | 118.00 | 123.85 |
| 21 | 3 | 408 | CLA | C3B-C4B-NB | -3.00 | 107.85 | 110.53 |
| 21 | A | 852 | CLA | O2D-CGD-O1D | -3.00 | 118.00 | 123.85 |
| 24 | L | 306 | BCR | C36-C18-C17 | -3.00 | 117.95 | 122.82 |
| 21 | c | 613 | CLA | O2D-CGD-O1D | -3.00 | 118.01 | 123.85 |
| 21 | A | 816 | CLA | O2D-CGD-O1D | -3.00 | 118.01 | 123.85 |
| 24 | 7 | 417 | BCR | C19-C18-C17 | 2.99 | 123.72 | 119.01 |
| 21 | 8 | 609 | CLA | O2D-CGD-O1D | -2.99 | 118.02 | 123.85 |
| 24 | G | 201 | BCR | C16-C15-C14 | 2.99 | 129.64 | 123.52 |
| 29 | 9 | 607 | CHL | CBC-CAC-C3C | -2.99 | 108.59 | 112.87 |
| 21 | B | 827 | CLA | O2D-CGD-O1D | -2.99 | 118.02 | 123.85 |
| 21 | G | 202 | CLA | O2D-CGD-O1D | -2.99 | 118.02 | 123.85 |
| 24 | 3 | 419 | BCR | C35-C13-C14 | -2.99 | 117.97 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 601 | CHL | C4-C3-C5 | 2.99 | 120.42 | 115.23 |
| 21 | G | 203 | CLA | O2D-CGD-O1D | -2.99 | 118.03 | 123.85 |
| 30 | 4 | 615 | LUT | C20-C13-C14 | -2.99 | 117.97 | 122.82 |
| 29 | 5 | 601 | CHL | O1D-CGD-CBD | -2.99 | 120.19 | 124.72 |
| 24 | M | 101 | BCR | C36-C18-C17 | -2.99 | 117.98 | 122.82 |
| 29 | 1 | 302 | CHL | OMC-CMC-C2C | -2.99 | 119.93 | 125.12 |
| 21 | A | 836 | CLA | C3B-C4B-NB | -2.99 | 107.86 | 110.53 |
| 29 | 1 | 302 | CHL | O2D-CGD-O1D | -2.99 | 118.03 | 123.85 |
| 21 | 9 | 611 | CLA | O2D-CGD-O1D | -2.99 | 118.04 | 123.85 |
| 21 | b | 312 | CLA | O2D-CGD-O1D | -2.99 | 118.04 | 123.85 |
| 24 | 7 | 418 | BCR | C35-C13-C14 | -2.99 | 117.98 | 122.82 |
| 32 | 9 | 617 | NEX | C12-C13-C14 | 2.99 | 123.70 | 119.01 |
| 31 | 7 | 416 | XAT | C19-C9-C8 | 2.98 | 122.65 | 118.09 |
| 21 | J | 102 | CLA | C3B-C4B-NB | -2.98 | 107.87 | 110.53 |
| 29 | 6 | 601 | CHL | O1D-CGD-CBD | -2.98 | 120.20 | 124.72 |
| 29 | a | 609 | CHL | OMC-CMC-C2C | -2.98 | 119.94 | 125.12 |
| 21 | c | 602 | CLA | O2D-CGD-O1D | -2.98 | 118.04 | 123.85 |
| 21 | K | 201 | CLA | O2D-CGD-O1D | -2.98 | 118.04 | 123.85 |
| 30 | 4 | 615 | LUT | C40-C33-C34 | -2.98 | 117.99 | 122.82 |
| 21 | 1 | 304 | CLA | O2D-CGD-O1D | -2.98 | 118.05 | 123.85 |
| 30 | 8 | 614 | LUT | C32-C33-C34 | 2.98 | 123.70 | 119.01 |
| 21 | A | 804 | CLA | O2D-CGD-O1D | -2.98 | 118.05 | 123.85 |
| 21 | A | 811 | CLA | C3B-C4B-NB | -2.98 | 107.87 | 110.53 |
| 31 | 9 | 616 | XAT | C7-C8-C9 | 2.98 | 130.15 | 125.53 |
| 21 | B | 804 | CLA | C3B-C4B-NB | -2.98 | 107.87 | 110.53 |
| 21 | A | 814 | CLA | O2D-CGD-O1D | -2.98 | 118.06 | 123.85 |
| 30 | 2 | 616 | LUT | C39-C29-C28 | 2.98 | 122.63 | 118.09 |
| 30 | a | 615 | LUT | C15-C35-C34 | 2.97 | 129.60 | 123.52 |
| 21 | 9 | 611 | CLA | C3B-C4B-NB | -2.97 | 107.88 | 110.53 |
| 21 | B | 818 | CLA | O2D-CGD-O1D | -2.97 | 118.06 | 123.85 |
| 24 | J | 103 | BCR | C35-C13-C14 | -2.97 | 118.00 | 122.82 |
| 21 | A | 821 | CLA | O2D-CGD-O1D | -2.97 | 118.06 | 123.85 |
| 21 | 4 | 611 | CLA | O2D-CGD-O1D | -2.97 | 118.06 | 123.85 |
| 32 | b | 318 | NEX | C40-C33-C34 | -2.97 | 118.00 | 122.82 |
| 21 | L | 303 | CLA | C3B-C4B-NB | -2.97 | 107.88 | 110.53 |
| 29 | 6 | 614 | CHL | OMC-CMC-C2C | -2.97 | 119.96 | 125.12 |
| 21 | 6 | 603 | CLA | O2D-CGD-O1D | -2.97 | 118.07 | 123.85 |
| 31 | 8 | 615 | XAT | C12-C13-C14 | 2.97 | 123.67 | 119.01 |
| 21 | 4 | 609 | CLA | C4B-C3B-C2B | -2.97 | 103.61 | 107.30 |
| 24 | L | 306 | BCR | C12-C13-C14 | 2.96 | 123.67 | 119.01 |
| 21 | K | 202 | CLA | C3B-C4B-NB | -2.96 | 107.88 | 110.53 |
| 24 | B | 846 | BCR | C11-C10-C9 | -2.96 | 123.12 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 601 | CHL | OMC-CMC-C2C | -2.96 | 119.97 | 125.12 |
| 24 | A | 854 | BCR | C36-C18-C17 | -2.96 | 118.02 | 122.82 |
| 21 | 9 | 610 | CLA | O2D-CGD-O1D | -2.96 | 118.08 | 123.85 |
| 31 | c | 617 | XAT | C12-C13-C14 | 2.96 | 123.67 | 119.01 |
| 24 | O | 205 | BCR | C35-C13-C14 | -2.96 | 118.02 | 122.82 |
| 21 | A | 829 | CLA | O2D-CGD-O1D | -2.96 | 118.09 | 123.85 |
| 24 | 8 | 616 | BCR | C12-C13-C14 | 2.96 | 123.67 | 119.01 |
| 21 | 1 | 315 | CLA | O2D-CGD-O1D | -2.96 | 118.09 | 123.85 |
| 24 | 6 | 618 | BCR | C12-C13-C14 | 2.96 | 123.66 | 119.01 |
| 24 | B | 845 | BCR | C16-C15-C14 | 2.96 | 129.57 | 123.52 |
| 24 | 6 | 618 | BCR | C36-C18-C17 | -2.96 | 118.03 | 122.82 |
| 29 | 9 | 608 | CHL | OMC-CMC-C2C | -2.96 | 119.99 | 125.12 |
| 29 | a | 601 | CHL | OMC-CMC-C2C | -2.96 | 119.99 | 125.12 |
| 21 | A | 841 | CLA | C3B-C4B-NB | -2.96 | 107.89 | 110.53 |
| 21 | 2 | 603 | CLA | O2D-CGD-O1D | -2.96 | 118.09 | 123.85 |
| 21 | 4 | 609 | CLA | C4-C3-C5 | 2.96 | 120.36 | 115.23 |
| 31 | 7 | 416 | XAT | C6-C7-C8 | -2.95 | 119.75 | 125.99 |
| 27 | B | 847 | DGD | C2G-O2G-C1B | -2.95 | 110.73 | 117.80 |
| 24 | B | 843 | BCR | C8-C7-C6 | -2.95 | 119.11 | 127.00 |
| 24 | 7 | 417 | BCR | C36-C18-C17 | -2.95 | 118.03 | 122.82 |
| 21 | 1 | 313 | CLA | C3B-C4B-NB | -2.95 | 107.90 | 110.53 |
| 29 | c | 609 | CHL | OMC-CMC-C2C | -2.95 | 120.00 | 125.12 |
| 21 | 3 | 415 | CLA | C3B-C4B-NB | -2.95 | 107.90 | 110.53 |
| 24 | K | 205 | BCR | C27-C26-C25 | -2.95 | 118.72 | 122.70 |
| 21 | 8 | 601 | CLA | C3B-C4B-NB | -2.95 | 107.90 | 110.53 |
| 21 | 1 | 312 | CLA | C3B-C4B-NB | -2.94 | 107.90 | 110.53 |
| 21 | 3 | 414 | CLA | C3B-C4B-NB | -2.94 | 107.90 | 110.53 |
| 24 | 7 | 417 | BCR | C35-C13-C14 | -2.94 | 118.05 | 122.82 |
| 30 | 5 | 615 | LUT | C15-C35-C34 | 2.94 | 129.54 | 123.52 |
| 21 | 6 | 613 | CLA | C3B-C4B-NB | -2.94 | 107.90 | 110.53 |
| 24 | O | 205 | BCR | C36-C18-C17 | -2.94 | 118.05 | 122.82 |
| 21 | A | 842 | CLA | O2D-CGD-O1D | -2.94 | 118.12 | 123.85 |
| 21 | a | 613 | CLA | C3B-C4B-NB | -2.94 | 107.91 | 110.53 |
| 24 | A | 846 | BCR | C19-C18-C17 | 2.94 | 123.63 | 119.01 |
| 29 | 2 | 601 | CHL | O1D-CGD-CBD | -2.94 | 120.27 | 124.72 |
| 21 | a | 610 | CLA | C3B-C4B-NB | -2.93 | 107.91 | 110.53 |
| 21 | A | 823 | CLA | C3B-C4B-NB | -2.93 | 107.91 | 110.53 |
| 21 | A | 802 | CLA | O2D-CGD-O1D | -2.93 | 118.14 | 123.85 |
| 21 | 4 | 610 | CLA | C3B-C4B-NB | -2.93 | 107.91 | 110.53 |
| 30 | 1 | 317 | LUT | C12-C13-C14 | 2.93 | 123.62 | 119.01 |
| 21 | B | 813 | CLA | C3B-C4B-NB | -2.93 | 107.92 | 110.53 |
| 21 | A | 840 | CLA | O2D-CGD-O1D | -2.93 | 118.15 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | 3 | 419 | BCR | C36-C18-C17 | -2.93 | 118.07 | 122.82 |
| 21 | H | 201 | CLA | O2D-CGD-O1D | -2.93 | 118.15 | 123.85 |
| 21 | J | 102 | CLA | O2D-CGD-O1D | -2.93 | 118.15 | 123.85 |
| 21 | 5 | 602 | CLA | O2D-CGD-O1D | -2.93 | 118.15 | 123.85 |
| 24 | F | 303 | BCR | C36-C18-C17 | -2.93 | 118.07 | 122.82 |
| 21 | 7 | 407 | CLA | CHD-C4C-C3C | -2.93 | 120.51 | 124.77 |
| 21 | A | 815 | CLA | C3B-C4B-NB | -2.93 | 107.92 | 110.53 |
| 21 | c | 612 | CLA | C3B-C4B-NB | -2.92 | 107.92 | 110.53 |
| 31 | 8 | 615 | XAT | C20-C13-C14 | -2.92 | 118.08 | 122.82 |
| 21 | 1 | 309 | CLA | O2D-CGD-O1D | -2.92 | 118.16 | 123.85 |
| 29 | 5 | 606 | CHL | OMC-CMC-C2C | -2.92 | 120.04 | 125.12 |
| 21 | 8 | 603 | CLA | C3B-C4B-NB | -2.92 | 107.92 | 110.53 |
| 21 | 1 | 316 | CLA | O2D-CGD-O1D | -2.92 | 118.16 | 123.85 |
| 21 | 7 | 407 | CLA | C4C-C3C-C2C | -2.92 | 102.64 | 106.89 |
| 29 | b | 308 | CHL | C4-C3-C5 | 2.92 | 120.30 | 115.23 |
| 29 | 9 | 606 | CHL | OMC-CMC-C2C | -2.92 | 120.05 | 125.12 |
| 21 | F | 305 | CLA | O2D-CGD-O1D | -2.92 | 118.17 | 123.85 |
| 21 | A | 810 | CLA | O2D-CGD-O1D | -2.92 | 118.17 | 123.85 |
| 30 | 1 | 317 | LUT | C40-C33-C34 | -2.92 | 118.09 | 122.82 |
| 21 | a | 614 | CLA | O2D-CGD-O1D | -2.92 | 118.17 | 123.85 |
| 21 | B | 829 | CLA | O2D-CGD-O1D | -2.92 | 118.17 | 123.85 |
| 21 | 4 | 612 | CLA | O2D-CGD-O1D | -2.91 | 118.17 | 123.85 |
| 32 | 9 | 617 | NEX | C20-C13-C14 | -2.91 | 118.09 | 122.82 |
| 21 | A | 811 | CLA | O2D-CGD-O1D | -2.91 | 118.18 | 123.85 |
| 29 | 9 | 605 | CHL | OMC-CMC-C2C | -2.91 | 120.06 | 125.12 |
| 29 | 1 | 307 | CHL | OMC-CMC-C2C | -2.91 | 120.06 | 125.12 |
| 29 | 4 | 607 | CHL | O2A-CGA-CBA | 2.91 | 120.71 | 111.83 |
| 21 | 4 | 613 | CLA | O2D-CGD-O1D | -2.91 | 118.18 | 123.85 |
| 29 | a | 606 | CHL | O1D-CGD-CBD | -2.91 | 120.31 | 124.72 |
| 21 | B | 831 | CLA | C3B-C4B-NB | -2.91 | 107.93 | 110.53 |
| 21 | A | 830 | CLA | C4-C3-C5 | 2.91 | 120.28 | 115.23 |
| 31 | 1 | 318 | XAT | C19-C9-C8 | 2.91 | 122.53 | 118.09 |
| 21 | 7 | 412 | CLA | CAA-C2A-C3A | -2.91 | 109.56 | 116.23 |
| 24 | B | 846 | BCR | C21-C20-C19 | -2.91 | 114.78 | 123.20 |
| 21 | A | 824 | CLA | C3B-C4B-NB | -2.91 | 107.94 | 110.53 |
| 31 | 1 | 318 | XAT | C35-C15-C14 | 2.90 | 129.46 | 123.52 |
| 21 | 5 | 605 | CLA | C3A-C2A-C1A | -2.90 | 103.33 | 106.30 |
| 30 | 5 | 615 | LUT | C20-C13-C14 | -2.90 | 118.11 | 122.82 |
| 21 | 1 | 309 | CLA | CAC-C3C-C4C | 2.90 | 128.57 | 124.79 |
| 21 | A | 813 | CLA | CHB-C4A-NA | 2.90 | 128.59 | 124.40 |
| 24 | K | 205 | BCR | C38-C26-C27 | 2.90 | 119.79 | 113.60 |
| 21 | 1 | 309 | CLA | CMA-C3A-C2A | -2.90 | 109.58 | 116.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 607 | CHL | OMC-CMC-C2C | -2.90 | 120.08 | 125.12 |
| 21 | 5 | 604 | CLA | O2D-CGD-O1D | -2.90 | 118.20 | 123.85 |
| 24 | B | 843 | BCR | C33-C5-C4 | 2.90 | 119.78 | 113.60 |
| 21 | 6 | 604 | CLA | O2D-CGD-O1D | -2.90 | 118.20 | 123.85 |
| 30 | 5 | 615 | LUT | C12-C13-C14 | 2.90 | 123.57 | 119.01 |
| 30 | a | 615 | LUT | C20-C13-C14 | -2.90 | 118.12 | 122.82 |
| 21 | b | 304 | CLA | O2D-CGD-O1D | -2.90 | 118.20 | 123.85 |
| 29 | a | 606 | CHL | OMC-CMC-C2C | -2.90 | 120.09 | 125.12 |
| 29 | c | 601 | CHL | CBC-CAC-C3C | -2.90 | 108.72 | 112.87 |
| 21 | 8 | 611 | CLA | C3B-C4B-NB | -2.90 | 107.94 | 110.53 |
| 21 | B | 808 | CLA | O2D-CGD-O1D | -2.90 | 118.21 | 123.85 |
| 21 | 1 | 313 | CLA | O2D-CGD-O1D | -2.90 | 118.21 | 123.85 |
| 21 | b | 313 | CLA | O2D-CGD-O1D | -2.90 | 118.21 | 123.85 |
| 21 | A | 830 | CLA | O2A-CGA-CBA | 2.90 | 120.66 | 111.83 |
| 21 | 1 | 308 | CLA | C3B-C4B-NB | -2.89 | 107.95 | 110.53 |
| 21 | 9 | 604 | CLA | O2D-CGD-O1D | -2.89 | 118.22 | 123.85 |
| 21 | a | 603 | CLA | O2D-CGD-O1D | -2.89 | 118.22 | 123.85 |
| 21 | 9 | 603 | CLA | O2D-CGD-O1D | -2.89 | 118.22 | 123.85 |
| 24 | A | 849 | BCR | C36-C18-C17 | -2.89 | 118.13 | 122.82 |
| 29 | c | 607 | CHL | O1D-CGD-CBD | -2.89 | 120.34 | 124.72 |
| 21 | 7 | 407 | CLA | C4B-C3B-C2B | -2.89 | 103.71 | 107.30 |
| 21 | 5 | 608 | CLA | O2D-CGD-O1D | -2.89 | 118.23 | 123.85 |
| 21 | 4 | 612 | CLA | C3B-C4B-NB | -2.89 | 107.95 | 110.53 |
| 29 | 2 | 605 | CHL | O1D-CGD-CBD | -2.89 | 120.35 | 124.72 |
| 24 | J | 101 | BCR | C19-C18-C17 | 2.89 | 123.55 | 119.01 |
| 21 | b | 303 | CLA | O2D-CGD-O1D | -2.88 | 118.23 | 123.85 |
| 21 | 3 | 412 | CLA | C3B-C4B-NB | -2.88 | 107.96 | 110.53 |
| 24 | A | 849 | BCR | C24-C23-C22 | 2.88 | 130.50 | 126.23 |
| 21 | 7 | 402 | CLA | O2D-CGD-O1D | -2.88 | 118.24 | 123.85 |
| 31 | 4 | 616 | XAT | C35-C15-C14 | 2.88 | 129.41 | 123.52 |
| 21 | 1 | 315 | CLA | C3B-C4B-NB | -2.88 | 107.96 | 110.53 |
| 29 | b | 309 | CHL | O2A-CGA-CBA | 2.88 | 120.61 | 111.83 |
| 21 | 5 | 604 | CLA | C3B-C4B-NB | -2.88 | 107.96 | 110.53 |
| 27 | B | 847 | DGD | O1G-C1A-C2A | 2.88 | 120.61 | 111.83 |
| 29 | 9 | 609 | CHL | OMC-CMC-C2C | -2.88 | 120.12 | 125.12 |
| 29 | b | 306 | CHL | OMC-CMC-C2C | -2.88 | 120.13 | 125.12 |
| 29 | 1 | 307 | CHL | O1D-CGD-CBD | -2.88 | 120.36 | 124.72 |
| 21 | a | 614 | CLA | C3B-C4B-NB | -2.88 | 107.96 | 110.53 |
| 21 | 5 | 611 | CLA | O2D-CGD-O1D | -2.87 | 118.25 | 123.85 |
| 24 | L | 301 | BCR | C12-C13-C14 | 2.87 | 123.53 | 119.01 |
| 21 | A | 809 | CLA | C3B-C4B-NB | -2.87 | 107.97 | 110.53 |
| 21 | 8 | 610 | CLA | C3B-C4B-NB | -2.87 | 107.97 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 606 | CHL | O1D-CGD-CBD | -2.87 | 120.37 | 124.72 |
| 24 | 6 | 618 | BCR | C35-C13-C14 | -2.87 | 118.17 | 122.82 |
| 21 | A | 832 | CLA | O2D-CGD-O1D | -2.87 | 118.26 | 123.85 |
| 21 | O | 202 | CLA | C3B-C4B-NB | -2.87 | 107.97 | 110.53 |
| 21 | 6 | 611 | CLA | C3B-C4B-NB | -2.87 | 107.97 | 110.53 |
| 21 | 1 | 306 | CLA | C3B-C4B-NB | -2.87 | 107.97 | 110.53 |
| 21 | 1 | 309 | CLA | O1D-CGD-CBD | -2.87 | 118.86 | 124.52 |
| 21 | 7 | 412 | CLA | C3B-C4B-NB | -2.87 | 107.97 | 110.53 |
| 24 | F | 303 | BCR | C16-C15-C14 | 2.86 | 129.38 | 123.52 |
| 29 | 4 | 605 | CHL | O1D-CGD-CBD | -2.86 | 120.38 | 124.72 |
| 29 | 4 | 607 | CHL | OMC-CMC-C2C | -2.86 | 120.15 | 125.12 |
| 24 | A | 850 | BCR | C19-C18-C17 | 2.86 | 123.51 | 119.01 |
| 30 | 1 | 317 | LUT | C20-C13-C14 | -2.86 | 118.18 | 122.82 |
| 21 | B | 820 | CLA | C3B-C4B-NB | -2.86 | 107.98 | 110.53 |
| 21 | F | 304 | CLA | C3B-C4B-NB | -2.86 | 107.98 | 110.53 |
| 21 | c | 610 | CLA | C3B-C4B-NB | -2.86 | 107.98 | 110.53 |
| 21 | B | 834 | CLA | O2D-CGD-O1D | -2.86 | 118.28 | 123.85 |
| 21 | a | 602 | CLA | O2D-CGD-O1D | -2.86 | 118.28 | 123.85 |
| 31 | 6 | 617 | XAT | C32-C33-C34 | 2.86 | 123.51 | 119.01 |
| 24 | 2 | 618 | BCR | C12-C13-C14 | 2.86 | 123.50 | 119.01 |
| 21 | B | 809 | CLA | C3B-C4B-NB | -2.86 | 107.98 | 110.53 |
| 29 | 2 | 601 | CHL | O2A-CGA-CBA | 2.86 | 120.54 | 111.83 |
| 21 | B | 815 | CLA | C1-C2-C3 | -2.86 | 121.52 | 126.20 |
| 21 | c | 602 | CLA | C3B-C4B-NB | -2.86 | 107.98 | 110.53 |
| 30 | 9 | 615 | LUT | C32-C33-C34 | 2.85 | 123.50 | 119.01 |
| 21 | B | 838 | CLA | O2D-CGD-O1D | -2.85 | 118.29 | 123.85 |
| 24 | L | 301 | BCR | C36-C18-C17 | -2.85 | 118.19 | 122.82 |
| 24 | J | 101 | BCR | C36-C18-C17 | -2.85 | 118.20 | 122.82 |
| 21 | b | 315 | CLA | O2D-CGD-O1D | -2.85 | 118.30 | 123.85 |
| 30 | a | 616 | LUT | C12-C13-C14 | 2.85 | 123.49 | 119.01 |
| 24 | B | 844 | BCR | C27-C26-C25 | -2.85 | 118.85 | 122.70 |
| 30 | 8 | 614 | LUT | C40-C33-C34 | -2.85 | 118.20 | 122.82 |
| 31 | c | 617 | XAT | C20-C13-C14 | -2.85 | 118.20 | 122.82 |
| 21 | B | 808 | CLA | C3B-C4B-NB | -2.85 | 107.99 | 110.53 |
| 21 | A | 837 | CLA | O2D-CGD-O1D | -2.85 | 118.30 | 123.85 |
| 21 | 4 | 604 | CLA | O2D-CGD-O1D | -2.85 | 118.30 | 123.85 |
| 21 | A | 812 | CLA | C3B-C4B-NB | -2.85 | 107.99 | 110.53 |
| 24 | A | 846 | BCR | C36-C18-C17 | -2.85 | 118.20 | 122.82 |
| 29 | c | 606 | CHL | OMC-CMC-C2C | -2.85 | 120.17 | 125.12 |
| 21 | B | 803 | CLA | O2D-CGD-O1D | -2.85 | 118.31 | 123.85 |
| 24 | L | 306 | BCR | C35-C13-C14 | -2.85 | 118.20 | 122.82 |
| 21 | 5 | 612 | CLA | C3B-C4B-NB | -2.85 | 107.99 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 9 | 614 | LUT | C35-C15-C14 | 2.84 | 129.34 | 123.52 |
| 29 | 6 | 607 | CHL | OMC-CMC-C2C | -2.84 | 120.18 | 125.12 |
| 21 | 2 | 612 | CLA | C3B-C4B-NB | -2.84 | 107.99 | 110.53 |
| 21 | 5 | 607 | CLA | C3B-C4B-NB | -2.84 | 107.99 | 110.53 |
| 21 | 8 | 611 | CLA | O2D-CGD-O1D | -2.84 | 118.32 | 123.85 |
| 29 | a | 608 | CHL | OMC-CMC-C2C | -2.84 | 120.19 | 125.12 |
| 24 | I | 101 | BCR | C35-C13-C14 | -2.84 | 118.22 | 122.82 |
| 29 | 4 | 605 | CHL | OMC-CMC-C2C | -2.84 | 120.19 | 125.12 |
| 21 | a | 611 | CLA | O2D-CGD-O1D | -2.84 | 118.33 | 123.85 |
| 21 | 7 | 410 | CLA | O2D-CGD-O1D | -2.84 | 118.33 | 123.85 |
| 21 | A | 832 | CLA | C3B-C4B-NB | -2.84 | 108.00 | 110.53 |
| 24 | 7 | 417 | BCR | C8-C9-C10 | 2.84 | 123.47 | 119.01 |
| 29 | 9 | 601 | CHL | OMC-CMC-C2C | -2.84 | 120.20 | 125.12 |
| 21 | 3 | 411 | CLA | O2D-CGD-O1D | -2.83 | 118.33 | 123.85 |
| 21 | A | 826 | CLA | C3B-C4B-NB | -2.83 | 108.00 | 110.53 |
| 21 | 9 | 612 | CLA | C3B-C4B-NB | -2.83 | 108.00 | 110.53 |
| 21 | O | 203 | CLA | CBD-CHA-C1A | 2.83 | 131.65 | 127.38 |
| 21 | O | 203 | CLA | C3B-C4B-NB | -2.83 | 108.00 | 110.53 |
| 21 | 4 | 608 | CLA | C3B-C4B-NB | -2.83 | 108.00 | 110.53 |
| 24 | 8 | 616 | BCR | C35-C13-C14 | -2.83 | 118.23 | 122.82 |
| 29 | 9 | 606 | CHL | O1D-CGD-CBD | -2.83 | 120.43 | 124.72 |
| 21 | B | 820 | CLA | O2D-CGD-O1D | -2.83 | 118.34 | 123.85 |
| 21 | 9 | 602 | CLA | C3B-C4B-NB | -2.83 | 108.01 | 110.53 |
| 21 | 8 | 612 | CLA | O2D-CGD-O1D | -2.83 | 118.35 | 123.85 |
| 21 | 5 | 605 | CLA | O2D-CGD-O1D | -2.83 | 118.35 | 123.85 |
| 24 | J | 104 | BCR | C30-C25-C24 | 2.82 | 123.31 | 115.65 |
| 21 | A | 822 | CLA | C3B-C4B-NB | -2.82 | 108.01 | 110.53 |
| 21 | 8 | 604 | CLA | O2D-CGD-O1D | -2.82 | 118.36 | 123.85 |
| 21 | A | 837 | CLA | C3B-C4B-NB | -2.82 | 108.01 | 110.53 |
| 31 | 6 | 617 | XAT | C20-C13-C14 | -2.82 | 118.25 | 122.82 |
| 21 | 3 | 413 | CLA | C3B-C4B-NB | -2.82 | 108.01 | 110.53 |
| 29 | a | 607 | CHL | OMC-CMC-C2C | -2.82 | 120.22 | 125.12 |
| 32 | c | 618 | NEX | C12-C13-C14 | 2.82 | 123.44 | 119.01 |
| 21 | c | 612 | CLA | O2D-CGD-O1D | -2.82 | 118.36 | 123.85 |
| 21 | a | 610 | CLA | O2D-CGD-O1D | -2.82 | 118.36 | 123.85 |
| 21 | 7 | 409 | CLA | C3B-C4B-NB | -2.82 | 108.02 | 110.53 |
| 21 | 9 | 612 | CLA | O2D-CGD-O1D | -2.82 | 118.37 | 123.85 |
| 29 | 2 | 605 | CHL | CBC-CAC-C3C | -2.82 | 108.84 | 112.87 |
| 24 | 7 | 418 | BCR | C8-C9-C10 | 2.82 | 123.44 | 119.01 |
| 21 | 9 | 610 | CLA | C3B-C4B-NB | -2.82 | 108.02 | 110.53 |
| 26 | A | 853 | LMU | C1B-O1B-C4' | -2.81 | 111.31 | 117.98 |
| 24 | I | 101 | BCR | C12-C13-C14 | 2.81 | 123.44 | 119.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 602 | CHL | O2A-CGA-CBA | 2.81 | 120.42 | 111.83 |
| 24 | B | 844 | BCR | C1-C6-C5 | -2.81 | 118.79 | 122.64 |
| 21 | A | 806 | CLA | C3B-C4B-NB | -2.81 | 108.02 | 110.53 |
| 21 | 5 | 614 | CLA | O2D-CGD-O1D | -2.81 | 118.38 | 123.85 |
| 30 | 9 | 615 | LUT | C40-C33-C34 | -2.81 | 118.26 | 122.82 |
| 24 | 8 | 616 | BCR | C36-C18-C17 | -2.81 | 118.26 | 122.82 |
| 24 | B | 844 | BCR | C33-C5-C6 | -2.81 | 121.42 | 124.48 |
| 29 | 1 | 307 | CHL | CBC-CAC-C3C | -2.81 | 108.85 | 112.87 |
| 24 | 2 | 618 | BCR | C35-C13-C14 | -2.81 | 118.27 | 122.82 |
| 29 | 1 | 302 | CHL | O2A-CGA-CBA | 2.80 | 120.39 | 111.83 |
| 21 | 2 | 604 | CLA | C3B-C4B-NB | -2.80 | 108.03 | 110.53 |
| 21 | a | 604 | CLA | C3B-C4B-NB | -2.80 | 108.03 | 110.53 |
| 21 | 2 | 604 | CLA | O2D-CGD-O1D | -2.80 | 118.39 | 123.85 |
| 24 | L | 301 | BCR | C35-C13-C14 | -2.80 | 118.28 | 122.82 |
| 21 | b | 311 | CLA | C3B-C4B-NB | -2.80 | 108.03 | 110.53 |
| 21 | A | 801 | CLA | C4-C3-C5 | 2.80 | 120.09 | 115.23 |
| 21 | 9 | 613 | CLA | O2D-CGD-O1D | -2.80 | 118.40 | 123.85 |
| 24 | L | 301 | BCR | C19-C18-C17 | 2.80 | 123.41 | 119.01 |
| 21 | 6 | 613 | CLA | O2D-CGD-O1D | -2.80 | 118.41 | 123.85 |
| 24 | J | 103 | BCR | C34-C9-C10 | -2.80 | 118.29 | 122.82 |
| 21 | 7 | 414 | CLA | C3B-C4B-NB | -2.80 | 108.03 | 110.53 |
| 21 | b | 314 | CLA | C3B-C4B-NB | -2.80 | 108.03 | 110.53 |
| 29 | 9 | 605 | CHL | O1D-CGD-CBD | -2.80 | 120.48 | 124.72 |
| 30 | 2 | 616 | LUT | C10-C11-C12 | 2.80 | 131.30 | 123.20 |
| 21 | G | 203 | CLA | C3B-C4B-NB | -2.79 | 108.03 | 110.53 |
| 24 | A | 848 | BCR | C36-C18-C17 | -2.79 | 118.29 | 122.82 |
| 21 | B | 837 | CLA | O2D-CGD-O1D | -2.79 | 117.74 | 124.08 |
| 21 | 6 | 612 | CLA | C3B-C4B-NB | -2.79 | 108.04 | 110.53 |
| 24 | J | 103 | BCR | C36-C18-C17 | -2.79 | 118.29 | 122.82 |
| 30 | a | 616 | LUT | C20-C13-C14 | -2.79 | 118.30 | 122.82 |
| 24 | 8 | 616 | BCR | C19-C18-C17 | 2.79 | 123.40 | 119.01 |
| 21 | b | 305 | CLA | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 21 | A | 828 | CLA | C1-C2-C3 | -2.79 | 121.63 | 126.20 |
| 21 | 7 | 410 | CLA | C3B-C4B-NB | -2.79 | 108.04 | 110.53 |
| 29 | a | 601 | CHL | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 29 | c | 605 | CHL | OMC-CMC-C2C | -2.79 | 120.28 | 125.12 |
| 29 | 8 | 607 | CHL | O2A-CGA-CBA | 2.79 | 120.33 | 111.83 |
| 21 | b | 314 | CLA | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 21 | c | 603 | CLA | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 29 | 4 | 606 | CHL | O1D-CGD-CBD | -2.79 | 120.50 | 124.72 |
| 32 | b | 318 | NEX | C12-C13-C14 | 2.79 | 123.39 | 119.01 |
| 24 | A | 847 | BCR | C36-C18-C17 | -2.79 | 118.30 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | 4 | 616 | XAT | C19-C9-C8 | 2.79 | 122.34 | 118.09 |
| 32 | c | 618 | NEX | C20-C13-C14 | -2.78 | 118.30 | 122.82 |
| 21 | B | 801 | CLA | C4C-C3C-C2C | -2.78 | 102.84 | 106.89 |
| 24 | 3 | 419 | BCR | C10-C11-C12 | 2.78 | 131.26 | 123.20 |
| 21 | 7 | 407 | CLA | CBC-CAC-C3C | 2.78 | 119.96 | 112.42 |
| 21 | B | 801 | CLA | CMA-C3A-C4A | -2.78 | 104.30 | 111.77 |
| 21 | b | 311 | CLA | O2D-CGD-O1D | -2.78 | 118.43 | 123.85 |
| 21 | 3 | 402 | CLA | C3B-C4B-NB | -2.78 | 108.05 | 110.53 |
| 24 | J | 103 | BCR | C19-C18-C17 | 2.78 | 123.38 | 119.01 |
| 29 | b | 310 | CHL | OMC-CMC-C2C | -2.78 | 120.29 | 125.12 |
| 21 | B | 805 | CLA | C3B-C4B-NB | -2.78 | 108.05 | 110.53 |
| 24 | B | 845 | BCR | C36-C18-C17 | -2.78 | 118.31 | 122.82 |
| 21 | G | 204 | CLA | C3B-C4B-NB | -2.78 | 108.05 | 110.53 |
| 21 | B | 801 | CLA | CHC-C1C-C2C | -2.78 | 119.05 | 126.95 |
| 30 | 3 | 416 | LUT | C32-C33-C34 | 2.78 | 123.38 | 119.01 |
| 21 | O | 202 | CLA | C3A-C2A-C1A | -2.78 | 103.46 | 106.30 |
| 30 | 6 | 616 | LUT | C39-C29-C28 | 2.77 | 122.33 | 118.09 |
| 21 | K | 204 | CLA | C3B-C4B-NB | -2.77 | 108.05 | 110.53 |
| 21 | L | 302 | CLA | C3B-C4B-NB | -2.77 | 108.05 | 110.53 |
| 26 | 3 | 420 | LMU | C1B-O1B-C4' | -2.77 | 111.40 | 117.98 |
| 21 | 2 | 610 | CLA | C3B-C4B-NB | -2.77 | 108.05 | 110.53 |
| 21 | A | 835 | CLA | CHB-C4A-NA | 2.77 | 128.40 | 124.40 |
| 21 | 5 | 609 | CLA | C3B-C4B-NB | -2.77 | 108.06 | 110.53 |
| 21 | a | 613 | CLA | O2D-CGD-O1D | -2.77 | 118.45 | 123.85 |
| 21 | A | 840 | CLA | C1-C2-C3 | -2.77 | 121.66 | 126.20 |
| 21 | A | 821 | CLA | C3B-C4B-NB | -2.77 | 108.06 | 110.53 |
| 29 | 4 | 614 | CHL | O1D-CGD-CBD | -2.77 | 120.52 | 124.72 |
| 24 | B | 846 | BCR | C38-C26-C25 | -2.77 | 121.46 | 124.48 |
| 21 | 1 | 314 | CLA | O2D-CGD-O1D | -2.77 | 117.80 | 124.08 |
| 31 | 7 | 416 | XAT | C40-C33-C34 | -2.77 | 118.33 | 122.82 |
| 21 | a | 602 | CLA | C3B-C4B-NB | -2.77 | 108.06 | 110.53 |
| 21 | 7 | 409 | CLA | CAA-C2A-C3A | -2.77 | 109.89 | 116.23 |
| 32 | b | 318 | NEX | C20-C13-C14 | -2.77 | 118.34 | 122.82 |
| 21 | B | 828 | CLA | C3B-C4B-NB | -2.76 | 108.06 | 110.53 |
| 24 | F | 303 | BCR | C34-C9-C8 | 2.76 | 122.31 | 118.09 |
| 24 | B | 844 | BCR | C38-C26-C27 | 2.76 | 119.49 | 113.60 |
| 21 | 8 | 602 | CLA | C3B-C4B-NB | -2.76 | 108.06 | 110.53 |
| 21 | L | 304 | CLA | O2D-CGD-O1D | -2.76 | 118.47 | 123.85 |
| 21 | A | 814 | CLA | C3B-C4B-NB | -2.76 | 108.06 | 110.53 |
| 21 | A | 836 | CLA | O2D-CGD-O1D | -2.76 | 118.47 | 123.85 |
| 21 | 3 | 406 | CLA | O2D-CGD-O1D | -2.76 | 117.82 | 124.08 |
| 21 | A | 827 | CLA | O2D-CGD-O1D | -2.76 | 117.83 | 124.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | B | 842 | BCR | C35-C13-C14 | -2.75 | 118.35 | 122.82 |
| 21 | B | 819 | CLA | C3B-C4B-NB | -2.75 | 108.07 | 110.53 |
| 21 | 2 | 611 | CLA | CMA-C3A-C2A | -2.75 | 109.91 | 116.23 |
| 24 | 3 | 418 | BCR | C36-C18-C17 | -2.75 | 118.36 | 122.82 |
| 21 | B | 822 | CLA | C3B-C4B-NB | -2.75 | 108.07 | 110.53 |
| 21 | 8 | 610 | CLA | O2D-CGD-O1D | -2.75 | 118.49 | 123.85 |
| 24 | L | 305 | BCR | C36-C18-C17 | -2.75 | 118.36 | 122.82 |
| 29 | b | 310 | CHL | C4-C3-C5 | 2.75 | 120.00 | 115.23 |
| 24 | G | 205 | BCR | C36-C18-C17 | -2.75 | 118.36 | 122.82 |
| 21 | B | 822 | CLA | O2D-CGD-O1D | -2.75 | 118.49 | 123.85 |
| 21 | A | 840 | CLA | C3B-C4B-NB | -2.75 | 108.07 | 110.53 |
| 21 | 9 | 613 | CLA | C3B-C4B-NB | -2.75 | 108.08 | 110.53 |
| 21 | c | 610 | CLA | O2D-CGD-O1D | -2.75 | 118.50 | 123.85 |
| 24 | 7 | 418 | BCR | C21-C20-C19 | 2.75 | 131.17 | 123.20 |
| 21 | 9 | 602 | CLA | O2D-CGD-O1D | -2.75 | 118.50 | 123.85 |
| 29 | a | 606 | CHL | O2D-CGD-O1D | -2.75 | 118.50 | 123.85 |
| 32 | 9 | 617 | NEX | C40-C33-C34 | -2.75 | 118.36 | 122.82 |
| 29 | a | 609 | CHL | O1D-CGD-CBD | -2.75 | 120.56 | 124.72 |
| 21 | 3 | 401 | CLA | CAA-C2A-C3A | -2.75 | 109.93 | 116.23 |
| 24 | K | 205 | BCR | C38-C26-C25 | -2.75 | 121.49 | 124.48 |
| 21 | 1 | 312 | CLA | O2D-CGD-O1D | -2.75 | 118.50 | 123.85 |
| 21 | c | 611 | CLA | C3B-C4B-NB | -2.75 | 108.08 | 110.53 |
| 24 | I | 101 | BCR | C36-C18-C17 | -2.75 | 118.37 | 122.82 |
| 24 | B | 844 | BCR | C23-C24-C25 | -2.75 | 119.67 | 127.00 |
| 24 | 3 | 418 | BCR | C35-C13-C14 | -2.74 | 118.37 | 122.82 |
| 21 | 3 | 401 | CLA | O2D-CGD-O1D | -2.74 | 117.86 | 124.08 |
| 21 | A | 829 | CLA | C3B-C4B-NB | -2.74 | 108.08 | 110.53 |
| 30 | 3 | 416 | LUT | C40-C33-C34 | -2.74 | 118.37 | 122.82 |
| 21 | 3 | 415 | CLA | O2D-CGD-O1D | -2.74 | 117.86 | 124.08 |
| 31 | 6 | 617 | XAT | C12-C13-C14 | 2.74 | 123.32 | 119.01 |
| 32 | 9 | 617 | NEX | C32-C33-C34 | 2.74 | 123.32 | 119.01 |
| 24 | B | 842 | BCR | C12-C13-C14 | 2.74 | 123.32 | 119.01 |
| 29 | 8 | 613 | CHL | OMC-CMC-C2C | -2.74 | 120.36 | 125.12 |
| 21 | 6 | 609 | CLA | CHB-C4A-NA | 2.74 | 128.35 | 124.40 |
| 21 | 3 | 403 | CLA | O2D-CGD-O1D | -2.74 | 118.52 | 123.85 |
| 29 | 8 | 605 | CHL | O1D-CGD-CBD | -2.74 | 120.57 | 124.72 |
| 29 | b | 306 | CHL | O1D-CGD-CBD | -2.74 | 120.57 | 124.72 |
| 21 | 3 | 411 | CLA | C3B-C4B-NB | -2.74 | 108.09 | 110.53 |
| 21 | 1 | 309 | CLA | CAA-C2A-C3A | -2.73 | 109.96 | 116.23 |
| 29 | 8 | 606 | CHL | O1D-CGD-CBD | -2.73 | 120.58 | 124.72 |
| 21 | a | 612 | CLA | O2D-CGD-O1D | -2.73 | 118.53 | 123.85 |
| 21 | 3 | 404 | CLA | O2D-CGD-O1D | -2.73 | 117.88 | 124.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 310 | CLA | C3B-C4B-NB | -2.73 | 108.09 | 110.53 |
| 21 | 8 | 618 | CLA | O2D-CGD-O1D | -2.73 | 118.53 | 123.85 |
| 30 | b | 316 | LUT | C40-C33-C34 | -2.73 | 118.39 | 122.82 |
| 29 | 6 | 606 | CHL | OMC-CMC-C2C | -2.73 | 120.38 | 125.12 |
| 21 | 7 | 407 | CLA | C2D-C1D-ND | 2.73 | 112.83 | 110.13 |
| 30 | a | 616 | LUT | C15-C35-C34 | 2.73 | 129.10 | 123.52 |
| 21 | 4 | 602 | CLA | C3B-C4B-NB | -2.73 | 108.09 | 110.53 |
| 24 | 3 | 418 | BCR | C12-C13-C14 | 2.73 | 123.30 | 119.01 |
| 21 | A | 801 | CLA | C3A-C2A-C1A | 2.73 | 105.42 | 101.34 |
| 24 | A | 848 | BCR | C19-C18-C17 | 2.73 | 123.30 | 119.01 |
| 21 | A | 810 | CLA | C3B-C4B-NB | -2.73 | 108.10 | 110.53 |
| 21 | B | 825 | CLA | C3B-C4B-NB | -2.73 | 108.10 | 110.53 |
| 31 | a | 618 | XAT | C40-C33-C34 | -2.72 | 118.40 | 122.82 |
| 29 | 6 | 606 | CHL | O1D-CGD-CBD | -2.72 | 120.59 | 124.72 |
| 21 | 4 | 613 | CLA | C3B-C4B-NB | -2.72 | 108.10 | 110.53 |
| 21 | 6 | 612 | CLA | O2D-CGD-O1D | -2.72 | 118.55 | 123.85 |
| 30 | b | 317 | LUT | C35-C15-C14 | 2.72 | 129.09 | 123.52 |
| 21 | 1 | 309 | CLA | C2A-C3A-C4A | 2.72 | 104.78 | 101.59 |
| 21 | 6 | 610 | CLA | C3B-C4B-NB | -2.72 | 108.10 | 110.53 |
| 21 | F | 304 | CLA | O2D-CGD-O1D | -2.72 | 118.55 | 123.85 |
| 24 | G | 201 | BCR | C36-C18-C17 | -2.72 | 118.41 | 122.82 |
| 29 | 6 | 602 | CHL | O1D-CGD-CBD | -2.72 | 120.60 | 124.72 |
| 24 | 4 | 617 | BCR | C36-C18-C17 | -2.72 | 118.41 | 122.82 |
| 21 | A | 817 | CLA | C3B-C4B-NB | -2.72 | 108.10 | 110.53 |
| 21 | b | 312 | CLA | C3B-C4B-NB | -2.72 | 108.10 | 110.53 |
| 31 | 5 | 616 | XAT | C20-C13-C14 | -2.72 | 118.41 | 122.82 |
| 24 | B | 845 | BCR | C19-C18-C17 | 2.72 | 123.28 | 119.01 |
| 30 | 8 | 614 | LUT | C20-C13-C14 | -2.72 | 118.42 | 122.82 |
| 21 | B | 823 | CLA | CHB-C4A-NA | 2.72 | 128.32 | 124.40 |
| 21 | 3 | 414 | CLA | CAA-C2A-C3A | -2.72 | 110.00 | 116.23 |
| 31 | 3 | 417 | XAT | C40-C33-C34 | -2.71 | 118.42 | 122.82 |
| 24 | G | 205 | BCR | C19-C18-C17 | 2.71 | 123.28 | 119.01 |
| 31 | 7 | 416 | XAT | C32-C33-C34 | 2.71 | 123.27 | 119.01 |
| 24 | B | 846 | BCR | C20-C21-C22 | -2.71 | 123.48 | 127.28 |
| 24 | A | 846 | BCR | C35-C13-C14 | -2.71 | 118.42 | 122.82 |
| 21 | 2 | 613 | CLA | C3B-C4B-NB | -2.71 | 108.11 | 110.53 |
| 21 | 3 | 409 | CLA | C4-C3-C5 | 2.71 | 119.93 | 115.23 |
| 21 | 5 | 612 | CLA | O2D-CGD-O1D | -2.71 | 118.58 | 123.85 |
| 24 | B | 846 | BCR | C4-C5-C6 | -2.71 | 119.05 | 122.70 |
| 29 | 6 | 605 | CHL | O1D-CGD-CBD | -2.71 | 120.62 | 124.72 |
| 21 | 3 | 412 | CLA | O2D-CGD-O1D | -2.71 | 117.94 | 124.08 |
| 31 | 4 | 616 | XAT | C40-C33-C34 | -2.70 | 118.43 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 8 | 601 | CLA | O2D-CGD-O1D | -2.70 | 118.58 | 123.85 |
| 29 | c | 608 | CHL | O1D-CGD-CBD | -2.70 | 120.62 | 124.72 |
| 21 | 1 | 303 | CLA | C3B-C4B-NB | -2.70 | 108.12 | 110.53 |
| 21 | 8 | 604 | CLA | C3B-C4B-NB | -2.70 | 108.12 | 110.53 |
| 21 | B | 811 | CLA | O2D-CGD-O1D | -2.70 | 118.59 | 123.85 |
| 29 | b | 307 | CHL | O1D-CGD-CBD | -2.70 | 120.62 | 124.72 |
| 24 | L | 305 | BCR | C19-C18-C17 | 2.70 | 123.26 | 119.01 |
| 21 | B | 809 | CLA | O2D-CGD-O1D | -2.70 | 117.95 | 124.08 |
| 24 | 4 | 617 | BCR | C19-C18-C17 | 2.70 | 123.26 | 119.01 |
| 24 | A | 850 | BCR | C35-C13-C14 | -2.70 | 118.44 | 122.82 |
| 21 | 5 | 603 | CLA | O2D-CGD-O1D | -2.70 | 118.60 | 123.85 |
| 21 | A | 808 | CLA | C3B-C4B-NB | -2.70 | 108.12 | 110.53 |
| 24 | A | 850 | BCR | C36-C18-C17 | -2.70 | 118.45 | 122.82 |
| 30 | 7 | 415 | LUT | C40-C33-C34 | -2.70 | 118.45 | 122.82 |
| 29 | b | 310 | CHL | CBC-CAC-C3C | -2.70 | 109.01 | 112.87 |
| 21 | a | 603 | CLA | C3B-C4B-NB | -2.70 | 108.12 | 110.53 |
| 21 | a | 611 | CLA | C3B-C4B-NB | -2.69 | 108.12 | 110.53 |
| 29 | 6 | 614 | CHL | O1D-CGD-CBD | -2.69 | 120.64 | 124.72 |
| 31 | 1 | 318 | XAT | C40-C33-C34 | -2.69 | 118.46 | 122.82 |
| 21 | 7 | 408 | CLA | O2D-CGD-O1D | -2.69 | 118.61 | 123.85 |
| 21 | A | 807 | CLA | C3B-C4B-NB | -2.69 | 108.13 | 110.53 |
| 21 | F | 305 | CLA | C3B-C4B-NB | -2.69 | 108.13 | 110.53 |
| 29 | 8 | 613 | CHL | O1D-CGD-CBD | -2.69 | 120.65 | 124.72 |
| 29 | 9 | 605 | CHL | CBC-CAC-C3C | -2.68 | 109.03 | 112.87 |
| 21 | 6 | 608 | CLA | O2D-CGD-O1D | -2.68 | 118.62 | 123.85 |
| 24 | 4 | 617 | BCR | C35-C13-C14 | -2.68 | 118.47 | 122.82 |
| 21 | 1 | 306 | CLA | C3A-C2A-C1A | -2.68 | 103.56 | 106.30 |
| 24 | A | 847 | BCR | C16-C15-C14 | 2.68 | 129.00 | 123.52 |
| 21 | 3 | 413 | CLA | O2D-CGD-O1D | -2.68 | 118.00 | 124.08 |
| 24 | 3 | 419 | BCR | C23-C22-C21 | 2.68 | 123.22 | 119.01 |
| 24 | I | 101 | BCR | C19-C18-C17 | 2.68 | 123.22 | 119.01 |
| 30 | b | 316 | LUT | C32-C33-C34 | 2.67 | 123.21 | 119.01 |
| 24 | G | 201 | BCR | C35-C13-C14 | -2.67 | 118.49 | 122.82 |
| 21 | F | 305 | CLA | CAA-C2A-C3A | -2.67 | 110.11 | 116.23 |
| 24 | B | 845 | BCR | C35-C13-C14 | -2.67 | 118.49 | 122.82 |
| 30 | c | 616 | LUT | C40-C33-C34 | -2.67 | 118.49 | 122.82 |
| 21 | K | 201 | CLA | C3B-C4B-NB | -2.67 | 108.15 | 110.53 |
| 21 | B | 813 | CLA | O2D-CGD-O1D | -2.66 | 118.03 | 124.08 |
| 24 | A | 854 | BCR | C35-C13-C14 | -2.66 | 118.50 | 122.82 |
| 24 | F | 301 | BCR | C36-C18-C17 | -2.66 | 118.50 | 122.82 |
| 29 | 2 | 601 | CHL | C1-C2-C3 | -2.66 | 121.84 | 126.20 |
| 30 | b | 317 | LUT | C40-C33-C34 | -2.66 | 118.50 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 5 | 606 | CHL | O1D-CGD-CBD | -2.66 | 120.69 | 124.72 |
| 31 | 2 | 617 | XAT | C40-C33-C34 | -2.66 | 118.50 | 122.82 |
| 30 | b | 316 | LUT | C20-C13-C14 | -2.66 | 118.51 | 122.82 |
| 21 | B | 801 | CLA | CMC-C2C-C1C | 2.66 | 129.19 | 125.03 |
| 21 | 1 | 308 | CLA | O2D-CGD-O1D | -2.66 | 118.05 | 124.08 |
| 29 | 2 | 605 | CHL | OMC-CMC-C2C | -2.66 | 120.50 | 125.12 |
| 30 | c | 616 | LUT | C20-C13-C14 | -2.65 | 118.52 | 122.82 |
| 21 | b | 315 | CLA | C3B-C4B-NB | -2.65 | 108.16 | 110.53 |
| 21 | B | 801 | CLA | CBC-CAC-C3C | -2.65 | 105.23 | 112.42 |
| 31 | c | 617 | XAT | C40-C33-C34 | -2.65 | 118.52 | 122.82 |
| 21 | 4 | 602 | CLA | O2D-CGD-O1D | -2.65 | 118.07 | 124.08 |
| 24 | J | 101 | BCR | C35-C13-C14 | -2.65 | 118.52 | 122.82 |
| 29 | 2 | 606 | CHL | O2D-CGD-O1D | -2.65 | 118.69 | 123.85 |
| 24 | A | 847 | BCR | C19-C18-C17 | 2.65 | 123.18 | 119.01 |
| 29 | b | 308 | CHL | O2A-CGA-CBA | 2.65 | 119.91 | 111.83 |
| 31 | c | 617 | XAT | C15-C35-C34 | 2.65 | 128.94 | 123.52 |
| 21 | b | 313 | CLA | C3B-C4B-NB | -2.65 | 108.17 | 110.53 |
| 21 | c | 613 | CLA | C3B-C4B-NB | -2.65 | 108.17 | 110.53 |
| 24 | B | 842 | BCR | C36-C18-C17 | -2.65 | 118.53 | 122.82 |
| 21 | B | 817 | CLA | C3B-C4B-NB | -2.65 | 108.17 | 110.53 |
| 24 | J | 104 | BCR | C2-C3-C4 | -2.65 | 105.46 | 111.28 |
| 30 | a | 616 | LUT | C39-C29-C28 | 2.65 | 122.13 | 118.09 |
| 30 | 7 | 415 | LUT | C1-C6-C5 | -2.65 | 119.02 | 122.64 |
| 24 | A | 848 | BCR | C16-C15-C14 | 2.64 | 128.93 | 123.52 |
| 21 | B | 807 | CLA | C3B-C4B-NB | -2.64 | 108.17 | 110.53 |
| 21 | 4 | 611 | CLA | C3B-C4B-NB | -2.64 | 108.17 | 110.53 |
| 29 | 1 | 307 | CHL | O2A-CGA-CBA | 2.64 | 119.89 | 111.83 |
| 21 | A | 819 | CLA | C3B-C4B-NB | -2.64 | 108.17 | 110.53 |
| 21 | K | 202 | CLA | CHB-C4A-NA | 2.64 | 128.21 | 124.40 |
| 30 | 6 | 616 | LUT | C40-C33-C34 | -2.64 | 118.54 | 122.82 |
| 24 | J | 103 | BCR | C8-C9-C10 | 2.64 | 123.16 | 119.01 |
| 24 | G | 201 | BCR | C19-C18-C17 | 2.64 | 123.16 | 119.01 |
| 29 | a | 605 | CHL | CBC-CAC-C3C | -2.64 | 109.10 | 112.87 |
| 31 | 4 | 616 | XAT | C32-C33-C34 | 2.64 | 123.16 | 119.01 |
| 29 | 6 | 602 | CHL | CBC-CAC-C3C | -2.64 | 109.10 | 112.87 |
| 30 | 5 | 615 | LUT | C40-C33-C34 | -2.63 | 118.55 | 122.82 |
| 24 | A | 854 | BCR | C23-C22-C21 | 2.63 | 123.15 | 119.01 |
| 21 | B | 815 | CLA | O2D-CGD-O1D | -2.63 | 118.11 | 124.08 |
| 21 | 1 | 311 | CLA | O2D-CGD-O1D | -2.63 | 118.11 | 124.08 |
| 21 | 9 | 610 | CLA | CMB-C2B-C1B | -2.63 | 121.41 | 125.42 |
| 29 | 4 | 607 | CHL | O1D-CGD-CBD | -2.63 | 120.73 | 124.72 |
| 21 | 4 | 604 | CLA | C3B-C4B-NB | -2.63 | 108.18 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 606 | CHL | O1D-CGD-CBD | -2.63 | 120.74 | 124.72 |
| 30 | 9 | 615 | LUT | C19-C9-C8 | 2.63 | 122.10 | 118.09 |
| 21 | G | 202 | CLA | CHB-C4A-NA | 2.63 | 128.19 | 124.40 |
| 29 | 6 | 602 | CHL | O2D-CGD-O1D | -2.63 | 118.74 | 123.85 |
| 29 | 6 | 607 | CHL | O2A-CGA-CBA | 2.63 | 119.84 | 111.83 |
| 21 | O | 204 | CLA | C3B-C4B-NB | -2.62 | 108.19 | 110.53 |
| 29 | b | 308 | CHL | O1D-CGD-CBD | -2.62 | 120.74 | 124.72 |
| 24 | G | 205 | BCR | C35-C13-C14 | -2.62 | 118.56 | 122.82 |
| 21 | B | 836 | CLA | CHB-C4A-NA | 2.62 | 128.19 | 124.40 |
| 21 | B | 821 | CLA | C3B-C4B-NB | -2.62 | 108.19 | 110.53 |
| 31 | 7 | 416 | XAT | C20-C13-C14 | -2.62 | 118.57 | 122.82 |
| 29 | a | 607 | CHL | O2D-CGD-O1D | -2.62 | 118.75 | 123.85 |
| 31 | 5 | 616 | XAT | C40-C33-C34 | -2.62 | 118.57 | 122.82 |
| 30 | a | 615 | LUT | C40-C33-C34 | -2.62 | 118.57 | 122.82 |
| 21 | 1 | 309 | CLA | CMD-C2D-C3D | -2.62 | 121.69 | 127.69 |
| 21 | B | 829 | CLA | CHB-C4A-NA | 2.62 | 128.18 | 124.40 |
| 24 | G | 201 | BCR | C12-C13-C14 | 2.62 | 123.12 | 119.01 |
| 21 | A | 817 | CLA | CHB-C4A-NA | 2.62 | 128.18 | 124.40 |
| 21 | L | 304 | CLA | C3B-C4B-NB | -2.61 | 108.20 | 110.53 |
| 29 | 9 | 606 | CHL | CBC-CAC-C3C | -2.61 | 109.13 | 112.87 |
| 24 | A | 850 | BCR | C12-C13-C14 | 2.61 | 123.12 | 119.01 |
| 31 | a | 618 | XAT | C32-C33-C34 | 2.61 | 123.12 | 119.01 |
| 24 | B | 843 | BCR | C1-C6-C7 | 2.61 | 122.73 | 115.65 |
| 21 | 7 | 411 | CLA | C3B-C4B-NB | -2.61 | 108.20 | 110.53 |
| 21 | 8 | 618 | CLA | C3B-C4B-NB | -2.61 | 108.20 | 110.53 |
| 29 | a | 606 | CHL | CBC-CAC-C3C | -2.61 | 109.14 | 112.87 |
| 21 | 1 | 311 | CLA | CAA-C2A-C3A | -2.61 | 110.24 | 116.23 |
| 21 | 5 | 611 | CLA | C3B-C4B-NB | -2.61 | 108.20 | 110.53 |
| 21 | 7 | 414 | CLA | CAA-C2A-C3A | -2.61 | 110.25 | 116.23 |
| 31 | 6 | 617 | XAT | C35-C15-C14 | 2.61 | 128.85 | 123.52 |
| 21 | A | 825 | CLA | C3B-C4B-NB | -2.61 | 108.20 | 110.53 |
| 21 | B | 824 | CLA | C3B-C4B-NB | -2.61 | 108.20 | 110.53 |
| 21 | A | 801 | CLA | O2A-CGA-CBA | 2.60 | 119.78 | 111.83 |
| 29 | 2 | 602 | CHL | O2D-CGD-O1D | -2.60 | 118.78 | 123.85 |
| 24 | O | 205 | BCR | C8-C9-C10 | 2.60 | 123.11 | 119.01 |
| 21 | 3 | 405 | CLA | O2D-CGD-O1D | -2.60 | 118.17 | 124.08 |
| 21 | B | 801 | CLA | C4B-C3B-C2B | -2.60 | 104.06 | 107.30 |
| 21 | B | 811 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |
| 21 | K | 203 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |
| 21 | 6 | 612 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |
| 24 | J | 101 | BCR | C12-C13-C14 | 2.60 | 123.10 | 119.01 |
| 21 | A | 841 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | b | 302 | CHL | O1D-CGD-CBD | -2.60 | 120.78 | 124.72 |
| 31 | 3 | 417 | XAT | C32-C33-C34 | 2.60 | 123.10 | 119.01 |
| 30 | 9 | 614 | LUT | C19-C9-C8 | 2.60 | 122.06 | 118.09 |
| 21 | B | 832 | CLA | CMB-C2B-C1B | -2.60 | 121.46 | 125.42 |
| 24 | A | 849 | BCR | C35-C13-C14 | -2.60 | 118.61 | 122.82 |
| 31 | 8 | 615 | XAT | C40-C33-C34 | -2.60 | 118.61 | 122.82 |
| 24 | B | 844 | BCR | C33-C5-C4 | 2.60 | 119.13 | 113.60 |
| 24 | L | 305 | BCR | C35-C13-C14 | -2.59 | 118.61 | 122.82 |
| 31 | 2 | 617 | XAT | C19-C9-C8 | 2.59 | 122.05 | 118.09 |
| 24 | B | 844 | BCR | C38-C26-C25 | -2.59 | 121.66 | 124.48 |
| 21 | 5 | 613 | CLA | CAA-C2A-C3A | -2.59 | 110.29 | 116.23 |
| 21 | 3 | 410 | CLA | CAA-C2A-C3A | -2.59 | 110.29 | 116.23 |
| 21 | 1 | 308 | CLA | CHB-C4A-NA | 2.59 | 128.14 | 124.40 |
| 29 | 2 | 614 | CHL | O1D-CGD-CBD | -2.59 | 120.80 | 124.72 |
| 21 | B | 804 | CLA | CHB-C4A-NA | 2.59 | 128.14 | 124.40 |
| 24 | F | 303 | BCR | C15-C16-C17 | 2.59 | 128.81 | 123.52 |
| 29 | 6 | 602 | CHL | C4-C3-C5 | 2.59 | 119.72 | 115.23 |
| 24 | B | 843 | BCR | C21-C20-C19 | -2.59 | 115.70 | 123.20 |
| 21 | 5 | 607 | CLA | O2D-CGD-O1D | -2.59 | 118.21 | 124.08 |
| 30 | c | 615 | LUT | C15-C35-C34 | 2.59 | 128.81 | 123.52 |
| 21 | c | 603 | CLA | C3B-C4B-NB | -2.59 | 108.22 | 110.53 |
| 21 | B | 833 | CLA | CHB-C4A-NA | 2.59 | 128.13 | 124.40 |
| 21 | 9 | 603 | CLA | CHB-C4A-NA | 2.59 | 128.13 | 124.40 |
| 30 | 5 | 615 | LUT | C19-C9-C10 | -2.58 | 118.63 | 122.82 |
| 21 | G | 204 | CLA | O2D-CGD-O1D | -2.58 | 118.22 | 124.08 |
| 24 | I | 101 | BCR | C8-C9-C10 | 2.58 | 123.07 | 119.01 |
| 29 | 9 | 607 | CHL | O1D-CGD-CBD | -2.58 | 120.81 | 124.72 |
| 21 | B | 834 | CLA | CHB-C4A-NA | 2.58 | 128.13 | 124.40 |
| 24 | A | 846 | BCR | C12-C13-C14 | 2.58 | 123.07 | 119.01 |
| 30 | 2 | 616 | LUT | C31-C30-C29 | 2.58 | 130.90 | 127.28 |
| 29 | 2 | 601 | CHL | O2D-CGD-O1D | -2.58 | 118.82 | 123.85 |
| 29 | 1 | 307 | CHL | O2D-CGD-O1D | -2.58 | 118.83 | 123.85 |
| 21 | 5 | 608 | CLA | CAA-C2A-C3A | -2.58 | 110.32 | 116.23 |
| 31 | 1 | 318 | XAT | C32-C33-C34 | 2.58 | 123.06 | 119.01 |
| 32 | c | 618 | NEX | C19-C9-C10 | -2.58 | 118.64 | 122.82 |
| 29 | 7 | 406 | CHL | O2D-CGD-CBD | 2.58 | 120.22 | 113.90 |
| 22 | A | 843 | PQN | C11-C3-C2 | -2.57 | 120.48 | 124.89 |
| 21 | 5 | 602 | CLA | CHB-C4A-NA | 2.57 | 128.12 | 124.40 |
| 29 | 9 | 601 | CHL | C4D-CHA-CBD | -2.57 | 106.37 | 108.97 |
| 21 | A | 804 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 21 | B | 816 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 21 | 5 | 609 | CLA | O2D-CGD-O1D | -2.57 | 118.24 | 124.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | c | 604 | CLA | C3B-C4B-NB | -2.57 | 108.23 | 110.53 |
| 21 | 4 | 603 | CLA | O2D-CGD-O1D | -2.57 | 118.24 | 124.08 |
| 21 | 4 | 608 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 21 | O | 201 | CLA | C3B-C4B-NB | -2.57 | 108.23 | 110.53 |
| 21 | 5 | 611 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 24 | B | 846 | BCR | C33-C5-C4 | 2.57 | 119.08 | 113.60 |
| 29 | 2 | 607 | CHL | O2A-CGA-CBA | 2.57 | 119.67 | 111.83 |
| 24 | J | 101 | BCR | C37-C22-C21 | -2.57 | 118.65 | 122.82 |
| 21 | 7 | 405 | CLA | O2D-CGD-O1D | -2.57 | 118.25 | 124.08 |
| 21 | a | 604 | CLA | O2D-CGD-O1D | -2.57 | 118.25 | 124.08 |
| 21 | K | 201 | CLA | CHB-C4A-NA | 2.57 | 128.10 | 124.40 |
| 21 | B | 825 | CLA | CHB-C4A-NA | 2.57 | 128.10 | 124.40 |
| 21 | 3 | 401 | CLA | CHB-C4A-NA | 2.57 | 128.10 | 124.40 |
| 24 | 4 | 617 | BCR | C12-C13-C14 | 2.57 | 123.05 | 119.01 |
| 30 | 9 | 614 | LUT | C39-C29-C28 | 2.57 | 122.01 | 118.09 |
| 21 | B | 836 | CLA | C3B-C4B-NB | -2.56 | 108.24 | 110.53 |
| 30 | 9 | 614 | LUT | C40-C33-C34 | -2.56 | 118.66 | 122.82 |
| 31 | 8 | 615 | XAT | C15-C35-C34 | 2.56 | 128.76 | 123.52 |
| 21 | O | 202 | CLA | O2D-CGD-O1D | -2.56 | 118.27 | 124.08 |
| 21 | 7 | 404 | CLA | O2D-CGD-O1D | -2.56 | 118.27 | 124.08 |
| 21 | G | 202 | CLA | C3B-C4B-NB | -2.56 | 108.25 | 110.53 |
| 31 | 6 | 617 | XAT | C7-C8-C9 | -2.56 | 121.56 | 125.53 |
| 30 | 6 | 616 | LUT | C8-C9-C10 | 2.56 | 123.03 | 119.01 |
| 29 | b | 310 | CHL | O2A-CGA-CBA | 2.56 | 119.64 | 111.83 |
| 21 | 5 | 610 | CLA | CAA-C2A-C3A | -2.56 | 110.36 | 116.23 |
| 21 | 7 | 409 | CLA | O2D-CGD-O1D | -2.56 | 118.28 | 124.08 |
| 21 | 7 | 401 | CLA | CHB-C4A-NA | 2.56 | 128.09 | 124.40 |
| 31 | c | 617 | XAT | C28-C29-C30 | 2.56 | 123.03 | 119.01 |
| 21 | 7 | 414 | CLA | O2D-CGD-O1D | -2.56 | 118.28 | 124.08 |
| 24 | B | 845 | BCR | C12-C13-C14 | 2.56 | 123.03 | 119.01 |
| 21 | A | 801 | CLA | CGD-CBD-CAD | 2.56 | 119.12 | 110.85 |
| 21 | 5 | 610 | CLA | O2D-CGD-O1D | -2.56 | 118.28 | 124.08 |
| 21 | B | 811 | CLA | C3B-C4B-NB | -2.56 | 108.25 | 110.53 |
| 21 | 2 | 603 | CLA | C3B-C4B-NB | -2.55 | 108.25 | 110.53 |
| 21 | 1 | 310 | CLA | O2D-CGD-O1D | -2.55 | 118.29 | 124.08 |
| 29 | 6 | 602 | CHL | O2A-CGA-CBA | 2.55 | 119.62 | 111.83 |
| 29 | b | 310 | CHL | O2D-CGD-CBD | 2.55 | 120.16 | 113.90 |
| 30 | c | 615 | LUT | C20-C13-C14 | -2.55 | 118.68 | 122.82 |
| 21 | A | 832 | CLA | CMB-C2B-C1B | -2.55 | 121.53 | 125.42 |
| 21 | B | 830 | CLA | C3B-C4B-NB | -2.55 | 108.25 | 110.53 |
| 21 | c | 614 | CLA | C3B-C4B-NB | -2.55 | 108.25 | 110.53 |
| 21 | 7 | 412 | CLA | O2D-CGD-O1D | -2.55 | 118.29 | 124.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 832 | CLA | CAA-C2A-C3A | -2.55 | 106.11 | 113.00 |
| 21 | 3 | 405 | CLA | CHB-C4A-NA | 2.55 | 128.08 | 124.40 |
| 21 | B | 814 | CLA | CHB-C4A-NA | 2.55 | 128.07 | 124.40 |
| 21 | 3 | 404 | CLA | CHB-C4A-NA | 2.55 | 128.07 | 124.40 |
| 30 | b | 317 | LUT | C32-C33-C34 | 2.54 | 123.01 | 119.01 |
| 31 | 5 | 616 | XAT | C12-C13-C14 | 2.54 | 123.01 | 119.01 |
| 29 | c | 601 | CHL | O1D-CGD-CBD | -2.54 | 120.87 | 124.72 |
| 21 | A | 804 | CLA | C3B-C4B-NB | -2.54 | 108.26 | 110.53 |
| 21 | A | 833 | CLA | C3B-C4B-NB | -2.54 | 108.26 | 110.53 |
| 21 | B | 840 | CLA | C3B-C4B-NB | -2.54 | 108.26 | 110.53 |
| 21 | 2 | 611 | CLA | CHB-C4A-NA | 2.54 | 128.07 | 124.40 |
| 24 | F | 303 | BCR | C7-C8-C9 | 2.54 | 130.00 | 126.23 |
| 24 | A | 848 | BCR | C34-C9-C8 | 2.54 | 121.97 | 118.09 |
| 31 | 2 | 617 | XAT | C20-C13-C14 | -2.54 | 118.70 | 122.82 |
| 21 | 7 | 411 | CLA | O2D-CGD-O1D | -2.54 | 118.32 | 124.08 |
| 21 | b | 311 | CLA | C1-C2-C3 | -2.54 | 122.03 | 126.20 |
| 29 | 9 | 601 | CHL | C3D-C4D-ND | -2.54 | 108.86 | 112.94 |
| 21 | 6 | 611 | CLA | CAA-C2A-C3A | -2.54 | 110.41 | 116.23 |
| 21 | B | 815 | CLA | CHB-C4A-NA | 2.54 | 128.06 | 124.40 |
| 21 | b | 304 | CLA | CHB-C4A-NA | 2.54 | 128.06 | 124.40 |
| 24 | F | 303 | BCR | C23-C22-C21 | 2.54 | 123.00 | 119.01 |
| 29 | 9 | 609 | CHL | O1D-CGD-CBD | -2.54 | 120.88 | 124.72 |
| 21 | A | 834 | CLA | C3B-C4B-NB | -2.54 | 108.27 | 110.53 |
| 21 | 4 | 611 | CLA | CHB-C4A-NA | 2.54 | 128.06 | 124.40 |
| 24 | B | 842 | BCR | C19-C18-C17 | 2.54 | 123.00 | 119.01 |
| 21 | b | 304 | CLA | C3B-C4B-NB | -2.54 | 108.27 | 110.53 |
| 21 | 5 | 610 | CLA | CAB-C3B-C2B | 2.53 | 130.27 | 123.53 |
| 30 | a | 616 | LUT | C40-C33-C34 | -2.53 | 118.71 | 122.82 |
| 21 | 4 | 602 | CLA | CHB-C4A-NA | 2.53 | 128.06 | 124.40 |
| 29 | 9 | 608 | CHL | CBC-CAC-C3C | -2.53 | 109.25 | 112.87 |
| 30 | b | 316 | LUT | C12-C13-C14 | 2.53 | 122.99 | 119.01 |
| 30 | 5 | 615 | LUT | C32-C33-C34 | 2.53 | 122.99 | 119.01 |
| 21 | 3 | 411 | CLA | CHB-C4A-NA | 2.53 | 128.05 | 124.40 |
| 21 | A | 814 | CLA | C1-C2-C3 | -2.53 | 122.05 | 126.20 |
| 24 | A | 849 | BCR | C21-C20-C19 | 2.53 | 130.53 | 123.20 |
| 24 | K | 205 | BCR | C23-C24-C25 | -2.53 | 120.24 | 127.00 |
| 21 | 3 | 410 | CLA | C3B-C4B-NB | -2.53 | 108.27 | 110.53 |
| 30 | c | 616 | LUT | C19-C9-C8 | 2.53 | 121.95 | 118.09 |
| 21 | 7 | 403 | CLA | O2D-CGD-O1D | -2.53 | 118.35 | 124.08 |
| 29 | 4 | 605 | CHL | O2D-CGD-O1D | -2.52 | 118.94 | 123.85 |
| 21 | L | 302 | CLA | CHB-C4A-NA | 2.52 | 128.04 | 124.40 |
| 31 | c | 617 | XAT | C32-C33-C34 | 2.52 | 122.97 | 119.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 802 | CLA | C3B-C4B-NB | -2.52 | 108.28 | 110.53 |
| 30 | 4 | 615 | LUT | C8-C9-C10 | 2.52 | 122.97 | 119.01 |
| 21 | 7 | 404 | CLA | C3B-C4B-NB | -2.52 | 108.28 | 110.53 |
| 30 | b | 317 | LUT | C39-C29-C28 | 2.52 | 121.93 | 118.09 |
| 21 | 7 | 407 | CLA | O2D-CGD-O1D | -2.52 | 118.37 | 124.08 |
| 21 | B | 821 | CLA | CHB-C4A-NA | 2.51 | 128.03 | 124.40 |
| 21 | 7 | 407 | CLA | C3C-C4C-NC | 2.51 | 113.65 | 110.43 |
| 21 | 9 | 613 | CLA | CHB-C4A-NA | 2.51 | 128.03 | 124.40 |
| 31 | 2 | 617 | XAT | C32-C33-C34 | 2.51 | 122.96 | 119.01 |
| 29 | b | 308 | CHL | CMA-C3A-C4A | -2.51 | 109.20 | 114.61 |
| 21 | B | 835 | CLA | CHB-C4A-NA | 2.51 | 128.02 | 124.40 |
| 21 | F | 304 | CLA | CHB-C4A-NA | 2.51 | 128.02 | 124.40 |
| 30 | b | 317 | LUT | C20-C13-C14 | -2.51 | 118.75 | 122.82 |
| 21 | 3 | 413 | CLA | CAA-C2A-C3A | -2.51 | 110.47 | 116.23 |
| 21 | 1 | 303 | CLA | CHB-C4A-NA | 2.51 | 128.02 | 124.40 |
| 29 | b | 309 | CHL | O1D-CGD-CBD | -2.51 | 120.92 | 124.72 |
| 29 | b | 302 | CHL | CBC-CAC-C3C | -2.51 | 109.28 | 112.87 |
| 21 | B | 814 | CLA | C3B-C4B-NB | -2.51 | 108.29 | 110.53 |
| 21 | 5 | 613 | CLA | O2D-CGD-O1D | -2.51 | 118.39 | 124.08 |
| 21 | 7 | 403 | CLA | CAB-C3B-C2B | 2.51 | 130.19 | 123.53 |
| 30 | 9 | 615 | LUT | C20-C13-C14 | -2.51 | 118.75 | 122.82 |
| 31 | 6 | 617 | XAT | C40-C33-C34 | -2.51 | 118.75 | 122.82 |
| 21 | B | 817 | CLA | CHB-C4A-NA | 2.50 | 128.01 | 124.40 |
| 29 | 9 | 605 | CHL | O2D-CGD-O1D | -2.50 | 118.97 | 123.85 |
| 21 | a | 604 | CLA | CHB-C4A-NA | 2.50 | 128.01 | 124.40 |
| 21 | A | 827 | CLA | C3B-C4B-NB | -2.50 | 108.30 | 110.53 |
| 24 | A | 848 | BCR | C35-C13-C14 | -2.50 | 118.77 | 122.82 |
| 21 | c | 613 | CLA | CHB-C4A-NA | 2.50 | 128.01 | 124.40 |
| 24 | B | 843 | BCR | C11-C12-C13 | -2.50 | 119.52 | 126.36 |
| 24 | A | 854 | BCR | C12-C13-C14 | 2.50 | 122.94 | 119.01 |
| 29 | 5 | 601 | CHL | O2D-CGD-O1D | -2.50 | 118.99 | 123.85 |
| 24 | L | 306 | BCR | C21-C20-C19 | 2.49 | 130.43 | 123.20 |
| 24 | B | 846 | BCR | C10-C11-C12 | -2.49 | 115.97 | 123.20 |
| 24 | A | 850 | BCR | C8-C9-C10 | 2.49 | 122.93 | 119.01 |
| 31 | 3 | 417 | XAT | C19-C9-C8 | 2.49 | 121.90 | 118.09 |
| 21 | 7 | 404 | CLA | CHB-C4A-NA | 2.49 | 128.00 | 124.40 |
| 21 | 6 | 609 | CLA | C3B-C4B-NB | -2.49 | 108.31 | 110.53 |
| 30 | 7 | 415 | LUT | C19-C9-C10 | -2.49 | 118.78 | 122.82 |
| 29 | b | 307 | CHL | OMC-CMC-C2C | -2.49 | 120.79 | 125.12 |
| 21 | 8 | 610 | CLA | CHB-C4A-NA | 2.49 | 128.00 | 124.40 |
| 21 | 1 | 309 | CLA | C3D-C4D-ND | 2.49 | 114.04 | 109.99 |
| 26 | A | 856 | LMU | C1B-O1B-C4' | -2.49 | 112.07 | 117.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 405 | CLA | C3B-C4B-NB | -2.49 | 108.31 | 110.53 |
| 24 | A | 849 | BCR | C34-C9-C8 | 2.49 | 121.89 | 118.09 |
| 21 | B | 805 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 21 | B | 813 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 30 | b | 317 | LUT | C19-C9-C8 | 2.49 | 121.89 | 118.09 |
| 29 | b | 307 | CHL | CBC-CAC-C3C | -2.49 | 109.31 | 112.87 |
| 21 | A | 814 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 21 | 7 | 410 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 21 | 4 | 609 | CLA | O2A-CGA-CBA | 2.49 | 119.42 | 111.83 |
| 21 | 1 | 315 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 21 | 7 | 408 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 21 | b | 313 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 21 | A | 831 | CLA | C1-C2-C3 | -2.49 | 122.12 | 126.20 |
| 21 | 3 | 415 | CLA | CAA-C2A-C3A | -2.49 | 110.53 | 116.23 |
| 31 | 4 | 616 | XAT | C20-C13-C14 | -2.49 | 118.79 | 122.82 |
| 21 | a | 613 | CLA | C1-C2-C3 | -2.48 | 122.13 | 126.20 |
| 22 | B | 841 | PQN | C11-C3-C2 | -2.48 | 120.63 | 124.89 |
| 21 | 8 | 602 | CLA | O2D-CGD-O1D | -2.48 | 118.45 | 124.08 |
| 30 | 7 | 415 | LUT | C32-C33-C34 | 2.48 | 122.92 | 119.01 |
| 21 | 4 | 601 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 21 | 9 | 612 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 21 | a | 612 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 21 | c | 611 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 31 | 1 | 318 | XAT | C7-C8-C9 | 2.48 | 129.38 | 125.53 |
| 21 | 1 | 305 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 21 | A | 839 | CLA | C3B-C4B-NB | -2.48 | 108.32 | 110.53 |
| 21 | 1 | 309 | CLA | C3B-C4B-NB | -2.48 | 108.32 | 110.53 |
| 21 | 9 | 604 | CLA | CHB-C4A-NA | 2.48 | 127.97 | 124.40 |
| 21 | 8 | 602 | CLA | CHB-C4A-NA | 2.48 | 127.97 | 124.40 |
| 21 | B | 814 | CLA | C1-C2-C3 | -2.47 | 122.14 | 126.20 |
| 21 | 1 | 311 | CLA | CAB-C3B-C2B | 2.47 | 130.11 | 123.53 |
| 21 | H | 201 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |
| 24 | A | 847 | BCR | C35-C13-C14 | -2.47 | 118.81 | 122.82 |
| 21 | 3 | 408 | CLA | C1-C2-C3 | -2.47 | 122.14 | 126.20 |
| 21 | 9 | 604 | CLA | C3B-C4B-NB | -2.47 | 108.32 | 110.53 |
| 21 | A | 840 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |
| 21 | B | 840 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |
| 21 | 5 | 607 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |
| 21 | A | 852 | CLA | C3B-C4B-NB | -2.47 | 108.32 | 110.53 |
| 21 | K | 203 | CLA | CAB-C3B-C2B | 2.47 | 130.10 | 123.53 |
| 30 | 6 | 616 | LUT | C15-C35-C34 | 2.47 | 128.58 | 123.52 |
| 21 | 4 | 610 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 2 | 607 | CHL | O1D-CGD-CBD | -2.47 | 120.98 | 124.72 |
| 24 | 3 | 418 | BCR | C19-C18-C17 | 2.47 | 122.89 | 119.01 |
| 30 | 8 | 614 | LUT | C39-C29-C28 | 2.47 | 121.86 | 118.09 |
| 21 | 3 | 406 | CLA | CAB-C3B-C2B | 2.47 | 130.10 | 123.53 |
| 29 | 2 | 607 | CHL | C5-C3-C4 | 2.47 | 120.27 | 114.59 |
| 21 | 1 | 314 | CLA | CAA-C2A-C3A | -2.47 | 110.57 | 116.23 |
| 31 | 5 | 616 | XAT | C32-C33-C34 | 2.47 | 122.89 | 119.01 |
| 29 | 4 | 607 | CHL | CBC-CAC-C3C | -2.47 | 109.34 | 112.87 |
| 21 | 3 | 402 | CLA | CHB-C4A-NA | 2.47 | 127.96 | 124.40 |
| 21 | 3 | 414 | CLA | CHB-C4A-NA | 2.47 | 127.96 | 124.40 |
| 31 | 4 | 616 | XAT | C6-C7-C8 | -2.47 | 120.78 | 125.99 |
| 21 | B | 823 | CLA | C3B-C4B-NB | -2.47 | 108.33 | 110.53 |
| 21 | 7 | 405 | CLA | CHB-C4A-NA | 2.47 | 127.96 | 124.40 |
| 21 | c | 603 | CLA | CHB-C4A-NA | 2.47 | 127.96 | 124.40 |
| 21 | 1 | 309 | CLA | CHB-C4A-NA | 2.47 | 127.96 | 124.40 |
| 31 | 8 | 615 | XAT | C32-C33-C34 | 2.47 | 122.89 | 119.01 |
| 24 | B | 843 | BCR | C30-C25-C26 | -2.47 | 119.27 | 122.64 |
| 21 | A | 824 | CLA | CHB-C4A-NA | 2.46 | 127.96 | 124.40 |
| 21 | B | 831 | CLA | O2A-CGA-O1A | -2.46 | 117.46 | 123.63 |
| 21 | B | 835 | CLA | C3B-C4B-NB | -2.46 | 108.33 | 110.53 |
| 21 | B | 819 | CLA | CHB-C4A-NA | 2.46 | 127.96 | 124.40 |
| 21 | 3 | 406 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 21 | 6 | 611 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 21 | A | 813 | CLA | C3B-C4B-NB | -2.46 | 108.33 | 110.53 |
| 21 | 8 | 603 | CLA | O2D-CGD-O1D | -2.46 | 118.49 | 124.08 |
| 21 | 4 | 603 | CLA | C3B-C4B-NB | -2.46 | 108.33 | 110.53 |
| 21 | 5 | 612 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 21 | A | 830 | CLA | C3B-C4B-NB | -2.46 | 108.33 | 110.53 |
| 24 | J | 104 | BCR | C16-C15-C14 | -2.46 | 118.48 | 123.52 |
| 21 | O | 203 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 21 | 6 | 613 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 29 | 2 | 607 | CHL | CMA-C3A-C4A | -2.46 | 109.31 | 114.61 |
| 21 | 1 | 314 | CLA | CMB-C2B-C3B | 2.46 | 130.07 | 123.53 |
| 21 | c | 612 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 21 | A | 837 | CLA | CHB-C4A-NA | 2.46 | 127.95 | 124.40 |
| 30 | c | 615 | LUT | C39-C29-C28 | 2.46 | 121.84 | 118.09 |
| 21 | A | 816 | CLA | C3B-C4B-NB | -2.46 | 108.34 | 110.53 |
| 21 | A | 816 | CLA | CHB-C4A-NA | 2.46 | 127.94 | 124.40 |
| 21 | L | 303 | CLA | CHB-C4A-NA | 2.46 | 127.94 | 124.40 |
| 21 | B | 812 | CLA | C1-C2-C3 | -2.45 | 122.17 | 126.20 |
| 21 | A | 809 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 21 | 7 | 414 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | a | 602 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 29 | 6 | 605 | CHL | O2D-CGD-O1D | -2.45 | 119.07 | 123.85 |
| 21 | 8 | 609 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 24 | F | 301 | BCR | C19-C18-C17 | 2.45 | 122.87 | 119.01 |
| 30 | c | 616 | LUT | C32-C33-C34 | 2.45 | 122.87 | 119.01 |
| 29 | 2 | 602 | CHL | C4-C3-C5 | 2.45 | 119.49 | 115.23 |
| 24 | J | 104 | BCR | C34-C9-C8 | 2.45 | 121.83 | 118.09 |
| 21 | 1 | 316 | CLA | CAB-C3B-C2B | 2.45 | 130.05 | 123.53 |
| 21 | A | 811 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 21 | 8 | 601 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 21 | a | 603 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 21 | A | 808 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 21 | 8 | 603 | CLA | CHB-C4A-NA | 2.45 | 127.94 | 124.40 |
| 30 | c | 615 | LUT | C40-C33-C34 | -2.45 | 118.85 | 122.82 |
| 30 | 3 | 416 | LUT | C20-C13-C14 | -2.45 | 118.85 | 122.82 |
| 24 | B | 843 | BCR | C1-C6-C5 | -2.45 | 119.29 | 122.64 |
| 30 | 9 | 614 | LUT | C7-C8-C9 | 2.45 | 129.86 | 126.23 |
| 21 | 1 | 316 | CLA | CMB-C2B-C3B | 2.45 | 130.04 | 123.53 |
| 30 | c | 616 | LUT | C12-C13-C14 | 2.45 | 122.86 | 119.01 |
| 29 | a | 609 | CHL | CBC-CAC-C3C | -2.45 | 109.37 | 112.87 |
| 32 | b | 318 | NEX | C19-C9-C10 | -2.45 | 118.85 | 122.82 |
| 21 | 9 | 604 | CLA | CMB-C2B-C1B | -2.45 | 121.69 | 125.42 |
| 21 | 5 | 608 | CLA | CHB-C4A-NA | 2.45 | 127.93 | 124.40 |
| 29 | c | 601 | CHL | O2A-CGA-CBA | 2.44 | 119.29 | 111.83 |
| 21 | B | 832 | CLA | C3B-C4B-NB | -2.44 | 108.35 | 110.53 |
| 21 | A | 821 | CLA | CHB-C4A-NA | 2.44 | 127.93 | 124.40 |
| 21 | 3 | 404 | CLA | CAB-C3B-C2B | 2.44 | 130.03 | 123.53 |
| 21 | 3 | 409 | CLA | O2D-CGD-O1D | -2.44 | 119.09 | 123.85 |
| 21 | B | 832 | CLA | CHB-C4A-NA | 2.44 | 127.93 | 124.40 |
| 21 | 2 | 610 | CLA | CHB-C4A-NA | 2.44 | 127.93 | 124.40 |
| 21 | 7 | 407 | CLA | CHB-C4A-NA | 2.44 | 127.93 | 124.40 |
| 24 | A | 849 | BCR | C12-C13-C14 | 2.44 | 122.85 | 119.01 |
| 24 | O | 205 | BCR | C21-C20-C19 | 2.44 | 130.28 | 123.20 |
| 21 | 7 | 403 | CLA | CMB-C2B-C3B | 2.44 | 130.02 | 123.53 |
| 21 | 9 | 611 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | B | 823 | CLA | O2D-CGD-CBD | 2.44 | 115.50 | 111.23 |
| 30 | 3 | 416 | LUT | C8-C9-C10 | 2.44 | 122.85 | 119.01 |
| 21 | 3 | 409 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 24 | L | 305 | BCR | C12-C13-C14 | 2.44 | 122.85 | 119.01 |
| 21 | A | 831 | CLA | O2D-CGD-CBD | 2.44 | 115.49 | 111.23 |
| 21 | O | 204 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | B | 810 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 8 | 605 | CHL | O2D-CGD-O1D | -2.44 | 119.10 | 123.85 |
| 21 | 4 | 609 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | 7 | 413 | CLA | CAA-C2A-C3A | -2.44 | 110.64 | 116.23 |
| 29 | b | 308 | CHL | O2D-CGD-O1D | -2.44 | 119.11 | 123.85 |
| 21 | B | 834 | CLA | CMB-C2B-C1B | -2.44 | 121.71 | 125.42 |
| 21 | J | 102 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | 1 | 313 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | 8 | 618 | CLA | CAA-C2A-C3A | -2.44 | 110.64 | 116.23 |
| 24 | B | 843 | BCR | C34-C9-C8 | 2.44 | 121.81 | 118.09 |
| 21 | G | 203 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | 2 | 608 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | a | 613 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 21 | B | 804 | CLA | O2A-CGA-O1A | -2.43 | 117.54 | 123.63 |
| 21 | 5 | 614 | CLA | CHB-C4A-NA | 2.43 | 127.91 | 124.40 |
| 21 | B | 801 | CLA | CMA-C3A-C2A | -2.43 | 104.57 | 113.98 |
| 21 | a | 614 | CLA | CAA-C2A-C3A | -2.43 | 110.65 | 116.23 |
| 21 | 8 | 608 | CLA | C3B-C4B-NB | -2.43 | 108.36 | 110.53 |
| 21 | 5 | 610 | CLA | CHB-C4A-NA | 2.43 | 127.91 | 124.40 |
| 21 | B | 828 | CLA | CMB-C2B-C1B | -2.43 | 121.72 | 125.42 |
| 29 | a | 605 | CHL | C3D-C4D-ND | -2.43 | 109.04 | 112.94 |
| 24 | B | 843 | BCR | C10-C11-C12 | -2.43 | 116.15 | 123.20 |
| 21 | 8 | 609 | CLA | C3B-C4B-NB | -2.43 | 108.36 | 110.53 |
| 21 | A | 801 | CLA | C2A-C1A-CHA | 2.43 | 128.09 | 123.87 |
| 21 | 1 | 311 | CLA | CHB-C4A-NA | 2.43 | 127.91 | 124.40 |
| 31 | 1 | 318 | XAT | C20-C13-C14 | -2.43 | 118.88 | 122.82 |
| 29 | c | 607 | CHL | O2D-CGD-O1D | -2.43 | 119.12 | 123.85 |
| 21 | A | 806 | CLA | CHB-C4A-NA | 2.43 | 127.91 | 124.40 |
| 30 | 6 | 616 | LUT | C10-C11-C12 | 2.43 | 130.24 | 123.20 |
| 29 | a | 601 | CHL | C3D-C4D-ND | -2.43 | 109.04 | 112.94 |
| 21 | 8 | 604 | CLA | CHB-C4A-NA | 2.43 | 127.90 | 124.40 |
| 31 | 8 | 615 | XAT | C8-C9-C10 | 2.43 | 122.83 | 119.01 |
| 30 | 3 | 416 | LUT | C11-C12-C13 | 2.43 | 133.02 | 126.36 |
| 21 | 2 | 611 | CLA | C3B-C4B-NB | -2.43 | 108.36 | 110.53 |
| 21 | 5 | 610 | CLA | CMB-C2B-C3B | 2.43 | 129.98 | 123.53 |
| 29 | 2 | 602 | CHL | CBC-CAC-C3C | -2.43 | 109.40 | 112.87 |
| 30 | 9 | 614 | LUT | C20-C13-C14 | -2.43 | 118.89 | 122.82 |
| 29 | 1 | 302 | CHL | CMA-C3A-C4A | -2.43 | 109.38 | 114.61 |
| 31 | 7 | 416 | XAT | C12-C13-C14 | 2.43 | 122.83 | 119.01 |
| 21 | 5 | 613 | CLA | CHB-C4A-NA | 2.43 | 127.90 | 124.40 |
| 21 | c | 604 | CLA | CHB-C4A-NA | 2.43 | 127.90 | 124.40 |
| 21 | 5 | 608 | CLA | CAB-C3B-C2B | 2.43 | 129.98 | 123.53 |
| 21 | A | 825 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 312 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 21 | 2 | 613 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 21 | 5 | 604 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 29 | b | 307 | CHL | O2D-CGD-O1D | -2.42 | 119.13 | 123.85 |
| 21 | B | 825 | CLA | C1-C2-C3 | -2.42 | 122.23 | 126.20 |
| 21 | A | 830 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 21 | F | 305 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 21 | A | 833 | CLA | C1-C2-C3 | -2.42 | 122.23 | 126.20 |
| 21 | 8 | 611 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | A | 807 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | 3 | 408 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | 7 | 405 | CLA | CAB-C3B-C2B | 2.42 | 129.97 | 123.53 |
| 24 | B | 844 | BCR | C4-C5-C6 | -2.42 | 119.43 | 122.70 |
| 21 | 1 | 316 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | A | 804 | CLA | C1-C2-C3 | -2.42 | 122.23 | 126.20 |
| 29 | 8 | 606 | CHL | CBC-CAC-C3C | -2.42 | 109.41 | 112.87 |
| 21 | 9 | 613 | CLA | C1-C2-C3 | -2.42 | 122.23 | 126.20 |
| 21 | 5 | 613 | CLA | CAB-C3B-C2B | 2.42 | 129.96 | 123.53 |
| 29 | 4 | 607 | CHL | C5-C3-C4 | 2.42 | 120.16 | 114.59 |
| 21 | b | 305 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | 4 | 612 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | 8 | 608 | CLA | CHB-C4A-NA | 2.42 | 127.89 | 124.40 |
| 21 | 7 | 405 | CLA | CMB-C2B-C3B | 2.42 | 129.96 | 123.53 |
| 21 | 5 | 608 | CLA | CMB-C2B-C3B | 2.42 | 129.95 | 123.53 |
| 29 | c | 609 | CHL | O2D-CGD-CBD | 2.42 | 119.83 | 113.90 |
| 31 | 2 | 617 | XAT | C6-C7-C8 | -2.41 | 120.89 | 125.99 |
| 21 | A | 828 | CLA | O2A-CGA-O1A | -2.41 | 117.59 | 123.63 |
| 21 | B | 818 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 21 | K | 204 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 21 | b | 314 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 21 | 5 | 605 | CLA | C3B-C4B-NB | -2.41 | 108.38 | 110.53 |
| 21 | B | 832 | CLA | O2A-CGA-O1A | -2.41 | 117.59 | 123.63 |
| 21 | A | 820 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 21 | a | 611 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 29 | 5 | 606 | CHL | O2D-CGD-O1D | -2.41 | 119.16 | 123.85 |
| 24 | M | 101 | BCR | C10-C11-C12 | 2.41 | 130.18 | 123.20 |
| 21 | A | 838 | CLA | C3B-C4B-NB | -2.41 | 108.38 | 110.53 |
| 21 | 1 | 314 | CLA | CAB-C3B-C2B | 2.41 | 129.94 | 123.53 |
| 24 | G | 205 | BCR | C12-C13-C14 | 2.41 | 122.80 | 119.01 |
| 21 | 7 | 409 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 21 | a | 610 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 21 | 2 | 609 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 827 | CLA | CHB-C4A-NA | 2.41 | 127.87 | 124.40 |
| 21 | B | 839 | CLA | C3B-C4B-NB | -2.41 | 108.38 | 110.53 |
| 24 | B | 846 | BCR | C33-C5-C6 | -2.40 | 121.86 | 124.48 |
| 21 | A | 826 | CLA | CHB-C4A-NA | 2.40 | 127.87 | 124.40 |
| 21 | B | 802 | CLA | C3B-C4B-NB | -2.40 | 108.38 | 110.53 |
| 21 | 2 | 609 | CLA | C3B-C4B-NB | -2.40 | 108.38 | 110.53 |
| 21 | A | 821 | CLA | O2A-CGA-O1A | -2.40 | 117.61 | 123.63 |
| 21 | G | 203 | CLA | C1-C2-C3 | -2.40 | 122.87 | 126.76 |
| 21 | A | 842 | CLA | CHB-C4A-NA | 2.40 | 127.87 | 124.40 |
| 21 | B | 839 | CLA | CHB-C4A-NA | 2.40 | 127.87 | 124.40 |
| 21 | 3 | 409 | CLA | C3D-C4D-ND | 2.40 | 113.89 | 109.99 |
| 30 | 2 | 616 | LUT | C40-C33-C34 | -2.40 | 118.93 | 122.82 |
| 21 | L | 304 | CLA | CHB-C4A-NA | 2.40 | 127.86 | 124.40 |
| 21 | B | 822 | CLA | CHB-C4A-NA | 2.40 | 127.86 | 124.40 |
| 21 | B | 836 | CLA | CMB-C2B-C1B | -2.40 | 121.77 | 125.42 |
| 29 | b | 309 | CHL | CBC-CAC-C3C | -2.40 | 109.44 | 112.87 |
| 24 | F | 301 | BCR | C35-C13-C14 | -2.40 | 118.93 | 122.82 |
| 21 | A | 823 | CLA | O2D-CGD-CBD | 2.40 | 115.42 | 111.23 |
| 29 | 2 | 602 | CHL | O1D-CGD-CBD | -2.40 | 121.09 | 124.72 |
| 29 | 9 | 608 | CHL | O1D-CGD-CBD | -2.40 | 121.09 | 124.72 |
| 32 | 9 | 617 | NEX | C19-C9-C10 | -2.39 | 118.94 | 122.82 |
| 21 | 7 | 408 | CLA | CAA-C2A-C3A | -2.39 | 110.74 | 116.23 |
| 21 | 4 | 609 | CLA | O2D-CGD-O1D | -2.39 | 119.19 | 123.85 |
| 21 | A | 805 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 21 | A | 819 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 24 | 4 | 617 | BCR | C34-C9-C8 | 2.39 | 121.74 | 118.09 |
| 29 | 4 | 606 | CHL | O2D-CGD-O1D | -2.39 | 119.20 | 123.85 |
| 21 | A | 839 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 21 | A | 834 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 29 | b | 302 | CHL | O2D-CGD-O1D | -2.39 | 119.20 | 123.85 |
| 21 | 5 | 614 | CLA | CAB-C3B-C2B | 2.39 | 129.88 | 123.53 |
| 21 | 7 | 403 | CLA | CHB-C4A-NA | 2.39 | 127.84 | 124.40 |
| 21 | 7 | 402 | CLA | C2A-C1A-CHA | 2.39 | 128.01 | 123.87 |
| 21 | b | 311 | CLA | CMB-C2B-C1B | -2.39 | 121.79 | 125.42 |
| 21 | B | 815 | CLA | O2A-CGA-O1A | -2.39 | 117.66 | 123.63 |
| 29 | 9 | 606 | CHL | O2D-CGD-O1D | -2.39 | 119.20 | 123.85 |
| 24 | B | 844 | BCR | C30-C25-C24 | 2.38 | 122.12 | 115.65 |
| 21 | 1 | 311 | CLA | CMB-C2B-C3B | 2.38 | 129.87 | 123.53 |
| 29 | 2 | 605 | CHL | O2D-CGD-O1D | -2.38 | 119.21 | 123.85 |
| 21 | 3 | 406 | CLA | CMB-C2B-C3B | 2.38 | 129.86 | 123.53 |
| 21 | F | 302 | CLA | CHB-C4A-NA | 2.38 | 127.84 | 124.40 |
| 21 | O | 201 | CLA | CHB-C4A-NA | 2.38 | 127.84 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 412 | CLA | CHB-C4A-NA | 2.38 | 127.84 | 124.40 |
| 21 | B | 826 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 21 | 7 | 413 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 21 | c | 602 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 29 | 3 | 407 | CHL | C4C-C3C-C2C | -2.38 | 103.98 | 113.37 |
| 21 | b | 305 | CLA | C3B-C4B-NB | -2.38 | 108.41 | 110.53 |
| 21 | B | 810 | CLA | CAB-C3B-C2B | 2.38 | 129.85 | 123.53 |
| 29 | 8 | 607 | CHL | C5-C3-C4 | 2.38 | 120.06 | 114.59 |
| 21 | B | 824 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 21 | 6 | 610 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 24 | L | 305 | BCR | C34-C9-C8 | 2.37 | 121.72 | 118.09 |
| 21 | 8 | 604 | CLA | CMB-C2B-C1B | -2.37 | 121.81 | 125.42 |
| 21 | A | 810 | CLA | CHB-C4A-NA | 2.37 | 127.83 | 124.40 |
| 21 | B | 803 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 21 | b | 312 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 24 | B | 843 | BCR | C4-C5-C6 | -2.37 | 119.50 | 122.70 |
| 29 | 6 | 606 | CHL | CBC-CAC-C3C | -2.37 | 109.48 | 112.87 |
| 21 | B | 831 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 21 | 4 | 613 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 29 | 3 | 407 | CHL | CMC-C2C-C1C | 2.37 | 129.00 | 124.73 |
| 30 | 6 | 616 | LUT | C32-C33-C34 | 2.37 | 122.73 | 119.01 |
| 21 | B | 809 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 21 | A | 852 | CLA | C1-C2-C3 | -2.37 | 122.32 | 126.20 |
| 29 | 2 | 614 | CHL | CMA-C3A-C4A | -2.37 | 109.51 | 114.61 |
| 24 | M | 101 | BCR | C21-C20-C19 | 2.37 | 130.06 | 123.20 |
| 21 | A | 815 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 29 | 3 | 407 | CHL | O2D-CGD-O1D | -2.37 | 118.71 | 124.08 |
| 21 | B | 838 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 21 | 7 | 411 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 21 | 1 | 310 | CLA | CHB-C4A-NA | 2.36 | 127.81 | 124.40 |
| 30 | 9 | 614 | LUT | C32-C33-C34 | 2.36 | 122.73 | 119.01 |
| 21 | O | 203 | CLA | C1-C2-C3 | -2.36 | 122.33 | 126.20 |
| 31 | 4 | 616 | XAT | C7-C8-C9 | 2.36 | 129.19 | 125.53 |
| 21 | A | 828 | CLA | C3B-C4B-NB | -2.36 | 108.42 | 110.53 |
| 21 | 7 | 413 | CLA | C3B-C4B-NB | -2.36 | 108.42 | 110.53 |
| 21 | 1 | 304 | CLA | CHB-C4A-NA | 2.36 | 127.80 | 124.40 |
| 21 | A | 838 | CLA | CHB-C4A-NA | 2.36 | 127.80 | 124.40 |
| 21 | 2 | 612 | CLA | CHB-C4A-NA | 2.36 | 127.80 | 124.40 |
| 21 | F | 302 | CLA | O1D-CGD-CBD | 2.36 | 129.16 | 124.52 |
| 21 | K | 203 | CLA | CMB-C2B-C3B | 2.36 | 129.79 | 123.53 |
| 30 | a | 615 | LUT | C32-C33-C34 | 2.35 | 122.71 | 119.01 |
| 21 | A | 822 | CLA | CHB-C4A-NA | 2.35 | 127.80 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 606 | CHL | CBC-CAC-C3C | -2.35 | 109.50 | 112.87 |
| 30 | 9 | 615 | LUT | C7-C8-C9 | 2.35 | 129.72 | 126.23 |
| 21 | a | 614 | CLA | CHB-C4A-NA | 2.35 | 127.80 | 124.40 |
| 21 | A | 838 | CLA | CMB-C2B-C1B | -2.35 | 121.83 | 125.42 |
| 24 | 4 | 617 | BCR | C7-C8-C9 | 2.35 | 129.72 | 126.23 |
| 21 | 3 | 415 | CLA | CHB-C4A-NA | 2.35 | 127.80 | 124.40 |
| 21 | 8 | 602 | CLA | C1-C2-C3 | -2.35 | 122.34 | 126.20 |
| 21 | 3 | 404 | CLA | C3B-C4B-NB | -2.35 | 107.89 | 110.33 |
| 21 | G | 204 | CLA | CHB-C4A-NA | 2.35 | 127.79 | 124.40 |
| 21 | 3 | 413 | CLA | CHB-C4A-NA | 2.35 | 127.79 | 124.40 |
| 29 | 6 | 614 | CHL | CBC-CAC-C3C | -2.35 | 109.51 | 112.87 |
| 24 | J | 104 | BCR | C28-C27-C26 | -2.35 | 109.87 | 114.06 |
| 21 | B | 825 | CLA | CMB-C2B-C1B | -2.35 | 121.84 | 125.42 |
| 29 | a | 605 | CHL | O2D-CGD-CBD | 2.35 | 119.66 | 113.90 |
| 21 | K | 202 | CLA | C1-C2-C3 | -2.35 | 122.96 | 126.76 |
| 24 | L | 306 | BCR | C8-C9-C10 | 2.35 | 122.70 | 119.01 |
| 21 | A | 833 | CLA | CHB-C4A-NA | 2.35 | 127.79 | 124.40 |
| 21 | c | 610 | CLA | CHB-C4A-NA | 2.35 | 127.79 | 124.40 |
| 30 | c | 615 | LUT | C12-C13-C14 | 2.34 | 122.69 | 119.01 |
| 29 | b | 302 | CHL | C3D-C4D-ND | -2.34 | 109.18 | 112.94 |
| 21 | 5 | 609 | CLA | CHB-C4A-NA | 2.34 | 127.78 | 124.40 |
| 21 | A | 852 | CLA | CMB-C2B-C1B | -2.34 | 121.85 | 125.42 |
| 24 | B | 844 | BCR | C24-C23-C22 | -2.34 | 122.78 | 126.23 |
| 21 | 5 | 613 | CLA | CMB-C2B-C3B | 2.34 | 129.75 | 123.53 |
| 21 | B | 802 | CLA | CHB-C4A-NA | 2.34 | 127.77 | 124.40 |
| 21 | b | 303 | CLA | CHB-C4A-NA | 2.34 | 127.77 | 124.40 |
| 21 | b | 311 | CLA | CHB-C4A-NA | 2.34 | 127.77 | 124.40 |
| 21 | 3 | 404 | CLA | CMB-C2B-C3B | 2.34 | 129.74 | 123.53 |
| 21 | A | 831 | CLA | C3B-C4B-NB | -2.34 | 108.44 | 110.53 |
| 29 | c | 608 | CHL | O2D-CGD-O1D | -2.34 | 119.30 | 123.85 |
| 29 | a | 608 | CHL | O1D-CGD-CBD | -2.33 | 121.18 | 124.72 |
| 21 | 8 | 612 | CLA | C3B-C4B-NB | -2.33 | 108.45 | 110.53 |
| 21 | 7 | 402 | CLA | CHB-C4A-NA | 2.33 | 127.77 | 124.40 |
| 21 | 9 | 602 | CLA | CHB-C4A-NA | 2.33 | 127.77 | 124.40 |
| 21 | 6 | 608 | CLA | CHB-C4A-NA | 2.33 | 127.77 | 124.40 |
| 31 | 6 | 617 | XAT | C10-C11-C12 | 2.33 | 129.96 | 123.20 |
| 21 | B | 806 | CLA | CHB-C4A-NA | 2.33 | 127.77 | 124.40 |
| 24 | B | 846 | BCR | C23-C24-C25 | -2.33 | 120.77 | 127.00 |
| 21 | B | 810 | CLA | CMB-C2B-C3B | 2.33 | 129.73 | 123.53 |
| 21 | B | 835 | CLA | CMB-C2B-C1B | -2.33 | 121.87 | 125.42 |
| 21 | B | 807 | CLA | CHB-C4A-NA | 2.33 | 127.76 | 124.40 |
| 21 | B | 812 | CLA | CHB-C4A-NA | 2.33 | 127.76 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | K | 202 | CLA | O2A-CGA-O1A | -2.33 | 117.81 | 123.63 |
| 29 | 6 | 606 | CHL | O2D-CGD-O1D | -2.33 | 119.32 | 123.85 |
| 24 | A | 847 | BCR | C34-C9-C8 | 2.33 | 121.64 | 118.09 |
| 21 | A | 831 | CLA | CHB-C4A-NA | 2.33 | 127.76 | 124.40 |
| 21 | 5 | 614 | CLA | C3B-C4B-NB | -2.33 | 107.91 | 110.33 |
| 29 | 7 | 406 | CHL | CBC-CAC-C3C | -2.33 | 109.54 | 112.87 |
| 21 | b | 311 | CLA | O2A-CGA-O1A | -2.33 | 117.81 | 123.63 |
| 29 | 6 | 607 | CHL | O1D-CGD-CBD | -2.33 | 121.20 | 124.72 |
| 21 | A | 841 | CLA | CAA-C2A-C3A | -2.33 | 106.72 | 113.00 |
| 21 | 2 | 609 | CLA | O2D-CGD-O1D | -2.32 | 119.32 | 123.85 |
| 29 | 8 | 606 | CHL | O2D-CGD-O1D | -2.32 | 119.32 | 123.85 |
| 24 | F | 301 | BCR | C34-C9-C8 | 2.32 | 121.64 | 118.09 |
| 24 | J | 104 | BCR | C37-C22-C23 | 2.32 | 121.64 | 118.09 |
| 29 | 9 | 607 | CHL | O2D-CGD-O1D | -2.32 | 119.33 | 123.85 |
| 21 | A | 802 | CLA | CHB-C4A-NA | 2.32 | 127.75 | 124.40 |
| 31 | 3 | 417 | XAT | C20-C13-C14 | -2.32 | 119.06 | 122.82 |
| 21 | 1 | 316 | CLA | C3B-C4B-NB | -2.32 | 107.92 | 110.33 |
| 21 | A | 832 | CLA | CHB-C4A-NA | 2.32 | 127.75 | 124.40 |
| 30 | 3 | 416 | LUT | C39-C29-C28 | 2.32 | 121.63 | 118.09 |
| 29 | 9 | 608 | CHL | O2D-CGD-O1D | -2.31 | 119.34 | 123.85 |
| 29 | 4 | 607 | CHL | CMA-C3A-C4A | -2.31 | 109.62 | 114.61 |
| 21 | A | 836 | CLA | CHB-C4A-NA | 2.31 | 127.74 | 124.40 |
| 21 | O | 202 | CLA | CHB-C4A-NA | 2.31 | 127.74 | 124.40 |
| 21 | 2 | 604 | CLA | CHB-C4A-NA | 2.31 | 127.74 | 124.40 |
| 21 | A | 838 | CLA | O2A-CGA-O1A | -2.31 | 117.84 | 123.63 |
| 23 | 1 | 301 | LHG | O7-C7-C8 | 2.31 | 116.49 | 111.48 |
| 21 | A | 818 | CLA | O2A-CGA-O1A | -2.31 | 117.84 | 123.63 |
| 29 | c | 607 | CHL | CBC-CAC-C3C | -2.31 | 109.56 | 112.87 |
| 21 | 5 | 614 | CLA | CMB-C2B-C3B | 2.31 | 129.67 | 123.53 |
| 21 | A | 840 | CLA | O2A-CGA-O1A | -2.31 | 117.85 | 123.63 |
| 30 | 3 | 416 | LUT | C15-C14-C13 | 2.31 | 130.51 | 127.28 |
| 21 | A | 830 | CLA | CAA-CBA-CGA | -2.31 | 106.66 | 113.21 |
| 21 | A | 816 | CLA | CMB-C2B-C1B | -2.31 | 121.91 | 125.42 |
| 29 | a | 609 | CHL | O2D-CGD-O1D | -2.30 | 119.36 | 123.85 |
| 21 | 5 | 610 | CLA | C3B-C4B-NB | -2.30 | 107.94 | 110.33 |
| 21 | A | 823 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 21 | 1 | 306 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 21 | A | 827 | CLA | CMB-C2B-C1B | -2.30 | 121.91 | 125.42 |
| 21 | 4 | 603 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 29 | c | 601 | CHL | O2D-CGD-O1D | -2.30 | 119.37 | 123.85 |
| 21 | 8 | 618 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 29 | 4 | 606 | CHL | CMA-C3A-C4A | -2.30 | 109.65 | 114.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 8 | 612 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 24 | K | 205 | BCR | C20-C19-C18 | -2.30 | 120.06 | 126.36 |
| 21 | 9 | 603 | CLA | C3B-C4B-NB | -2.30 | 108.48 | 110.53 |
| 21 | A | 817 | CLA | O2A-CGA-O1A | -2.30 | 117.88 | 123.63 |
| 21 | A | 808 | CLA | CMB-C2B-C1B | -2.30 | 121.92 | 125.42 |
| 30 | 1 | 317 | LUT | C8-C9-C10 | 2.30 | 122.62 | 119.01 |
| 21 | 1 | 311 | CLA | C3B-C4B-NB | -2.29 | 107.95 | 110.33 |
| 21 | 3 | 409 | CLA | O2A-CGA-CBA | 2.29 | 118.83 | 111.83 |
| 21 | B | 827 | CLA | C3B-C4B-NB | -2.29 | 108.48 | 110.53 |
| 21 | 3 | 410 | CLA | O2D-CGD-O1D | -2.29 | 118.88 | 124.08 |
| 29 | 8 | 613 | CHL | O2D-CGD-O1D | -2.29 | 119.39 | 123.85 |
| 21 | 7 | 403 | CLA | C3B-C4B-NB | -2.29 | 107.95 | 110.33 |
| 21 | B | 835 | CLA | C1-C2-C3 | -2.29 | 122.44 | 126.20 |
| 21 | 4 | 604 | CLA | CHB-C4A-NA | 2.29 | 127.71 | 124.40 |
| 29 | c | 606 | CHL | O2D-CGD-O1D | -2.29 | 119.39 | 123.85 |
| 21 | 5 | 608 | CLA | C3B-C4B-NB | -2.29 | 107.95 | 110.33 |
| 29 | 4 | 614 | CHL | CMA-C3A-C4A | -2.29 | 109.68 | 114.61 |
| 21 | 3 | 410 | CLA | CHB-C4A-NA | 2.29 | 127.70 | 124.40 |
| 24 | K | 205 | BCR | C10-C11-C12 | -2.29 | 116.57 | 123.20 |
| 21 | O | 203 | CLA | O2A-CGA-O1A | -2.29 | 117.90 | 123.63 |
| 21 | A | 835 | CLA | CMB-C2B-C3B | 2.29 | 131.93 | 126.55 |
| 21 | B | 835 | CLA | O2A-CGA-O1A | -2.29 | 117.91 | 123.63 |
| 29 | 9 | 609 | CHL | CBC-CAC-C3C | -2.29 | 109.60 | 112.87 |
| 21 | 9 | 610 | CLA | O2A-CGA-O1A | -2.29 | 117.91 | 123.63 |
| 29 | 6 | 601 | CHL | C3D-C4D-ND | -2.28 | 109.27 | 112.94 |
| 30 | a | 616 | LUT | C32-C33-C34 | 2.28 | 122.60 | 119.01 |
| 21 | 2 | 603 | CLA | CHB-C4A-NA | 2.28 | 127.69 | 124.40 |
| 29 | 6 | 602 | CHL | CMA-C3A-C4A | -2.28 | 109.69 | 114.61 |
| 21 | A | 834 | CLA | O2D-CGD-CBD | 2.28 | 115.22 | 111.23 |
| 21 | B | 839 | CLA | CAA-C2A-C3A | -2.28 | 106.84 | 113.00 |
| 30 | 6 | 616 | LUT | C31-C30-C29 | 2.28 | 130.48 | 127.28 |
| 24 | F | 303 | BCR | C35-C13-C14 | -2.28 | 119.12 | 122.82 |
| 21 | 7 | 412 | CLA | CHB-C4A-NA | 2.28 | 127.69 | 124.40 |
| 29 | 7 | 406 | CHL | C4C-C3C-C2C | -2.28 | 104.37 | 113.37 |
| 21 | 9 | 610 | CLA | CHB-C4A-NA | 2.28 | 127.69 | 124.40 |
| 24 | J | 104 | BCR | C3-C2-C1 | -2.27 | 106.38 | 114.43 |
| 29 | b | 306 | CHL | O2D-CGD-O1D | -2.27 | 119.42 | 123.85 |
| 21 | B | 820 | CLA | CHB-C4A-NA | 2.27 | 127.68 | 124.40 |
| 21 | B | 834 | CLA | C3B-C4B-NB | -2.27 | 108.50 | 110.53 |
| 29 | 9 | 601 | CHL | O2D-CGD-O1D | -2.27 | 119.42 | 123.85 |
| 31 | c | 617 | XAT | C36-C21-C22 | -2.27 | 104.97 | 108.97 |
| 21 | 1 | 304 | CLA | CMB-C2B-C1B | -2.27 | 121.96 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | c | 608 | CHL | C3D-C4D-ND | -2.27 | 109.29 | 112.94 |
| 21 | B | 826 | CLA | C3B-C4B-NB | -2.27 | 108.50 | 110.53 |
| 21 | 3 | 403 | CLA | CHB-C4A-NA | 2.27 | 127.68 | 124.40 |
| 24 | K | 205 | BCR | C1-C6-C5 | -2.27 | 119.53 | 122.64 |
| 21 | 3 | 401 | CLA | CMB-C2B-C1B | -2.27 | 121.97 | 125.42 |
| 21 | B | 823 | CLA | C1-C2-C3 | -2.27 | 122.48 | 126.20 |
| 24 | F | 301 | BCR | C16-C15-C14 | 2.27 | 128.16 | 123.52 |
| 24 | J | 104 | BCR | C24-C25-C26 | -2.27 | 116.34 | 121.56 |
| 21 | B | 802 | CLA | O2A-CGA-O1A | -2.27 | 117.96 | 123.63 |
| 21 | B | 840 | CLA | CMB-C2B-C1B | -2.27 | 121.97 | 125.42 |
| 21 | A | 821 | CLA | C1-C2-C3 | -2.27 | 122.49 | 126.20 |
| 21 | B | 826 | CLA | O2A-CGA-O1A | -2.26 | 117.97 | 123.63 |
| 21 | 7 | 413 | CLA | CMB-C2B-C1B | -2.26 | 121.97 | 125.42 |
| 21 | B | 810 | CLA | C1-C2-C3 | -2.26 | 122.49 | 126.20 |
| 31 | 3 | 417 | XAT | C39-C29-C28 | 2.26 | 121.55 | 118.09 |
| 29 | a | 608 | CHL | O2D-CGD-O1D | -2.26 | 119.44 | 123.85 |
| 21 | B | 824 | CLA | O2A-CGA-O1A | -2.26 | 117.97 | 123.63 |
| 21 | B | 808 | CLA | CHB-C4A-NA | 2.26 | 127.66 | 124.40 |
| 21 | 1 | 314 | CLA | CMA-C3A-C2A | -2.26 | 111.05 | 116.23 |
| 21 | B | 838 | CLA | O2A-CGA-O1A | -2.26 | 117.97 | 123.63 |
| 21 | 8 | 618 | CLA | CMA-C3A-C2A | -2.26 | 111.05 | 116.23 |
| 21 | A | 821 | CLA | CMB-C2B-C1B | -2.26 | 121.98 | 125.42 |
| 29 | a | 605 | CHL | CMA-C3A-C4A | -2.26 | 109.74 | 114.61 |
| 21 | B | 821 | CLA | O2D-CGD-CBD | 2.26 | 115.18 | 111.23 |
| 21 | A | 801 | CLA | CED-O2D-CGD | 2.26 | 121.04 | 115.92 |
| 21 | B | 827 | CLA | CHB-C4A-NA | 2.26 | 127.66 | 124.40 |
| 29 | 4 | 614 | CHL | O2D-CGD-O1D | -2.26 | 119.45 | 123.85 |
| 21 | B | 801 | CLA | CAC-C3C-C4C | 2.26 | 127.73 | 124.79 |
| 29 | b | 310 | CHL | CMA-C3A-C4A | -2.26 | 109.75 | 114.61 |
| 21 | B | 839 | CLA | O2A-CGA-O1A | -2.26 | 117.99 | 123.63 |
| 24 | 6 | 618 | BCR | C23-C22-C21 | 2.25 | 122.55 | 119.01 |
| 21 | B | 816 | CLA | O2A-CGA-O1A | -2.25 | 117.99 | 123.63 |
| 21 | 7 | 414 | CLA | CMB-C2B-C1B | -2.25 | 121.99 | 125.42 |
| 30 | 7 | 415 | LUT | C39-C29-C28 | 2.25 | 121.53 | 118.09 |
| 29 | b | 306 | CHL | CBC-CAC-C3C | -2.25 | 109.65 | 112.87 |
| 29 | b | 306 | CHL | CMA-C3A-C4A | -2.25 | 109.77 | 114.61 |
| 21 | 3 | 402 | CLA | O2A-CGA-O1A | -2.25 | 118.00 | 123.63 |
| 24 | B | 844 | BCR | C21-C20-C19 | -2.25 | 116.69 | 123.20 |
| 29 | b | 308 | CHL | C1-O2A-CGA | 2.24 | 122.08 | 116.65 |
| 31 | 6 | 617 | XAT | C6-C7-C8 | 2.24 | 130.74 | 125.99 |
| 21 | 7 | 405 | CLA | C3B-C4B-NB | -2.24 | 108.00 | 110.33 |
| 29 | c | 608 | CHL | CBC-CAC-C3C | -2.24 | 109.66 | 112.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 31 | 1 | 318 | XAT | C11-C10-C9 | 2.24 | 130.42 | 127.28 |
| 29 | b | 310 | CHL | C1-C2-C3 | -2.24 | 122.53 | 126.20 |
| 21 | A | 815 | CLA | CMB-C2B-C1B | -2.24 | 122.01 | 125.42 |
| 30 | c | 616 | LUT | C7-C8-C9 | 2.24 | 129.55 | 126.23 |
| 32 | c | 618 | NEX | C30-C31-C32 | 2.24 | 129.69 | 123.20 |
| 21 | 1 | 314 | CLA | CHB-C4A-NA | 2.24 | 127.63 | 124.40 |
| 21 | 6 | 604 | CLA | CHB-C4A-NA | 2.24 | 127.63 | 124.40 |
| 21 | A | 802 | CLA | O1D-CGD-CBD | 2.24 | 128.93 | 124.52 |
| 21 | 5 | 613 | CLA | C3B-C4B-NB | -2.24 | 108.01 | 110.33 |
| 21 | F | 302 | CLA | C1-C2-C3 | -2.24 | 122.53 | 126.20 |
| 30 | 9 | 615 | LUT | C12-C13-C14 | 2.24 | 122.53 | 119.01 |
| 21 | 7 | 411 | CLA | C1-C2-C3 | -2.24 | 122.53 | 126.20 |
| 21 | O | 204 | CLA | O2D-CGD-O1D | -2.24 | 119.01 | 124.08 |
| 21 | K | 202 | CLA | CAA-CBA-CGA | -2.24 | 106.86 | 113.21 |
| 29 | b | 309 | CHL | O2D-CGD-O1D | -2.24 | 119.50 | 123.85 |
| 29 | a | 605 | CHL | C4D-CHA-CBD | -2.23 | 106.71 | 108.97 |
| 29 | 1 | 302 | CHL | C5-C3-C4 | 2.23 | 119.73 | 114.59 |
| 24 | B | 843 | BCR | C38-C26-C27 | 2.23 | 118.36 | 113.60 |
| 29 | 2 | 601 | CHL | CMA-C3A-C4A | -2.23 | 109.80 | 114.61 |
| 21 | B | 830 | CLA | CHB-C4A-NA | 2.23 | 127.62 | 124.40 |
| 29 | a | 601 | CHL | C4D-CHA-CBD | -2.23 | 106.72 | 108.97 |
| 21 | B | 817 | CLA | C1-C2-C3 | -2.23 | 122.54 | 126.20 |
| 21 | B | 828 | CLA | CHB-C4A-NA | 2.23 | 127.62 | 124.40 |
| 21 | b | 315 | CLA | CHB-C4A-NA | 2.23 | 127.62 | 124.40 |
| 21 | B | 828 | CLA | O2A-CGA-O1A | -2.23 | 118.05 | 123.63 |
| 29 | 2 | 606 | CHL | CMA-C3A-C4A | -2.23 | 109.81 | 114.61 |
| 24 | A | 847 | BCR | C37-C22-C23 | 2.23 | 121.49 | 118.09 |
| 29 | 9 | 606 | CHL | CMA-C3A-C4A | -2.23 | 109.81 | 114.61 |
| 21 | c | 602 | CLA | C1-C2-C3 | -2.23 | 122.55 | 126.20 |
| 29 | 6 | 605 | CHL | CBC-CAC-C3C | -2.23 | 109.69 | 112.87 |
| 21 | B | 810 | CLA | O2A-CGA-O1A | -2.23 | 118.06 | 123.63 |
| 21 | c | 614 | CLA | CHB-C4A-NA | 2.22 | 127.61 | 124.40 |
| 31 | 2 | 617 | XAT | C12-C13-C14 | 2.22 | 122.50 | 119.01 |
| 21 | 9 | 602 | CLA | O2A-CGA-O1A | -2.22 | 118.07 | 123.63 |
| 24 | 3 | 418 | BCR | C37-C22-C23 | 2.22 | 121.48 | 118.09 |
| 21 | B | 812 | CLA | O2A-CGA-O1A | -2.22 | 118.08 | 123.63 |
| 21 | B | 806 | CLA | CMB-C2B-C1B | -2.22 | 122.04 | 125.42 |
| 24 | B | 846 | BCR | C8-C7-C6 | -2.22 | 121.08 | 127.00 |
| 21 | 1 | 304 | CLA | C1-C2-C3 | -2.22 | 122.56 | 126.20 |
| 21 | B | 840 | CLA | O2A-CGA-O1A | -2.22 | 118.08 | 123.63 |
| 21 | L | 303 | CLA | O2D-CGD-CBD | 2.22 | 115.11 | 111.23 |
| 24 | B | 843 | BCR | C20-C19-C18 | -2.22 | 120.29 | 126.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | 7 | 418 | BCR | C24-C23-C22 | 2.22 | 129.51 | 126.23 |
| 21 | 5 | 603 | CLA | CHB-C4A-NA | 2.21 | 127.60 | 124.40 |
| 21 | 7 | 408 | CLA | C3B-C4B-NB | -2.21 | 108.55 | 110.53 |
| 31 | 1 | 318 | XAT | C6-C7-C8 | -2.21 | 121.31 | 125.99 |
| 21 | B | 825 | CLA | O2A-CGA-O1A | -2.21 | 118.09 | 123.63 |
| 29 | 2 | 614 | CHL | O2D-CGD-O1D | -2.21 | 119.54 | 123.85 |
| 24 | I | 101 | BCR | C15-C16-C17 | 2.21 | 128.05 | 123.52 |
| 21 | 8 | 611 | CLA | C1-C2-C3 | -2.21 | 122.57 | 126.20 |
| 24 | A | 848 | BCR | C12-C13-C14 | 2.21 | 122.49 | 119.01 |
| 24 | J | 104 | BCR | C15-C16-C17 | -2.21 | 118.99 | 123.52 |
| 29 | c | 609 | CHL | C3D-C4D-ND | -2.21 | 109.39 | 112.94 |
| 31 | a | 618 | XAT | C15-C35-C34 | 2.21 | 128.04 | 123.52 |
| 29 | b | 307 | CHL | CMA-C3A-C4A | -2.21 | 109.85 | 114.61 |
| 21 | 6 | 609 | CLA | CMB-C2B-C1B | -2.21 | 122.05 | 125.42 |
| 30 | b | 316 | LUT | C39-C29-C28 | 2.21 | 121.46 | 118.09 |
| 24 | G | 201 | BCR | C8-C9-C10 | 2.21 | 122.48 | 119.01 |
| 21 | A | 803 | CLA | C1-C2-C3 | -2.21 | 122.58 | 126.20 |
| 21 | 4 | 609 | CLA | C3D-C4D-ND | 2.21 | 113.58 | 109.99 |
| 21 | A | 812 | CLA | CHB-C4A-NA | 2.21 | 127.58 | 124.40 |
| 29 | 1 | 307 | CHL | C5-C3-C4 | 2.21 | 119.66 | 114.59 |
| 29 | 9 | 607 | CHL | C3D-C4D-ND | -2.21 | 109.40 | 112.94 |
| 21 | 8 | 602 | CLA | O2A-CGA-O1A | -2.21 | 118.11 | 123.63 |
| 21 | B | 801 | CLA | CHB-C4A-NA | 2.21 | 127.58 | 124.40 |
| 21 | B | 807 | CLA | CAA-C2A-C3A | -2.20 | 107.05 | 113.00 |
| 24 | B | 843 | BCR | C36-C18-C17 | -2.20 | 119.25 | 122.82 |
| 21 | 3 | 406 | CLA | C3B-C4B-NB | -2.20 | 108.05 | 110.33 |
| 30 | b | 317 | LUT | C12-C13-C14 | 2.20 | 122.47 | 119.01 |
| 21 | 3 | 401 | CLA | C3B-C4B-NB | -2.20 | 108.57 | 110.53 |
| 29 | c | 605 | CHL | CBC-CAC-C3C | -2.20 | 109.73 | 112.87 |
| 21 | B | 831 | CLA | CAC-C3C-C4C | 2.20 | 127.65 | 124.79 |
| 30 | c | 616 | LUT | C39-C29-C28 | 2.20 | 121.44 | 118.09 |
| 21 | A | 803 | CLA | O2A-CGA-O1A | -2.19 | 118.14 | 123.63 |
| 21 | A | 813 | CLA | CMB-C2B-C1B | -2.19 | 122.08 | 125.42 |
| 21 | 5 | 602 | CLA | O2A-CGA-O1A | -2.19 | 118.14 | 123.63 |
| 24 | F | 303 | BCR | C11-C10-C9 | 2.19 | 130.35 | 127.28 |
| 21 | 2 | 608 | CLA | O2A-CGA-O1A | -2.19 | 118.15 | 123.63 |
| 24 | 6 | 618 | BCR | C8-C9-C10 | 2.19 | 122.45 | 119.01 |
| 21 | B | 821 | CLA | C1-C2-C3 | -2.19 | 122.61 | 126.20 |
| 24 | K | 205 | BCR | C33-C5-C4 | 2.19 | 118.26 | 113.60 |
| 21 | L | 304 | CLA | CMB-C2B-C1B | -2.19 | 122.09 | 125.42 |
| 31 | 7 | 416 | XAT | C11-C10-C9 | 2.19 | 130.35 | 127.28 |
| 29 | 7 | 406 | CHL | CMA-C3A-C2A | -2.19 | 111.22 | 116.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 303 | CLA | O2A-CGA-O1A | -2.19 | 118.16 | 123.63 |
| 29 | 2 | 607 | CHL | O2D-CGD-O1D | -2.18 | 119.60 | 123.85 |
| 21 | 9 | 610 | CLA | CMB-C2B-C3B | 2.18 | 131.69 | 126.55 |
| 21 | A | 837 | CLA | O2A-CGA-O1A | -2.18 | 118.17 | 123.63 |
| 24 | A | 847 | BCR | C12-C13-C14 | 2.18 | 122.44 | 119.01 |
| 21 | B | 837 | CLA | CHB-C4A-NA | 2.18 | 127.55 | 124.40 |
| 24 | I | 101 | BCR | C37-C22-C23 | 2.18 | 121.42 | 118.09 |
| 24 | 2 | 618 | BCR | C15-C16-C17 | -2.18 | 119.06 | 123.52 |
| 21 | B | 831 | CLA | O2D-CGD-CBD | 2.18 | 115.04 | 111.23 |
| 21 | B | 808 | CLA | CMB-C2B-C1B | -2.18 | 122.10 | 125.42 |
| 21 | A | 809 | CLA | O2A-CGA-O1A | -2.18 | 118.17 | 123.63 |
| 21 | A | 829 | CLA | O2A-CGA-O1A | -2.18 | 118.18 | 123.63 |
| 21 | A | 826 | CLA | O2A-CGA-O1A | -2.18 | 118.18 | 123.63 |
| 21 | A | 829 | CLA | CHB-C4A-NA | 2.18 | 127.54 | 124.40 |
| 21 | 5 | 605 | CLA | CHB-C4A-NA | 2.18 | 127.54 | 124.40 |
| 21 | 3 | 408 | CLA | O2A-CGA-O1A | -2.18 | 118.19 | 123.63 |
| 29 | a | 605 | CHL | O2D-CGD-O1D | -2.17 | 119.15 | 124.08 |
| 21 | A | 818 | CLA | CMB-C2B-C1B | -2.17 | 122.11 | 125.42 |
| 30 | 7 | 415 | LUT | C15-C35-C34 | 2.17 | 127.97 | 123.52 |
| 21 | A | 832 | CLA | CMB-C2B-C3B | 2.17 | 131.66 | 126.55 |
| 24 | B | 846 | BCR | C1-C6-C5 | -2.17 | 119.67 | 122.64 |
| 21 | A | 803 | CLA | CMB-C2B-C1B | -2.17 | 122.11 | 125.42 |
| 21 | A | 852 | CLA | O2A-CGA-O1A | -2.17 | 118.20 | 123.63 |
| 21 | A | 814 | CLA | O2A-CGA-O1A | -2.17 | 118.21 | 123.63 |
| 29 | b | 308 | CHL | C3D-C4D-ND | -2.17 | 109.46 | 112.94 |
| 24 | L | 301 | BCR | C34-C9-C8 | 2.16 | 121.39 | 118.09 |
| 21 | B | 808 | CLA | C1-C2-C3 | -2.16 | 122.65 | 126.20 |
| 21 | A | 825 | CLA | CMB-C2B-C1B | -2.16 | 122.13 | 125.42 |
| 29 | c | 601 | CHL | CMA-C3A-C4A | -2.16 | 109.96 | 114.61 |
| 21 | A | 802 | CLA | O2A-CGA-O1A | -2.16 | 118.22 | 123.63 |
| 21 | 4 | 611 | CLA | CMB-C2B-C1B | -2.16 | 122.13 | 125.42 |
| 29 | 6 | 614 | CHL | O2D-CGD-O1D | -2.16 | 119.65 | 123.85 |
| 21 | B | 834 | CLA | CMB-C2B-C3B | 2.16 | 131.62 | 126.55 |
| 31 | 3 | 417 | XAT | C35-C15-C14 | 2.15 | 127.93 | 123.52 |
| 21 | B | 806 | CLA | O2D-CGD-CBD | 2.15 | 114.99 | 111.23 |
| 21 | A | 809 | CLA | CMB-C2B-C1B | -2.15 | 122.14 | 125.42 |
| 31 | a | 618 | XAT | C10-C11-C12 | 2.15 | 129.43 | 123.20 |
| 30 | 9 | 614 | LUT | C11-C10-C9 | 2.15 | 130.29 | 127.28 |
| 29 | b | 310 | CHL | O2D-CGD-O1D | -2.15 | 119.21 | 124.08 |
| 21 | A | 812 | CLA | O2A-CGA-O1A | -2.15 | 118.26 | 123.63 |
| 29 | 6 | 607 | CHL | O2D-CGD-O1D | -2.15 | 119.67 | 123.85 |
| 29 | 6 | 607 | CHL | C5-C3-C4 | 2.15 | 119.53 | 114.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 809 | CLA | O2A-CGA-O1A | -2.15 | 118.26 | 123.63 |
| 21 | A | 852 | CLA | CMB-C2B-C3B | 2.14 | 131.59 | 126.55 |
| 21 | 4 | 609 | CLA | C2A-C1A-CHA | 2.14 | 127.59 | 123.87 |
| 21 | A | 805 | CLA | O2D-CGD-CBD | 2.14 | 114.97 | 111.23 |
| 29 | 2 | 602 | CHL | CMA-C3A-C4A | -2.14 | 110.00 | 114.61 |
| 29 | c | 601 | CHL | C3D-C4D-ND | -2.14 | 109.51 | 112.94 |
| 24 | 8 | 616 | BCR | C37-C22-C23 | 2.14 | 121.36 | 118.09 |
| 21 | 8 | 602 | CLA | CMB-C2B-C1B | -2.14 | 122.16 | 125.42 |
| 29 | 8 | 607 | CHL | CMA-C3A-C4A | -2.14 | 110.00 | 114.61 |
| 21 | 3 | 412 | CLA | O2A-CGA-O1A | -2.14 | 118.28 | 123.63 |
| 21 | c | 610 | CLA | CMB-C2B-C1B | -2.14 | 122.17 | 125.42 |
| 21 | b | 303 | CLA | O2A-CGA-O1A | -2.13 | 118.29 | 123.63 |
| 31 | 4 | 616 | XAT | C12-C13-C14 | 2.13 | 122.37 | 119.01 |
| 29 | 9 | 607 | CHL | CMA-C3A-C4A | -2.13 | 110.01 | 114.61 |
| 29 | 9 | 601 | CHL | CMA-C3A-C4A | -2.13 | 110.02 | 114.61 |
| 21 | A | 818 | CLA | CHB-C1B-NB | 2.13 | 127.25 | 124.05 |
| 21 | B | 801 | CLA | O2A-CGA-O1A | -2.13 | 118.30 | 123.63 |
| 21 | A | 826 | CLA | CMB-C2B-C1B | -2.13 | 122.17 | 125.42 |
| 29 | c | 607 | CHL | C3D-C4D-ND | -2.13 | 109.52 | 112.94 |
| 21 | B | 824 | CLA | CMB-C2B-C1B | -2.13 | 122.18 | 125.42 |
| 24 | 7 | 418 | BCR | C10-C11-C12 | 2.13 | 129.37 | 123.20 |
| 21 | 2 | 609 | CLA | CBA-CAA-C2A | -2.13 | 110.53 | 114.28 |
| 30 | c | 615 | LUT | C32-C33-C34 | 2.13 | 122.35 | 119.01 |
| 24 | J | 104 | BCR | C10-C11-C12 | -2.13 | 117.04 | 123.20 |
| 21 | 6 | 604 | CLA | C3B-C4B-NB | -2.12 | 108.63 | 110.53 |
| 29 | 5 | 606 | CHL | C3D-C4D-ND | -2.12 | 109.53 | 112.94 |
| 29 | 9 | 609 | CHL | O2D-CGD-O1D | -2.12 | 119.72 | 123.85 |
| 21 | B | 829 | CLA | C3B-C4B-NB | -2.12 | 108.64 | 110.53 |
| 24 | B | 843 | BCR | C8-C9-C10 | -2.12 | 115.67 | 119.01 |
| 29 | b | 309 | CHL | CMA-C3A-C4A | -2.12 | 110.04 | 114.61 |
| 21 | 9 | 610 | CLA | C1-C2-C3 | -2.12 | 122.72 | 126.20 |
| 21 | A | 819 | CLA | C1-C2-C3 | -2.12 | 122.72 | 126.20 |
| 24 | B | 843 | BCR | C37-C22-C23 | 2.12 | 121.32 | 118.09 |
| 21 | 1 | 305 | CLA | O2A-CGA-O1A | -2.12 | 118.33 | 123.63 |
| 29 | c | 605 | CHL | C3D-C4D-ND | -2.12 | 109.54 | 112.94 |
| 29 | 3 | 407 | CHL | CMA-C3A-C2A | -2.12 | 111.38 | 116.23 |
| 21 | 7 | 401 | CLA | O2D-CGD-CBD | 2.12 | 114.93 | 111.23 |
| 21 | 6 | 603 | CLA | CHB-C4A-NA | 2.12 | 127.45 | 124.40 |
| 29 | 1 | 307 | CHL | CMA-C3A-C4A | -2.12 | 110.05 | 114.61 |
| 29 | 7 | 406 | CHL | O2D-CGD-O1D | -2.12 | 119.28 | 124.08 |
| 21 | a | 602 | CLA | CMB-C2B-C1B | -2.12 | 122.20 | 125.42 |
| 30 | 9 | 615 | LUT | C39-C29-C28 | 2.12 | 121.32 | 118.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 826 | CLA | C1-C2-C3 | -2.12 | 122.73 | 126.20 |
| 21 | A | 809 | CLA | O2D-CGD-CBD | 2.11 | 114.93 | 111.23 |
| 21 | B | 837 | CLA | C1-C2-C3 | -2.11 | 122.73 | 126.20 |
| 21 | K | 202 | CLA | O2D-CGD-CBD | 2.11 | 114.92 | 111.23 |
| 21 | A | 819 | CLA | O2D-CGD-CBD | 2.11 | 114.92 | 111.23 |
| 21 | A | 825 | CLA | C1-C2-C3 | -2.11 | 122.74 | 126.20 |
| 21 | 4 | 602 | CLA | O2A-CGA-O1A | -2.11 | 118.35 | 123.63 |
| 24 | B | 844 | BCR | C15-C16-C17 | -2.11 | 119.20 | 123.52 |
| 29 | 8 | 607 | CHL | O1D-CGD-CBD | -2.11 | 121.52 | 124.72 |
| 21 | B | 805 | CLA | O2A-CGA-O1A | -2.11 | 118.35 | 123.63 |
| 21 | B | 836 | CLA | CMB-C2B-C3B | 2.11 | 131.51 | 126.55 |
| 21 | G | 203 | CLA | O2A-CGA-O1A | -2.11 | 118.36 | 123.63 |
| 29 | 8 | 606 | CHL | C3D-C4D-ND | -2.11 | 109.56 | 112.94 |
| 21 | B | 826 | CLA | CMB-C2B-C1B | -2.10 | 122.22 | 125.42 |
| 29 | 7 | 406 | CHL | C3D-C4D-ND | -2.10 | 109.56 | 112.94 |
| 21 | B | 835 | CLA | CMB-C2B-C3B | 2.10 | 131.50 | 126.55 |
| 29 | 6 | 606 | CHL | CMA-C3A-C4A | -2.10 | 110.08 | 114.61 |
| 29 | 6 | 602 | CHL | C3D-C4D-ND | -2.10 | 109.56 | 112.94 |
| 29 | 2 | 602 | CHL | C1-O2A-CGA | 2.10 | 121.74 | 116.65 |
| 21 | B | 832 | CLA | CMB-C2B-C3B | 2.10 | 131.50 | 126.55 |
| 29 | 9 | 609 | CHL | CMA-C3A-C4A | -2.10 | 110.08 | 114.61 |
| 21 | 4 | 608 | CLA | CMB-C2B-C1B | -2.10 | 122.22 | 125.42 |
| 29 | 3 | 407 | CHL | CAA-C2A-C1A | -2.10 | 109.72 | 114.49 |
| 29 | a | 606 | CHL | O2A-CGA-CBA | 2.10 | 120.63 | 114.00 |
| 21 | B | 823 | CLA | O2A-CGA-O1A | -2.10 | 118.38 | 123.63 |
| 24 | G | 205 | BCR | C34-C9-C8 | 2.10 | 121.29 | 118.09 |
| 29 | 2 | 606 | CHL | C3D-C4D-ND | -2.10 | 109.57 | 112.94 |
| 21 | B | 810 | CLA | C3B-C4B-NB | -2.10 | 108.15 | 110.33 |
| 29 | 9 | 608 | CHL | CMA-C3A-C4A | -2.10 | 110.09 | 114.61 |
| 21 | B | 807 | CLA | O2A-CGA-O1A | -2.10 | 118.39 | 123.63 |
| 21 | 4 | 602 | CLA | CMB-C2B-C1B | -2.10 | 122.23 | 125.42 |
| 21 | 1 | 311 | CLA | CMA-C3A-C2A | -2.09 | 111.43 | 116.23 |
| 21 | B | 806 | CLA | C3B-C4B-NB | -2.09 | 108.66 | 110.53 |
| 21 | K | 203 | CLA | C3B-C4B-NB | -2.09 | 108.16 | 110.33 |
| 29 | b | 302 | CHL | C4D-CHA-CBD | -2.09 | 106.86 | 108.97 |
| 29 | 1 | 302 | CHL | C3D-C4D-ND | -2.09 | 109.58 | 112.94 |
| 21 | 9 | 613 | CLA | O2A-CGA-O1A | -2.09 | 118.40 | 123.63 |
| 21 | A | 816 | CLA | CMB-C2B-C3B | 2.09 | 131.47 | 126.55 |
| 21 | B | 826 | CLA | O2D-CGD-CBD | 2.09 | 114.89 | 111.23 |
| 21 | O | 201 | CLA | CMB-C2B-C1B | -2.09 | 122.24 | 125.42 |
| 21 | 7 | 411 | CLA | O2A-CGA-O1A | -2.09 | 118.40 | 123.63 |
| 21 | 1 | 310 | CLA | CMB-C2B-C1B | -2.09 | 122.24 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | L | 301 | BCR | C37-C22-C23 | 2.09 | 121.28 | 118.09 |
| 21 | B | 813 | CLA | CMB-C2B-C1B | -2.09 | 122.24 | 125.42 |
| 21 | B | 827 | CLA | O2A-CGA-O1A | -2.09 | 118.41 | 123.63 |
| 21 | 2 | 611 | CLA | CMB-C2B-C1B | -2.09 | 122.24 | 125.42 |
| 21 | b | 311 | CLA | CMB-C2B-C3B | 2.09 | 131.46 | 126.55 |
| 21 | A | 828 | CLA | CMB-C2B-C1B | -2.09 | 122.24 | 125.42 |
| 21 | B | 801 | CLA | C4-C3-C5 | 2.08 | 118.85 | 115.23 |
| 21 | A | 838 | CLA | CMB-C2B-C3B | 2.08 | 131.45 | 126.55 |
| 24 | J | 104 | BCR | C7-C6-C5 | 2.08 | 126.36 | 121.56 |
| 21 | B | 827 | CLA | CMB-C2B-C1B | -2.08 | 122.25 | 125.42 |
| 21 | 2 | 609 | CLA | CMB-C2B-C3B | 2.08 | 131.45 | 126.55 |
| 21 | A | 818 | CLA | O2D-CGD-CBD | 2.08 | 114.87 | 111.23 |
| 21 | B | 806 | CLA | O2A-CGA-O1A | -2.08 | 118.42 | 123.63 |
| 24 | B | 844 | BCR | C1-C6-C7 | 2.08 | 121.29 | 115.65 |
| 21 | B | 837 | CLA | O2A-CGA-O1A | -2.08 | 118.43 | 123.63 |
| 21 | a | 613 | CLA | O2A-CGA-O1A | -2.08 | 118.43 | 123.63 |
| 21 | b | 314 | CLA | O2A-CGA-O1A | -2.08 | 118.43 | 123.63 |
| 30 | 7 | 415 | LUT | C7-C8-C9 | 2.08 | 129.31 | 126.23 |
| 24 | 3 | 419 | BCR | C21-C20-C19 | 2.08 | 129.22 | 123.20 |
| 21 | A | 804 | CLA | O2D-CGD-CBD | 2.08 | 114.86 | 111.23 |
| 21 | A | 801 | CLA | CMA-C3A-C2A | -2.08 | 105.95 | 113.98 |
| 21 | 3 | 403 | CLA | C3B-C4B-NB | -2.08 | 108.68 | 110.53 |
| 21 | a | 604 | CLA | O2A-CGA-O1A | -2.08 | 118.43 | 123.63 |
| 21 | 3 | 409 | CLA | CMB-C2B-C3B | 2.08 | 131.43 | 126.55 |
| 30 | 4 | 615 | LUT | C39-C29-C28 | 2.08 | 121.26 | 118.09 |
| 21 | c | 603 | CLA | O2A-CGA-O1A | -2.08 | 118.44 | 123.63 |
| 21 | A | 803 | CLA | CMB-C2B-C3B | 2.07 | 131.43 | 126.55 |
| 21 | B | 825 | CLA | CMB-C2B-C3B | 2.07 | 131.43 | 126.55 |
| 29 | c | 606 | CHL | CMA-C3A-C4A | -2.07 | 110.15 | 114.61 |
| 29 | 3 | 407 | CHL | C1A-CHA-CBD | 2.07 | 137.67 | 132.36 |
| 24 | 8 | 616 | BCR | C8-C9-C10 | 2.07 | 122.27 | 119.01 |
| 30 | 2 | 616 | LUT | C15-C35-C34 | 2.07 | 127.75 | 123.52 |
| 21 | 1 | 304 | CLA | C3B-C4B-NB | -2.07 | 108.68 | 110.53 |
| 21 | A | 814 | CLA | CMB-C2B-C1B | -2.07 | 122.27 | 125.42 |
| 30 | c | 615 | LUT | C19-C9-C8 | 2.07 | 121.25 | 118.09 |
| 21 | c | 603 | CLA | CMB-C2B-C1B | -2.07 | 122.27 | 125.42 |
| 21 | A | 801 | CLA | CHB-C4A-NA | 2.07 | 127.39 | 124.40 |
| 29 | a | 606 | CHL | C3D-C4D-ND | -2.07 | 109.62 | 112.94 |
| 31 | 9 | 616 | XAT | C6-C7-C8 | -2.07 | 121.62 | 125.99 |
| 21 | 3 | 409 | CLA | CHA-C4D-ND | -2.07 | 128.28 | 132.55 |
| 29 | c | 606 | CHL | C3D-C4D-ND | -2.07 | 109.62 | 112.94 |
| 21 | A | 824 | CLA | O2A-CGA-O1A | -2.07 | 118.46 | 123.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | b | 301 | LMU | C1B-O1B-C4' | -2.07 | 113.08 | 117.98 |
| 21 | A | 810 | CLA | O2A-CGA-O1A | -2.06 | 118.02 | 123.33 |
| 21 | B | 830 | CLA | CMB-C2B-C1B | -2.06 | 122.28 | 125.42 |
| 29 | 4 | 607 | CHL | C3D-C4D-ND | -2.06 | 109.63 | 112.94 |
| 21 | B | 821 | CLA | O2A-CGA-O1A | -2.06 | 118.48 | 123.63 |
| 21 | b | 314 | CLA | CMB-C2B-C1B | -2.06 | 122.28 | 125.42 |
| 29 | 4 | 614 | CHL | CAA-C2A-C3A | -2.06 | 111.51 | 116.23 |
| 29 | 4 | 607 | CHL | O2D-CGD-O1D | -2.06 | 119.84 | 123.85 |
| 21 | F | 302 | CLA | O2A-CGA-O1A | -2.06 | 118.48 | 123.63 |
| 21 | A | 827 | CLA | O2A-CGA-O1A | -2.06 | 118.48 | 123.63 |
| 31 | 1 | 318 | XAT | C12-C13-C14 | 2.06 | 122.24 | 119.01 |
| 29 | 6 | 607 | CHL | C3D-C4D-ND | -2.06 | 109.64 | 112.94 |
| 29 | 8 | 606 | CHL | CMA-C3A-C4A | -2.06 | 110.18 | 114.61 |
| 29 | 9 | 609 | CHL | C3D-C4D-ND | -2.06 | 109.64 | 112.94 |
| 29 | 2 | 614 | CHL | O2A-CGA-CBA | 2.05 | 120.49 | 114.00 |
| 29 | 8 | 607 | CHL | O2D-CGD-O1D | -2.05 | 119.85 | 123.85 |
| 21 | B | 832 | CLA | C1-C2-C3 | -2.05 | 122.83 | 126.20 |
| 21 | A | 839 | CLA | O2D-CGD-CBD | 2.05 | 114.82 | 111.23 |
| 24 | 4 | 617 | BCR | C37-C22-C23 | 2.05 | 121.22 | 118.09 |
| 29 | 2 | 607 | CHL | CBC-CAC-C3C | -2.05 | 109.94 | 112.87 |
| 21 | 2 | 608 | CLA | C1-C2-C3 | -2.05 | 122.84 | 126.20 |
| 29 | c | 609 | CHL | O2D-CGD-O1D | -2.05 | 119.43 | 124.08 |
| 21 | A | 803 | CLA | CHB-C4A-NA | 2.05 | 127.36 | 124.40 |
| 21 | 5 | 605 | CLA | C2A-C1A-CHA | 2.05 | 125.89 | 122.71 |
| 21 | 9 | 611 | CLA | O2A-CGA-O1A | -2.05 | 118.50 | 123.63 |
| 21 | 4 | 612 | CLA | O2A-CGA-O1A | -2.05 | 118.50 | 123.63 |
| 21 | 1 | 304 | CLA | CMB-C2B-C3B | 2.05 | 131.37 | 126.55 |
| 21 | A | 827 | CLA | CMB-C2B-C3B | 2.05 | 131.36 | 126.55 |
| 24 | B | 846 | BCR | C30-C25-C26 | -2.05 | 119.84 | 122.64 |
| 21 | B | 817 | CLA | O2D-CGD-CBD | 2.05 | 114.81 | 111.23 |
| 21 | A | 825 | CLA | O2A-CGA-O1A | -2.05 | 118.51 | 123.63 |
| 21 | a | 603 | CLA | CMA-C3A-C2A | -2.04 | 111.54 | 116.23 |
| 21 | A | 808 | CLA | CMB-C2B-C3B | 2.04 | 131.36 | 126.55 |
| 21 | B | 802 | CLA | O1D-CGD-CBD | 2.04 | 128.55 | 124.52 |
| 29 | 8 | 613 | CHL | CMA-C3A-C4A | -2.04 | 110.21 | 114.61 |
| 31 | a | 618 | XAT | C28-C29-C30 | 2.04 | 122.22 | 119.01 |
| 21 | B | 814 | CLA | O2A-CGA-O1A | -2.04 | 118.52 | 123.63 |
| 21 | B | 829 | CLA | O1D-CGD-CBD | 2.04 | 128.54 | 124.52 |
| 29 | b | 308 | CHL | CBC-CAC-C3C | -2.04 | 109.95 | 112.87 |
| 21 | A | 834 | CLA | O2A-CGA-O1A | -2.04 | 118.53 | 123.63 |
| 29 | 6 | 614 | CHL | CMA-C3A-C4A | -2.04 | 110.22 | 114.61 |
| 21 | L | 302 | CLA | O2A-CGA-O1A | -2.04 | 118.09 | 123.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 9 | 605 | CHL | CMA-C3A-C4A | -2.04 | 110.22 | 114.61 |
| 30 | 6 | 616 | LUT | C27-C28-C29 | 2.04 | 130.71 | 126.32 |
| 24 | 2 | 618 | BCR | C29-C30-C25 | 2.04 | 113.40 | 110.44 |
| 21 | A | 837 | CLA | C1-C2-C3 | -2.04 | 122.86 | 126.20 |
| 21 | A | 819 | CLA | O2A-CGA-O1A | -2.04 | 118.54 | 123.63 |
| 29 | 9 | 605 | CHL | C3D-C4D-ND | -2.04 | 109.67 | 112.94 |
| 21 | 5 | 602 | CLA | C1-C2-C3 | -2.03 | 122.86 | 126.20 |
| 29 | 1 | 307 | CHL | C3D-C4D-ND | -2.03 | 109.67 | 112.94 |
| 21 | c | 611 | CLA | O2A-CGA-O1A | -2.03 | 118.54 | 123.63 |
| 31 | 2 | 617 | XAT | C39-C29-C28 | 2.03 | 121.19 | 118.09 |
| 31 | 7 | 416 | XAT | O4-C6-C7 | -2.03 | 111.05 | 116.88 |
| 21 | A | 813 | CLA | CMB-C2B-C3B | 2.03 | 131.33 | 126.55 |
| 21 | A | 842 | CLA | O2A-CGA-O1A | -2.03 | 118.54 | 123.63 |
| 21 | A | 801 | CLA | CAA-C2A-C3A | -2.03 | 107.51 | 113.00 |
| 31 | 2 | 617 | XAT | C7-C8-C9 | 2.03 | 128.68 | 125.53 |
| 21 | 6 | 609 | CLA | O1D-CGD-CBD | 2.03 | 128.52 | 124.52 |
| 21 | 1 | 315 | CLA | O2A-CGA-O1A | -2.03 | 118.11 | 123.33 |
| 29 | 8 | 607 | CHL | CBC-CAC-C3C | -2.03 | 109.97 | 112.87 |
| 21 | A | 826 | CLA | O2D-CGD-CBD | 2.03 | 114.78 | 111.23 |
| 21 | 9 | 611 | CLA | C1-C2-C3 | -2.03 | 122.87 | 126.20 |
| 29 | 2 | 607 | CHL | C3D-C4D-ND | -2.03 | 109.69 | 112.94 |
| 29 | a | 601 | CHL | CBC-CAC-C3C | -2.03 | 109.97 | 112.87 |
| 24 | K | 205 | BCR | C30-C25-C24 | 2.03 | 121.15 | 115.65 |
| 29 | 9 | 608 | CHL | C3D-C4D-ND | -2.03 | 109.69 | 112.94 |
| 21 | A | 803 | CLA | C3B-C4B-NB | -2.03 | 108.72 | 110.53 |
| 21 | A | 805 | CLA | CMB-C2B-C1B | -2.03 | 122.33 | 125.42 |
| 29 | c | 607 | CHL | CMA-C3A-C4A | -2.02 | 110.25 | 114.61 |
| 21 | 3 | 402 | CLA | C1-C2-C3 | -2.02 | 122.88 | 126.20 |
| 21 | B | 808 | CLA | O2A-CGA-O1A | -2.02 | 118.57 | 123.63 |
| 24 | L | 305 | BCR | C30-C25-C24 | 2.02 | 121.14 | 115.65 |
| 21 | A | 805 | CLA | O2A-CGA-O1A | -2.02 | 118.57 | 123.63 |
| 21 | 5 | 611 | CLA | CMB-C2B-C1B | -2.02 | 122.34 | 125.42 |
| 24 | 2 | 618 | BCR | C23-C22-C21 | 2.02 | 122.19 | 119.01 |
| 24 | J | 104 | BCR | C4-C5-C6 | -2.02 | 119.97 | 122.70 |
| 21 | B | 803 | CLA | O2A-CGA-O1A | -2.02 | 118.58 | 123.63 |
| 21 | 2 | 612 | CLA | O2A-CGA-O1A | -2.02 | 118.14 | 123.33 |
| 30 | 5 | 615 | LUT | C39-C29-C28 | 2.02 | 121.17 | 118.09 |
| 21 | 1 | 309 | CLA | CHA-C4D-ND | -2.02 | 128.39 | 132.55 |
| 21 | c | 613 | CLA | O2A-CGA-O1A | -2.02 | 118.59 | 123.63 |
| 21 | 7 | 413 | CLA | CMB-C2B-C3B | 2.01 | 131.29 | 126.55 |
| 30 | 2 | 616 | LUT | C32-C33-C34 | 2.01 | 122.18 | 119.01 |
| 31 | 4 | 616 | XAT | C39-C29-C28 | 2.01 | 121.17 | 118.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 826 | CLA | CMB-C2B-C3B | 2.01 | 131.29 | 126.55 |
| 29 | b | 309 | CHL | C3D-C4D-ND | -2.01 | 109.71 | 112.94 |
| 21 | A | 835 | CLA | O2A-CGA-O1A | -2.01 | 118.59 | 123.63 |
| 21 | 2 | 604 | CLA | CMB-C2B-C1B | -2.01 | 122.36 | 125.42 |
| 21 | 1 | 314 | CLA | C3B-C4B-NB | -2.01 | 108.24 | 110.33 |
| 31 | 5 | 616 | XAT | C19-C9-C8 | 2.01 | 121.16 | 118.09 |
| 21 | 7 | 402 | CLA | C3B-C4B-NB | -2.01 | 108.73 | 110.53 |
| 21 | A | 852 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.40 |
| 21 | B | 840 | CLA | CMB-C2B-C3B | 2.01 | 131.28 | 126.55 |
| 21 | a | 602 | CLA | O2A-CGA-O1A | -2.01 | 118.60 | 123.63 |
| 21 | 5 | 607 | CLA | O1A-CGA-CBA | 2.01 | 129.47 | 123.09 |
| 21 | A | 818 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.40 |
| 21 | 1 | 310 | CLA | O2A-CGA-O1A | -2.01 | 118.17 | 123.33 |
| 21 | B | 836 | CLA | CAA-C2A-C3A | -2.01 | 107.58 | 113.00 |
| 21 | c | 602 | CLA | O2A-CGA-O1A | -2.01 | 118.61 | 123.63 |
| 21 | 2 | 612 | CLA | O2D-CGD-CBD | 2.01 | 114.74 | 111.23 |
| 29 | 8 | 607 | CHL | C3D-C4D-ND | -2.01 | 109.72 | 112.94 |
| 21 | A | 806 | CLA | O2A-CGA-O1A | -2.01 | 118.61 | 123.63 |
| 29 | 2 | 605 | CHL | C3D-C4D-ND | -2.01 | 109.72 | 112.94 |
| 24 | B | 842 | BCR | C1-C6-C5 | -2.00 | 119.90 | 122.64 |
| 29 | 8 | 613 | CHL | CMA-C3A-C2A | -2.00 | 111.63 | 116.23 |
| 29 | 6 | 614 | CHL | CED-O2D-CGD | 2.00 | 120.46 | 115.92 |
| 29 | b | 306 | CHL | C3D-C4D-ND | -2.00 | 109.72 | 112.94 |
| 21 | B | 804 | CLA | C1-C2-C3 | -2.00 | 122.91 | 126.20 |
| 24 | A | 854 | BCR | C34-C9-C8 | 2.00 | 121.15 | 118.09 |
| 21 | 3 | 409 | CLA | C2A-C1A-CHA | 2.00 | 127.34 | 123.87 |
| 21 | b | 303 | CLA | C1-C2-C3 | -2.00 | 122.92 | 126.20 |
| 24 | J | 104 | BCR | C32-C1-C6 | -2.00 | 107.10 | 110.24 |
| 29 | a | 608 | CHL | C3D-C4D-ND | -2.00 | 109.73 | 112.94 |
| 21 | A | 828 | CLA | CHB-C4A-NA | 2.00 | 127.29 | 124.40 |
| 21 | 8 | 604 | CLA | CMB-C2B-C3B | 2.00 | 131.26 | 126.55 |
| 30 | 1 | 317 | LUT | C39-C29-C28 | 2.00 | 121.14 | 118.09 |
| 29 | c | 609 | CHL | CMA-C3A-C4A | -2.00 | 110.30 | 114.61 |
| 21 | B | 806 | CLA | CMB-C2B-C3B | 2.00 | 131.25 | 126.55 |
| 21 | A | 807 | CLA | C1-C2-C3 | -2.00 | 122.92 | 126.20 |

All (368) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | A | 802 | CLA | ND |
| 21 | A | 803 | CLA | ND |
| 21 | A | 804 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 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 |
| 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 | 852 | CLA | ND |
| 21 | B | 801 | CLA | ND |
| 21 | B | 802 | CLA | ND |
| 21 | B | 803 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 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 |
| 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 | F | 302 | CLA | ND |
| 21 | F | 304 | CLA | ND |
| 21 | F | 305 | CLA | ND |
| 21 | G | 202 | CLA | ND |
| 21 | G | 203 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | G | 204 | CLA | ND |
| 21 | H | 201 | CLA | ND |
| 21 | J | 102 | CLA | ND |
| 21 | K | 201 | CLA | ND |
| 21 | K | 202 | CLA | ND |
| 21 | K | 203 | CLA | ND |
| 21 | K | 204 | CLA | ND |
| 21 | L | 302 | CLA | ND |
| 21 | L | 303 | CLA | ND |
| 21 | L | 304 | CLA | ND |
| 21 | O | 201 | CLA | ND |
| 21 | O | 202 | CLA | ND |
| 21 | O | 203 | CLA | ND |
| 21 | O | 204 | CLA | ND |
| 21 | 1 | 303 | CLA | ND |
| 21 | 1 | 304 | CLA | ND |
| 21 | 1 | 305 | CLA | ND |
| 21 | 1 | 306 | CLA | ND |
| 21 | 1 | 308 | CLA | ND |
| 21 | 1 | 309 | CLA | ND |
| 21 | 1 | 310 | CLA | ND |
| 21 | 1 | 311 | CLA | ND |
| 21 | 1 | 312 | CLA | ND |
| 21 | 1 | 313 | CLA | ND |
| 21 | 1 | 314 | CLA | ND |
| 21 | 1 | 315 | CLA | ND |
| 21 | 1 | 316 | CLA | ND |
| 21 | 2 | 603 | CLA | ND |
| 21 | 2 | 604 | CLA | ND |
| 21 | 2 | 608 | CLA | ND |
| 21 | 2 | 609 | CLA | ND |
| 21 | 2 | 610 | CLA | ND |
| 21 | 2 | 611 | CLA | ND |
| 21 | 2 | 612 | CLA | ND |
| 21 | 2 | 613 | CLA | ND |
| 21 | 3 | 401 | CLA | ND |
| 21 | 3 | 402 | CLA | ND |
| 21 | 3 | 403 | CLA | ND |
| 21 | 3 | 404 | CLA | ND |
| 21 | 3 | 405 | CLA | ND |
| 21 | 3 | 406 | CLA | ND |
| 21 | 3 | 408 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | 3 | 409 | CLA | ND |
| 21 | 3 | 410 | CLA | ND |
| 21 | 3 | 411 | CLA | ND |
| 21 | 3 | 412 | CLA | ND |
| 21 | 3 | 413 | CLA | ND |
| 21 | 3 | 414 | CLA | ND |
| 21 | 3 | 415 | CLA | ND |
| 21 | 4 | 601 | CLA | ND |
| 21 | 4 | 602 | CLA | ND |
| 21 | 4 | 603 | CLA | ND |
| 21 | 4 | 604 | CLA | ND |
| 21 | 4 | 608 | CLA | ND |
| 21 | 4 | 610 | CLA | ND |
| 21 | 4 | 611 | CLA | ND |
| 21 | 4 | 612 | CLA | ND |
| 21 | 4 | 613 | CLA | ND |
| 21 | 5 | 602 | CLA | ND |
| 21 | 5 | 603 | CLA | ND |
| 21 | 5 | 604 | CLA | ND |
| 21 | 5 | 605 | CLA | ND |
| 21 | 5 | 607 | CLA | ND |
| 21 | 5 | 608 | 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 | 6 | 603 | CLA | ND |
| 21 | 6 | 604 | CLA | ND |
| 21 | 6 | 608 | 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 | 7 | 401 | CLA | ND |
| 21 | 7 | 402 | CLA | ND |
| 21 | 7 | 403 | CLA | ND |
| 21 | 7 | 404 | CLA | ND |
| 21 | 7 | 405 | CLA | ND |
| 21 | 7 | 408 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | 7 | 409 | CLA | ND |
| 21 | 7 | 410 | CLA | ND |
| 21 | 7 | 411 | CLA | ND |
| 21 | 7 | 412 | CLA | ND |
| 21 | 7 | 413 | CLA | ND |
| 21 | 7 | 414 | CLA | ND |
| 21 | 8 | 601 | 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 | 618 | CLA | ND |
| 21 | 9 | 602 | CLA | ND |
| 21 | 9 | 603 | CLA | ND |
| 21 | 9 | 604 | CLA | ND |
| 21 | 9 | 610 | CLA | ND |
| 21 | 9 | 611 | CLA | ND |
| 21 | 9 | 612 | CLA | ND |
| 21 | 9 | 613 | CLA | ND |
| 21 | a | 602 | CLA | ND |
| 21 | a | 603 | CLA | ND |
| 21 | a | 604 | CLA | ND |
| 21 | a | 610 | CLA | ND |
| 21 | a | 611 | CLA | ND |
| 21 | a | 612 | CLA | ND |
| 21 | a | 613 | CLA | ND |
| 21 | a | 614 | CLA | ND |
| 21 | b | 303 | CLA | ND |
| 21 | b | 304 | CLA | ND |
| 21 | b | 305 | CLA | ND |
| 21 | b | 311 | CLA | ND |
| 21 | b | 312 | CLA | ND |
| 21 | b | 313 | CLA | ND |
| 21 | b | 314 | CLA | ND |
| 21 | b | 315 | CLA | ND |
| 21 | c | 602 | CLA | ND |
| 21 | c | 603 | CLA | ND |
| 21 | c | 604 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | c | 610 | CLA | ND |
| 21 | c | 611 | CLA | ND |
| 21 | c | 612 | CLA | ND |
| 21 | c | 613 | CLA | ND |
| 21 | c | 614 | CLA | ND |
| 29 | 1 | 302 | CHL | NA |
| 29 | 1 | 302 | CHL | NC |
| 29 | 1 | 302 | CHL | ND |
| 29 | 1 | 307 | CHL | NA |
| 29 | 1 | 307 | CHL | NC |
| 29 | 1 | 307 | CHL | ND |
| 29 | 2 | 601 | CHL | NA |
| 29 | 2 | 601 | CHL | NC |
| 29 | 2 | 601 | CHL | ND |
| 29 | 2 | 602 | CHL | NA |
| 29 | 2 | 602 | CHL | NC |
| 29 | 2 | 602 | CHL | ND |
| 29 | 2 | 605 | CHL | NA |
| 29 | 2 | 605 | CHL | NC |
| 29 | 2 | 605 | CHL | ND |
| 29 | 2 | 606 | CHL | NA |
| 29 | 2 | 606 | CHL | NC |
| 29 | 2 | 606 | CHL | ND |
| 29 | 2 | 607 | CHL | NA |
| 29 | 2 | 607 | CHL | NC |
| 29 | 2 | 607 | CHL | ND |
| 29 | 2 | 614 | CHL | NA |
| 29 | 2 | 614 | CHL | NC |
| 29 | 2 | 614 | CHL | ND |
| 29 | 3 | 407 | CHL | NA |
| 29 | 3 | 407 | CHL | NC |
| 29 | 3 | 407 | CHL | ND |
| 29 | 4 | 605 | CHL | NA |
| 29 | 4 | 605 | CHL | NC |
| 29 | 4 | 605 | CHL | ND |
| 29 | 4 | 606 | CHL | NA |
| 29 | 4 | 606 | CHL | NC |
| 29 | 4 | 606 | CHL | ND |
| 29 | 4 | 607 | CHL | NA |
| 29 | 4 | 607 | CHL | NC |
| 29 | 4 | 607 | CHL | ND |
| 29 | 4 | 614 | CHL | NA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 29 | 4 | 614 | CHL | NC |
| 29 | 4 | 614 | CHL | ND |
| 29 | 5 | 601 | CHL | NA |
| 29 | 5 | 601 | CHL | NC |
| 29 | 5 | 601 | CHL | ND |
| 29 | 5 | 606 | CHL | NA |
| 29 | 5 | 606 | CHL | NC |
| 29 | 5 | 606 | CHL | ND |
| 29 | 6 | 601 | CHL | NA |
| 29 | 6 | 601 | CHL | NC |
| 29 | 6 | 601 | CHL | ND |
| 29 | 6 | 602 | CHL | NA |
| 29 | 6 | 602 | CHL | NC |
| 29 | 6 | 602 | CHL | ND |
| 29 | 6 | 605 | CHL | NA |
| 29 | 6 | 605 | CHL | NC |
| 29 | 6 | 605 | CHL | ND |
| 29 | 6 | 606 | CHL | NA |
| 29 | 6 | 606 | CHL | NC |
| 29 | 6 | 606 | CHL | ND |
| 29 | 6 | 607 | CHL | NA |
| 29 | 6 | 607 | CHL | NC |
| 29 | 6 | 607 | CHL | ND |
| 29 | 6 | 614 | CHL | NA |
| 29 | 6 | 614 | CHL | NC |
| 29 | 6 | 614 | CHL | ND |
| 29 | 7 | 406 | CHL | NA |
| 29 | 7 | 406 | CHL | NC |
| 29 | 7 | 406 | CHL | ND |
| 29 | 8 | 605 | CHL | NA |
| 29 | 8 | 605 | CHL | NC |
| 29 | 8 | 605 | CHL | ND |
| 29 | 8 | 606 | CHL | NA |
| 29 | 8 | 606 | CHL | NC |
| 29 | 8 | 606 | CHL | ND |
| 29 | 8 | 607 | CHL | NA |
| 29 | 8 | 607 | CHL | NC |
| 29 | 8 | 607 | CHL | ND |
| 29 | 8 | 613 | CHL | NA |
| 29 | 8 | 613 | CHL | NC |
| 29 | 8 | 613 | CHL | ND |
| 29 | 9 | 601 | CHL | NA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 29 | 9 | 601 | CHL | NC |
| 29 | 9 | 601 | CHL | ND |
| 29 | 9 | 605 | CHL | NA |
| 29 | 9 | 605 | CHL | NC |
| 29 | 9 | 605 | CHL | ND |
| 29 | 9 | 606 | CHL | NA |
| 29 | 9 | 606 | CHL | NC |
| 29 | 9 | 606 | CHL | ND |
| 29 | 9 | 607 | CHL | NA |
| 29 | 9 | 607 | CHL | NC |
| 29 | 9 | 607 | CHL | ND |
| 29 | 9 | 608 | CHL | NA |
| 29 | 9 | 608 | CHL | NC |
| 29 | 9 | 608 | CHL | ND |
| 29 | 9 | 609 | CHL | NA |
| 29 | 9 | 609 | CHL | NC |
| 29 | 9 | 609 | CHL | ND |
| 29 | a | 601 | CHL | NA |
| 29 | a | 601 | CHL | NC |
| 29 | a | 601 | CHL | ND |
| 29 | a | 605 | CHL | NA |
| 29 | a | 605 | CHL | NC |
| 29 | a | 605 | CHL | ND |
| 29 | a | 606 | CHL | NA |
| 29 | a | 606 | CHL | NC |
| 29 | a | 606 | CHL | ND |
| 29 | a | 607 | CHL | NA |
| 29 | a | 607 | CHL | NC |
| 29 | a | 607 | CHL | ND |
| 29 | a | 608 | CHL | NA |
| 29 | a | 608 | CHL | NC |
| 29 | a | 608 | CHL | ND |
| 29 | a | 609 | CHL | NA |
| 29 | a | 609 | CHL | NC |
| 29 | a | 609 | CHL | ND |
| 29 | b | 302 | CHL | NA |
| 29 | b | 302 | CHL | NC |
| 29 | b | 302 | CHL | ND |
| 29 | b | 306 | CHL | NA |
| 29 | b | 306 | CHL | NC |
| 29 | b | 306 | CHL | ND |
| 29 | b | 307 | CHL | NA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 29 | b | 307 | CHL | NC |
| 29 | b | 307 | CHL | ND |
| 29 | b | 308 | CHL | NA |
| 29 | b | 308 | CHL | NC |
| 29 | b | 308 | CHL | ND |
| 29 | b | 309 | CHL | NA |
| 29 | b | 309 | CHL | NC |
| 29 | b | 309 | CHL | ND |
| 29 | b | 310 | CHL | NA |
| 29 | b | 310 | CHL | NC |
| 29 | b | 310 | CHL | ND |
| 29 | c | 601 | CHL | NA |
| 29 | c | 601 | CHL | NC |
| 29 | c | 601 | CHL | ND |
| 29 | c | 605 | CHL | NA |
| 29 | c | 605 | CHL | NC |
| 29 | c | 605 | CHL | ND |
| 29 | c | 606 | CHL | NA |
| 29 | c | 606 | CHL | NC |
| 29 | c | 606 | CHL | ND |
| 29 | c | 607 | CHL | NA |
| 29 | c | 607 | CHL | NC |
| 29 | c | 607 | CHL | ND |
| 29 | c | 608 | CHL | NA |
| 29 | c | 608 | CHL | NC |
| 29 | c | 608 | CHL | ND |
| 29 | c | 609 | CHL | NA |
| 29 | c | 609 | CHL | NC |
| 29 | c | 609 | CHL | ND |

All (1947) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 801 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 802 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 804 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 805 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 806 | CLA | CAD-CBD-CGD-O1D |
| 21 | A | 806 | CLA | CAD-CBD-CGD-O2D |
| 21 | A | 807 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 807 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 807 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 817 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 817 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 818 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 818 | CLA | C2-C3-C5-C6 |
| 21 | A | 818 | CLA | C4-C3-C5-C6 |
| 21 | A | 819 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 819 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 826 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 827 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 827 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 827 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 832 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 832 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 834 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 834 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 837 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 837 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 837 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 838 | CLA | C2-C3-C5-C6 |
| 21 | A | 838 | CLA | C4-C3-C5-C6 |
| 21 | A | 841 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 842 | CLA | C2-C1-O2A-CGA |
| 21 | A | 842 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 842 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 852 | CLA | C4-C3-C5-C6 |
| 21 | B | 802 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 802 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 802 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 804 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 804 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 807 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 811 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 816 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 816 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 817 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 817 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 818 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 818 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 818 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 827 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 827 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 830 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 830 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 832 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 834 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 834 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 836 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 836 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 839 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 839 | CLA | CAD-CBD-CGD-O1D |
| 21 | B | 839 | CLA | CAD-CBD-CGD-O2D |
| 21 | G | 202 | CLA | C1A-C2A-CAA-CBA |
| 21 | G | 202 | CLA | C3A-C2A-CAA-CBA |
| 21 | G | 202 | CLA | CBD-CGD-O2D-CED |
| 21 | G | 203 | CLA | CBD-CGD-O2D-CED |
| 21 | J | 102 | CLA | C1A-C2A-CAA-CBA |
| 21 | J | 102 | CLA | C3A-C2A-CAA-CBA |
| 21 | J | 102 | CLA | CAD-CBD-CGD-O1D |
| 21 | J | 102 | CLA | CAD-CBD-CGD-O2D |
| 21 | K | 202 | CLA | C1A-C2A-CAA-CBA |
| 21 | L | 302 | CLA | C1A-C2A-CAA-CBA |
| 21 | L | 302 | CLA | CHA-CBD-CGD-O1D |
| 21 | L | 302 | CLA | CHA-CBD-CGD-O2D |
| 21 | O | 201 | CLA | CAD-CBD-CGD-O1D |
| 21 | O | 201 | CLA | CAD-CBD-CGD-O2D |
| 21 | O | 202 | CLA | CAD-CBD-CGD-O2D |
| 21 | 1 | 303 | CLA | C3A-C2A-CAA-CBA |
| 21 | 1 | 303 | CLA | CHA-CBD-CGD-O1D |
| 21 | 1 | 303 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 305 | CLA | C1A-C2A-CAA-CBA |
| 21 | 1 | 305 | CLA | C3A-C2A-CAA-CBA |
| 21 | 1 | 306 | CLA | CBD-CGD-O2D-CED |
| 21 | 1 | 312 | CLA | CBD-CGD-O2D-CED |
| 21 | 1 | 316 | CLA | CBD-CGD-O2D-CED |
| 21 | 2 | 603 | CLA | CBD-CGD-O2D-CED |
| 21 | 2 | 608 | CLA | C1A-C2A-CAA-CBA |
| 21 | 2 | 608 | CLA | C3A-C2A-CAA-CBA |
| 21 | 2 | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 2 | 609 | CLA | C3A-C2A-CAA-CBA |
| 21 | 2 | 609 | CLA | C4C-C3C-CAC-CBC |
| 21 | 2 | 609 | CLA | CBD-CGD-O2D-CED |
| 21 | 2 | 609 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 405 | CLA | CAD-CBD-CGD-O2D |
| 21 | 3 | 409 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 3 | 409 | CLA | C3A-C2A-CAA-CBA |
| 21 | 3 | 409 | CLA | CBD-CGD-O2D-CED |
| 21 | 3 | 411 | CLA | CBD-CGD-O2D-CED |
| 21 | 4 | 602 | CLA | C3A-C2A-CAA-CBA |
| 21 | 4 | 609 | CLA | C3A-C2A-CAA-CBA |
| 21 | 4 | 609 | CLA | CBD-CGD-O2D-CED |
| 21 | 4 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 602 | CLA | C3A-C2A-CAA-CBA |
| 21 | 5 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 5 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 5 | 607 | CLA | C1A-C2A-CAA-CBA |
| 21 | 5 | 607 | CLA | C3A-C2A-CAA-CBA |
| 21 | 5 | 608 | CLA | CBD-CGD-O2D-CED |
| 21 | 5 | 612 | CLA | C1A-C2A-CAA-CBA |
| 21 | 5 | 612 | CLA | C3A-C2A-CAA-CBA |
| 21 | 5 | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 603 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 604 | CLA | C1A-C2A-CAA-CBA |
| 21 | 6 | 604 | CLA | C3A-C2A-CAA-CBA |
| 21 | 6 | 608 | CLA | C3A-C2A-CAA-CBA |
| 21 | 6 | 608 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 608 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 6 | 609 | CLA | C3A-C2A-CAA-CBA |
| 21 | 6 | 609 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 613 | CLA | CBD-CGD-O2D-CED |
| 21 | 7 | 401 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 401 | CLA | CHA-CBD-CGD-O1D |
| 21 | 7 | 401 | CLA | CHA-CBD-CGD-O2D |
| 21 | 7 | 402 | CLA | C1A-C2A-CAA-CBA |
| 21 | 7 | 402 | CLA | C3A-C2A-CAA-CBA |
| 21 | 7 | 402 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 402 | CLA | CAD-CBD-CGD-O1D |
| 21 | 7 | 402 | CLA | CAD-CBD-CGD-O2D |
| 21 | 7 | 405 | CLA | C1A-C2A-CAA-CBA |
| 21 | 7 | 405 | CLA | C3A-C2A-CAA-CBA |
| 21 | 7 | 407 | CLA | C3A-C2A-CAA-CBA |
| 21 | 7 | 407 | CLA | CAD-CBD-CGD-O2D |
| 21 | 8 | 601 | CLA | CAD-CBD-CGD-O1D |
| 21 | 8 | 601 | CLA | CAD-CBD-CGD-O2D |
| 21 | 8 | 602 | CLA | C1A-C2A-CAA-CBA |
| 21 | 8 | 602 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 8 | 602 | CLA | CAD-CBD-CGD-O2D |
| 21 | 8 | 604 | CLA | C1A-C2A-CAA-CBA |
| 21 | 8 | 604 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 608 | CLA | C1A-C2A-CAA-CBA |
| 21 | 8 | 608 | CLA | C3A-C2A-CAA-CBA |
| 21 | 8 | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 8 | 611 | CLA | CBD-CGD-O2D-CED |
| 21 | 8 | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | 8 | 618 | CLA | C2B-C3B-CAB-CBB |
| 21 | 8 | 618 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 618 | CLA | CBD-CGD-O2D-CED |
| 21 | 9 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 9 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | a | 602 | CLA | CBD-CGD-O2D-CED |
| 21 | a | 604 | CLA | C1A-C2A-CAA-CBA |
| 21 | a | 604 | CLA | C3A-C2A-CAA-CBA |
| 21 | b | 303 | CLA | CBD-CGD-O2D-CED |
| 21 | b | 313 | CLA | CHA-CBD-CGD-O1D |
| 21 | b | 313 | CLA | CHA-CBD-CGD-O2D |
| 21 | b | 314 | CLA | CBD-CGD-O2D-CED |
| 21 | c | 604 | CLA | CAD-CBD-CGD-O1D |
| 21 | c | 604 | CLA | CAD-CBD-CGD-O2D |
| 21 | c | 610 | CLA | CBD-CGD-O2D-CED |
| 21 | c | 614 | CLA | CAD-CBD-CGD-O1D |
| 21 | c | 614 | CLA | CAD-CBD-CGD-O2D |
| 23 | A | 844 | LHG | C4-O6-P-O3 |
| 23 | A | 844 | LHG | C4-O6-P-O5 |
| 23 | A | 855 | LHG | O10-C23-O8-C6 |
| 23 | A | 855 | LHG | C24-C23-O8-C6 |
| 23 | 1 | 301 | LHG | C4-O6-P-O3 |
| 23 | 1 | 301 | LHG | C4-O6-P-O4 |
| 23 | 1 | 301 | LHG | O9-C7-O7-C5 |
| 23 | 1 | 301 | LHG | C8-C7-O7-C5 |
| 23 | 1 | 319 | LHG | C4-O6-P-O3 |
| 23 | 1 | 319 | LHG | C4-O6-P-O4 |
| 23 | 1 | 319 | LHG | O10-C23-O8-C6 |
| 23 | 1 | 319 | LHG | C24-C23-O8-C6 |
| 23 | 2 | 619 | LHG | C3-O3-P-O5 |
| 23 | 2 | 619 | LHG | C3-O3-P-O6 |
| 23 | 4 | 618 | LHG | C4-O6-P-O3 |
| 23 | 4 | 618 | LHG | C4-O6-P-O5 |
| 23 | 4 | 618 | LHG | O7-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | 4 | 619 | LHG | C2-C3-O3-P |
| 23 | 4 | 619 | LHG | C5-C4-O6-P |
| 23 | 4 | 619 | LHG | O9-C7-O7-C5 |
| 23 | 4 | 619 | LHG | C8-C7-O7-C5 |
| 23 | 4 | 619 | LHG | O10-C23-O8-C6 |
| 23 | 4 | 619 | LHG | C24-C23-O8-C6 |
| 23 | 5 | 617 | LHG | C2-C3-O3-P |
| 23 | 5 | 617 | LHG | C4-O6-P-O5 |
| 23 | 5 | 617 | LHG | O10-C23-O8-C6 |
| 23 | 5 | 617 | LHG | C24-C23-O8-C6 |
| 23 | 6 | 619 | LHG | C3-O3-P-O5 |
| 23 | 8 | 617 | LHG | C2-C3-O3-P |
| 23 | 8 | 617 | LHG | C4-O6-P-O3 |
| 23 | 8 | 617 | LHG | C4-O6-P-O4 |
| 23 | 8 | 617 | LHG | C5-C4-O6-P |
| 23 | 8 | 617 | LHG | O10-C23-O8-C6 |
| 23 | 8 | 617 | LHG | C24-C23-O8-C6 |
| 23 | 9 | 618 | LHG | C3-O3-P-O5 |
| 23 | 9 | 618 | LHG | O10-C23-O8-C6 |
| 23 | 9 | 618 | LHG | C24-C23-O8-C6 |
| 23 | a | 617 | LHG | C3-O3-P-O5 |
| 23 | a | 617 | LHG | O10-C23-O8-C6 |
| 23 | a | 617 | LHG | C24-C23-O8-C6 |
| 23 | b | 319 | LHG | C4-O6-P-O3 |
| 23 | b | 319 | LHG | C4-O6-P-O5 |
| 23 | b | 319 | LHG | O10-C23-O8-C6 |
| 23 | b | 319 | LHG | C24-C23-O8-C6 |
| 23 | c | 619 | LHG | O10-C23-O8-C6 |
| 23 | c | 619 | LHG | C24-C23-O8-C6 |
| 24 | B | 843 | BCR | C7-C8-C9-C34 |
| 24 | B | 843 | BCR | C11-C12-C13-C14 |
| 24 | B | 844 | BCR | C11-C12-C13-C14 |
| 24 | B | 846 | BCR | C7-C8-C9-C10 |
| 24 | B | 846 | BCR | C7-C8-C9-C34 |
| 24 | J | 103 | BCR | C9-C10-C11-C12 |
| 24 | J | 104 | BCR | C11-C12-C13-C14 |
| 24 | J | 104 | BCR | C11-C12-C13-C35 |
| 24 | J | 104 | BCR | C23-C24-C25-C26 |
| 24 | J | 104 | BCR | C23-C24-C25-C30 |
| 24 | M | 101 | BCR | C1-C6-C7-C8 |
| 24 | M | 101 | BCR | C5-C6-C7-C8 |
| 24 | 6 | 618 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | 8 | 616 | BCR | C20-C21-C22-C37 |
| 24 | 8 | 616 | BCR | C23-C24-C25-C26 |
| 24 | 8 | 616 | BCR | C23-C24-C25-C30 |
| 27 | B | 847 | DGD | O6D-C1D-O3G-C3G |
| 28 | J | 105 | LMG | C2-C1-O1-C7 |
| 28 | J | 105 | LMG | O6-C1-O1-C7 |
| 28 | J | 105 | LMG | O10-C28-O8-C9 |
| 28 | J | 105 | LMG | C29-C28-O8-C9 |
| 29 | 2 | 602 | CHL | C1A-C2A-CAA-CBA |
| 29 | 2 | 602 | CHL | C3A-C2A-CAA-CBA |
| 29 | 4 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 5 | 601 | CHL | C1C-C2C-CMC-OMC |
| 29 | 5 | 601 | CHL | C3C-C2C-CMC-OMC |
| 29 | 6 | 605 | CHL | CHA-CBD-CGD-O1D |
| 29 | 6 | 605 | CHL | CHA-CBD-CGD-O2D |
| 29 | 6 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 9 | 601 | CHL | CBD-CGD-O2D-CED |
| 29 | 9 | 606 | CHL | C1A-C2A-CAA-CBA |
| 29 | 9 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | a | 608 | CHL | CBD-CGD-O2D-CED |
| 29 | c | 608 | CHL | C3A-C2A-CAA-CBA |
| 29 | c | 609 | CHL | C1C-C2C-CMC-OMC |
| 29 | c | 609 | CHL | C3C-C2C-CMC-OMC |
| 30 | 7 | 415 | LUT | C9-C10-C11-C12 |
| 30 | 7 | 415 | LUT | C21-C26-C27-C28 |
| 30 | 7 | 415 | LUT | C25-C26-C27-C28 |
| 30 | a | 615 | LUT | C25-C26-C27-C28 |
| 30 | a | 615 | LUT | C26-C27-C28-C29 |
| 31 | 5 | 616 | XAT | O4-C6-C7-C8 |
| 31 | 6 | 617 | XAT | C5-C6-C7-C8 |
| 31 | 6 | 617 | XAT | O4-C6-C7-C8 |
| 31 | 9 | 616 | XAT | C25-C26-C27-C28 |
| 31 | c | 617 | XAT | O24-C26-C27-C28 |
| 21 | 2 | 609 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 801 | CLA | O1D-CGD-O2D-CED |
| 21 | 1 | 306 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 409 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 603 | CLA | O1D-CGD-O2D-CED |
| 21 | 8 | 611 | CLA | O1D-CGD-O2D-CED |
| 21 | b | 313 | CLA | O1D-CGD-O2D-CED |
| 21 | c | 610 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 807 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | G | 203 | CLA | O1D-CGD-O2D-CED |
| 21 | 2 | 603 | CLA | O1D-CGD-O2D-CED |
| 21 | 4 | 609 | CLA | O1D-CGD-O2D-CED |
| 21 | 5 | 608 | CLA | O1D-CGD-O2D-CED |
| 21 | 7 | 408 | CLA | O1D-CGD-O2D-CED |
| 21 | 8 | 604 | CLA | O1D-CGD-O2D-CED |
| 21 | 8 | 612 | CLA | O1D-CGD-O2D-CED |
| 29 | 8 | 607 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 811 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 819 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 834 | CLA | CBD-CGD-O2D-CED |
| 21 | F | 302 | CLA | CBD-CGD-O2D-CED |
| 21 | 1 | 313 | CLA | CBD-CGD-O2D-CED |
| 21 | 3 | 403 | CLA | CBD-CGD-O2D-CED |
| 21 | 4 | 604 | CLA | CBD-CGD-O2D-CED |
| 21 | 5 | 605 | CLA | CBD-CGD-O2D-CED |
| 21 | 5 | 611 | CLA | CBD-CGD-O2D-CED |
| 21 | 5 | 614 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 608 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 611 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | 7 | 408 | CLA | CBD-CGD-O2D-CED |
| 21 | 7 | 410 | CLA | CBD-CGD-O2D-CED |
| 21 | 8 | 604 | CLA | CBD-CGD-O2D-CED |
| 21 | 9 | 602 | CLA | CBD-CGD-O2D-CED |
| 21 | 9 | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | 9 | 613 | CLA | CBD-CGD-O2D-CED |
| 21 | a | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | b | 313 | CLA | CBD-CGD-O2D-CED |
| 21 | c | 613 | CLA | CBD-CGD-O2D-CED |
| 29 | 2 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 8 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 9 | 608 | CHL | CBD-CGD-O2D-CED |
| 29 | b | 309 | CHL | CBD-CGD-O2D-CED |
| 21 | B | 823 | CLA | C4C-C3C-CAC-CBC |
| 21 | 4 | 604 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 609 | CLA | O1D-CGD-O2D-CED |
| 21 | 5 | 605 | CLA | O1D-CGD-O2D-CED |
| 21 | 5 | 614 | CLA | O1D-CGD-O2D-CED |
| 21 | 7 | 410 | CLA | O1D-CGD-O2D-CED |
| 21 | 9 | 613 | CLA | O1D-CGD-O2D-CED |
| 21 | a | 612 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | 8 | 613 | CHL | CBD-CGD-O2D-CED |
| 21 | A | 806 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 821 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 814 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 816 | CLA | O1A-CGA-O2A-C1 |
| 21 | 3 | 403 | CLA | O1A-CGA-O2A-C1 |
| 21 | 3 | 408 | CLA | O1A-CGA-O2A-C1 |
| 21 | 4 | 609 | CLA | O1A-CGA-O2A-C1 |
| 21 | 5 | 604 | CLA | O1A-CGA-O2A-C1 |
| 21 | a | 611 | CLA | O1A-CGA-O2A-C1 |
| 21 | c | 611 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 802 | CLA | O1D-CGD-O2D-CED |
| 21 | 1 | 316 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 411 | CLA | O1D-CGD-O2D-CED |
| 21 | 5 | 612 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 611 | CLA | O1D-CGD-O2D-CED |
| 21 | a | 602 | CLA | O1D-CGD-O2D-CED |
| 21 | b | 314 | CLA | O1D-CGD-O2D-CED |
| 21 | c | 613 | CLA | O1D-CGD-O2D-CED |
| 29 | 4 | 607 | CHL | O1D-CGD-O2D-CED |
| 21 | 1 | 312 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 613 | CLA | O1D-CGD-O2D-CED |
| 29 | 6 | 607 | CHL | O1D-CGD-O2D-CED |
| 29 | 9 | 601 | CHL | O1D-CGD-O2D-CED |
| 21 | a | 611 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 817 | CLA | C3-C5-C6-C7 |
| 21 | A | 828 | CLA | C3-C5-C6-C7 |
| 21 | B | 808 | CLA | C3-C5-C6-C7 |
| 21 | 5 | 602 | CLA | C3-C5-C6-C7 |
| 21 | 8 | 602 | CLA | C3-C5-C6-C7 |
| 21 | 8 | 611 | CLA | C3-C5-C6-C7 |
| 21 | b | 303 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 828 | CLA | CBA-CGA-O2A-C1 |
| 21 | 3 | 408 | CLA | CBA-CGA-O2A-C1 |
| 21 | 5 | 604 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 816 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 821 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 803 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 812 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 818 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 839 | CLA | CBD-CGD-O2D-CED |
| 21 | 1 | 315 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 2 | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | 8 | 609 | CLA | CBD-CGD-O2D-CED |
| 21 | a | 613 | CLA | CBD-CGD-O2D-CED |
| 21 | c | 612 | CLA | CBD-CGD-O2D-CED |
| 21 | c | 614 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 823 | CLA | C2C-C3C-CAC-CBC |
| 21 | 8 | 618 | CLA | O1D-CGD-O2D-CED |
| 29 | a | 608 | CHL | O1D-CGD-O2D-CED |
| 21 | G | 202 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 408 | CLA | C4-C3-C5-C6 |
| 21 | 9 | 611 | CLA | C4-C3-C5-C6 |
| 29 | b | 308 | CHL | C4-C3-C5-C6 |
| 21 | A | 852 | CLA | C2-C3-C5-C6 |
| 21 | 3 | 408 | CLA | C2-C3-C5-C6 |
| 21 | 9 | 611 | CLA | C2-C3-C5-C6 |
| 29 | b | 308 | CHL | C2-C3-C5-C6 |
| 21 | 5 | 611 | CLA | O1D-CGD-O2D-CED |
| 29 | b | 309 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 822 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 827 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 842 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 852 | CLA | C3-C5-C6-C7 |
| 21 | B | 818 | CLA | C2A-CAA-CBA-CGA |
| 21 | 1 | 316 | CLA | C2A-CAA-CBA-CGA |
| 21 | 2 | 609 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 609 | CLA | C3-C5-C6-C7 |
| 21 | 5 | 611 | CLA | C2A-CAA-CBA-CGA |
| 21 | 8 | 610 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 842 | CLA | C3-C5-C6-C7 |
| 21 | B | 809 | CLA | C3-C5-C6-C7 |
| 21 | B | 814 | CLA | C3-C5-C6-C7 |
| 21 | O | 203 | CLA | C3-C5-C6-C7 |
| 28 | 6 | 615 | LMG | O6-C1-O1-C7 |
| 29 | 2 | 607 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 806 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 821 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 842 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 803 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 814 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 816 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 836 | CLA | CBA-CGA-O2A-C1 |
| 21 | 1 | 303 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 3 | 403 | CLA | CBA-CGA-O2A-C1 |
| 21 | 4 | 609 | CLA | CBA-CGA-O2A-C1 |
| 21 | a | 611 | CLA | CBA-CGA-O2A-C1 |
| 21 | c | 611 | CLA | CBA-CGA-O2A-C1 |
| 24 | J | 101 | BCR | C19-C20-C21-C22 |
| 30 | 5 | 615 | LUT | C9-C10-C11-C12 |
| 21 | A | 828 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 842 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 803 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 817 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 826 | CLA | O1A-CGA-O2A-C1 |
| 26 | b | 301 | LMU | O5B-C5B-C6B-O6B |
| 21 | B | 819 | CLA | O1D-CGD-O2D-CED |
| 21 | 1 | 313 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 403 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 801 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 602 | CLA | C3-C5-C6-C7 |
| 21 | A | 831 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 833 | CLA | CBD-CGD-O2D-CED |
| 21 | J | 102 | CLA | CBD-CGD-O2D-CED |
| 29 | 9 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 9 | 609 | CHL | CBD-CGD-O2D-CED |
| 29 | c | 608 | CHL | CBD-CGD-O2D-CED |
| 28 | 6 | 615 | LMG | C2-C1-O1-C7 |
| 21 | A | 811 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 608 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 612 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 838 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 817 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 826 | CLA | CBA-CGA-O2A-C1 |
| 29 | 1 | 307 | CHL | CBA-CGA-O2A-C1 |
| 21 | A | 814 | CLA | CBD-CGD-O2D-CED |
| 29 | 6 | 605 | CHL | CBD-CGD-O2D-CED |
| 29 | a | 609 | CHL | CBD-CGD-O2D-CED |
| 21 | B | 820 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 838 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 806 | CLA | C3-C5-C6-C7 |
| 21 | B | 830 | CLA | C3-C5-C6-C7 |
| 21 | A | 824 | CLA | CBD-CGD-O2D-CED |
| 21 | b | 311 | CLA | CBD-CGD-O2D-CED |
| 21 | b | 315 | CLA | CBD-CGD-O2D-CED |
| 29 | 8 | 605 | CHL | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | F | 302 | CLA | O1D-CGD-O2D-CED |
| 21 | 9 | 612 | CLA | O1D-CGD-O2D-CED |
| 29 | 9 | 608 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 817 | CLA | C4-C3-C5-C6 |
| 21 | B | 830 | CLA | C4-C3-C5-C6 |
| 21 | 3 | 409 | CLA | C4-C3-C5-C6 |
| 21 | A | 817 | CLA | C2-C3-C5-C6 |
| 21 | B | 830 | CLA | C2-C3-C5-C6 |
| 21 | B | 836 | CLA | O1A-CGA-O2A-C1 |
| 21 | 1 | 303 | CLA | O1A-CGA-O2A-C1 |
| 29 | 1 | 307 | CHL | O1A-CGA-O2A-C1 |
| 21 | A | 817 | CLA | CBD-CGD-O2D-CED |
| 29 | 2 | 605 | CHL | C2A-CAA-CBA-CGA |
| 29 | 4 | 606 | CHL | C2A-CAA-CBA-CGA |
| 21 | 9 | 602 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 819 | CLA | CBA-CGA-O2A-C1 |
| 21 | a | 604 | CLA | CBA-CGA-O2A-C1 |
| 29 | 2 | 607 | CHL | CBA-CGA-O2A-C1 |
| 21 | A | 806 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 834 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 841 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 852 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 817 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 822 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 826 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 828 | CLA | CBD-CGD-O2D-CED |
| 21 | 2 | 604 | CLA | CBD-CGD-O2D-CED |
| 21 | 3 | 402 | CLA | CBD-CGD-O2D-CED |
| 21 | 5 | 602 | CLA | CBD-CGD-O2D-CED |
| 21 | 6 | 604 | CLA | CBD-CGD-O2D-CED |
| 29 | 4 | 614 | CHL | CBD-CGD-O2D-CED |
| 29 | 6 | 614 | CHL | CBD-CGD-O2D-CED |
| 29 | 2 | 607 | CHL | O1A-CGA-O2A-C1 |
| 21 | a | 611 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 819 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 828 | CLA | CBD-CGD-O2D-CED |
| 21 | K | 203 | CLA | CBD-CGD-O2D-CED |
| 29 | c | 606 | CHL | CBD-CGD-O2D-CED |
| 24 | J | 104 | BCR | C9-C10-C11-C12 |
| 21 | a | 604 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 834 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 812 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 817 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 823 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 841 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 807 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 825 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 830 | CLA | CBA-CGA-O2A-C1 |
| 21 | G | 203 | CLA | CBA-CGA-O2A-C1 |
| 21 | 4 | 602 | CLA | CBA-CGA-O2A-C1 |
| 29 | 2 | 602 | CHL | CBA-CGA-O2A-C1 |
| 29 | 6 | 602 | CHL | CBA-CGA-O2A-C1 |
| 29 | b | 308 | CHL | CBA-CGA-O2A-C1 |
| 21 | A | 840 | CLA | CBD-CGD-O2D-CED |
| 21 | b | 304 | CLA | CBD-CGD-O2D-CED |
| 26 | b | 301 | LMU | C4B-C5B-C6B-O6B |
| 21 | A | 816 | CLA | O1D-CGD-O2D-CED |
| 29 | 8 | 613 | CHL | O1D-CGD-O2D-CED |
| 21 | 4 | 609 | CLA | C4-C3-C5-C6 |
| 21 | 3 | 409 | CLA | C2-C3-C5-C6 |
| 21 | 4 | 609 | CLA | C2-C3-C5-C6 |
| 21 | A | 806 | CLA | C11-C10-C8-C9 |
| 21 | A | 809 | CLA | C6-C7-C8-C9 |
| 21 | A | 825 | CLA | C11-C12-C13-C14 |
| 21 | A | 825 | CLA | C14-C13-C15-C16 |
| 21 | A | 826 | CLA | C6-C7-C8-C9 |
| 21 | A | 840 | CLA | C11-C12-C13-C14 |
| 21 | B | 802 | CLA | C14-C13-C15-C16 |
| 21 | B | 804 | CLA | C6-C7-C8-C9 |
| 21 | B | 805 | CLA | C6-C7-C8-C9 |
| 21 | B | 812 | CLA | C11-C12-C13-C14 |
| 21 | B | 836 | CLA | C14-C13-C15-C16 |
| 21 | B | 838 | CLA | C6-C7-C8-C9 |
| 21 | 1 | 303 | CLA | C6-C7-C8-C9 |
| 21 | a | 613 | CLA | O1D-CGD-O2D-CED |
| 21 | c | 612 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 821 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 839 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 827 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 823 | CLA | O1A-CGA-O2A-C1 |
| 29 | b | 302 | CHL | CBD-CGD-O2D-CED |
| 24 | A | 849 | BCR | C37-C22-C23-C24 |
| 24 | B | 843 | BCR | C11-C12-C13-C35 |
| 24 | B | 843 | BCR | C36-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 844 | BCR | C11-C12-C13-C35 |
| 24 | I | 101 | BCR | C7-C8-C9-C34 |
| 24 | J | 104 | BCR | C37-C22-C23-C24 |
| 24 | K | 205 | BCR | C37-C22-C23-C24 |
| 24 | L | 306 | BCR | C37-C22-C23-C24 |
| 24 | O | 205 | BCR | C7-C8-C9-C34 |
| 24 | O | 205 | BCR | C37-C22-C23-C24 |
| 24 | 3 | 419 | BCR | C37-C22-C23-C24 |
| 24 | 7 | 418 | BCR | C37-C22-C23-C24 |
| 30 | 2 | 616 | LUT | C7-C8-C9-C19 |
| 30 | 7 | 415 | LUT | C27-C28-C29-C39 |
| 30 | a | 615 | LUT | C27-C28-C29-C39 |
| 30 | a | 616 | LUT | C7-C8-C9-C19 |
| 31 | 6 | 617 | XAT | C11-C12-C13-C20 |
| 31 | 9 | 616 | XAT | C7-C8-C9-C19 |
| 24 | B | 843 | BCR | C7-C8-C9-C10 |
| 24 | B | 844 | BCR | C7-C8-C9-C10 |
| 24 | I | 101 | BCR | C7-C8-C9-C10 |
| 24 | J | 104 | BCR | C21-C22-C23-C24 |
| 24 | K | 205 | BCR | C21-C22-C23-C24 |
| 24 | L | 306 | BCR | C21-C22-C23-C24 |
| 24 | M | 101 | BCR | C7-C8-C9-C10 |
| 24 | O | 205 | BCR | C7-C8-C9-C10 |
| 24 | O | 205 | BCR | C21-C22-C23-C24 |
| 24 | 3 | 419 | BCR | C21-C22-C23-C24 |
| 24 | 7 | 418 | BCR | C21-C22-C23-C24 |
| 30 | 2 | 616 | LUT | C7-C8-C9-C10 |
| 30 | 7 | 415 | LUT | C27-C28-C29-C30 |
| 30 | a | 616 | LUT | C7-C8-C9-C10 |
| 31 | 9 | 616 | XAT | C7-C8-C9-C10 |
| 21 | A | 809 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 818 | CLA | C3-C5-C6-C7 |
| 21 | K | 204 | CLA | C2A-CAA-CBA-CGA |
| 21 | 3 | 409 | CLA | C3-C5-C6-C7 |
| 29 | 4 | 607 | CHL | C2A-CAA-CBA-CGA |
| 29 | 6 | 605 | CHL | C2A-CAA-CBA-CGA |
| 29 | b | 308 | CHL | C3-C5-C6-C7 |
| 21 | A | 817 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 825 | CLA | O1A-CGA-O2A-C1 |
| 29 | b | 306 | CHL | CBD-CGD-O2D-CED |
| 23 | A | 844 | LHG | O7-C5-C6-O8 |
| 21 | B | 803 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 806 | CLA | C2-C1-O2A-CGA |
| 21 | B | 803 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 812 | CLA | O1D-CGD-O2D-CED |
| 21 | 8 | 609 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 807 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 819 | CLA | C12-C13-C15-C16 |
| 21 | 8 | 611 | CLA | C4-C3-C5-C6 |
| 23 | 9 | 618 | LHG | C7-C8-C9-C10 |
| 24 | B | 843 | BCR | C13-C14-C15-C16 |
| 29 | c | 601 | CHL | O2A-C1-C2-C3 |
| 21 | B | 818 | CLA | O1D-CGD-O2D-CED |
| 21 | c | 614 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 805 | CLA | C3-C5-C6-C7 |
| 21 | A | 834 | CLA | C5-C6-C7-C8 |
| 21 | B | 807 | CLA | C5-C6-C7-C8 |
| 21 | B | 812 | CLA | C10-C11-C12-C13 |
| 21 | A | 819 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 841 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 830 | CLA | O1A-CGA-O2A-C1 |
| 29 | 2 | 602 | CHL | O1A-CGA-O2A-C1 |
| 29 | 6 | 602 | CHL | O1A-CGA-O2A-C1 |
| 29 | b | 308 | CHL | O1A-CGA-O2A-C1 |
| 29 | 4 | 605 | CHL | CBD-CGD-O2D-CED |
| 21 | A | 814 | CLA | C5-C6-C7-C8 |
| 21 | B | 823 | CLA | C8-C10-C11-C12 |
| 21 | B | 823 | CLA | C15-C16-C17-C18 |
| 21 | 4 | 612 | CLA | C5-C6-C7-C8 |
| 21 | A | 824 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 832 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 803 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 827 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 838 | CLA | C2A-CAA-CBA-CGA |
| 21 | G | 203 | CLA | C2A-CAA-CBA-CGA |
| 21 | L | 302 | CLA | C2A-CAA-CBA-CGA |
| 21 | 7 | 401 | CLA | C2A-CAA-CBA-CGA |
| 21 | 7 | 402 | CLA | C2A-CAA-CBA-CGA |
| 21 | 7 | 407 | CLA | C2A-CAA-CBA-CGA |
| 21 | c | 604 | CLA | C2A-CAA-CBA-CGA |
| 21 | c | 611 | CLA | C2A-CAA-CBA-CGA |
| 29 | 5 | 601 | CHL | C2A-CAA-CBA-CGA |
| 29 | 6 | 601 | CHL | C2A-CAA-CBA-CGA |
| 29 | 6 | 606 | CHL | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | 6 | 614 | CHL | C2A-CAA-CBA-CGA |
| 29 | 8 | 607 | CHL | C2A-CAA-CBA-CGA |
| 29 | 9 | 606 | CHL | C2A-CAA-CBA-CGA |
| 29 | 9 | 608 | CHL | C2A-CAA-CBA-CGA |
| 29 | c | 607 | CHL | C2A-CAA-CBA-CGA |
| 29 | c | 608 | CHL | C2A-CAA-CBA-CGA |
| 21 | 1 | 315 | CLA | O1D-CGD-O2D-CED |
| 21 | 2 | 612 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 806 | CLA | C5-C6-C7-C8 |
| 21 | B | 809 | CLA | C5-C6-C7-C8 |
| 21 | B | 836 | CLA | C13-C15-C16-C17 |
| 21 | c | 613 | CLA | C13-C15-C16-C17 |
| 23 | 4 | 618 | LHG | C23-C24-C25-C26 |
| 21 | A | 812 | CLA | O1A-CGA-O2A-C1 |
| 21 | G | 203 | CLA | O1A-CGA-O2A-C1 |
| 21 | 4 | 602 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 807 | CLA | C8-C10-C11-C12 |
| 21 | A | 819 | CLA | C8-C10-C11-C12 |
| 21 | A | 825 | CLA | C10-C11-C12-C13 |
| 21 | A | 825 | CLA | C13-C15-C16-C17 |
| 21 | B | 806 | CLA | C8-C10-C11-C12 |
| 21 | B | 809 | CLA | C10-C11-C12-C13 |
| 21 | B | 812 | CLA | C5-C6-C7-C8 |
| 21 | B | 817 | CLA | C13-C15-C16-C17 |
| 21 | B | 825 | CLA | C13-C15-C16-C17 |
| 21 | A | 807 | CLA | CBA-CGA-O2A-C1 |
| 21 | 9 | 611 | CLA | C8-C10-C11-C12 |
| 23 | 4 | 619 | LHG | C23-C24-C25-C26 |
| 21 | B | 817 | CLA | C15-C16-C17-C18 |
| 21 | B | 809 | CLA | C8-C10-C11-C12 |
| 21 | F | 305 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 827 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 833 | CLA | O1D-CGD-O2D-CED |
| 21 | J | 102 | CLA | O1D-CGD-O2D-CED |
| 29 | 9 | 609 | CHL | O1D-CGD-O2D-CED |
| 29 | c | 608 | CHL | O1D-CGD-O2D-CED |
| 21 | B | 820 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 829 | CLA | C5-C6-C7-C8 |
| 21 | A | 841 | CLA | C10-C11-C12-C13 |
| 21 | A | 841 | CLA | C13-C15-C16-C17 |
| 21 | 1 | 305 | CLA | CBA-CGA-O2A-C1 |
| 21 | 3 | 409 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | 2 | 601 | CHL | CBA-CGA-O2A-C1 |
| 21 | B | 807 | CLA | C3-C5-C6-C7 |
| 21 | 9 | 611 | CLA | C3-C5-C6-C7 |
| 21 | A | 840 | CLA | C8-C10-C11-C12 |
| 21 | 4 | 609 | CLA | C2A-CAA-CBA-CGA |
| 21 | 9 | 604 | CLA | C2A-CAA-CBA-CGA |
| 29 | a | 605 | CHL | C2A-CAA-CBA-CGA |
| 29 | b | 302 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 831 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 817 | CLA | C10-C11-C12-C13 |
| 21 | B | 807 | CLA | C10-C11-C12-C13 |
| 21 | B | 835 | CLA | C10-C11-C12-C13 |
| 21 | B | 840 | CLA | C15-C16-C17-C18 |
| 21 | 5 | 602 | CLA | C5-C6-C7-C8 |
| 21 | B | 805 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 807 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 814 | CLA | O1D-CGD-O2D-CED |
| 29 | 9 | 607 | CHL | O1D-CGD-O2D-CED |
| 21 | B | 801 | CLA | C5-C6-C7-C8 |
| 21 | B | 804 | CLA | C15-C16-C17-C18 |
| 21 | 8 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 836 | CLA | C4-C3-C5-C6 |
| 29 | 6 | 605 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 814 | CLA | C15-C16-C17-C18 |
| 21 | A | 819 | CLA | C13-C15-C16-C17 |
| 21 | B | 817 | CLA | C5-C6-C7-C8 |
| 21 | A | 804 | CLA | C3-C5-C6-C7 |
| 21 | 3 | 408 | CLA | C3-C5-C6-C7 |
| 27 | B | 847 | DGD | C2B-C1B-O2G-C2G |
| 21 | B | 831 | CLA | C2C-C3C-CAC-CBC |
| 29 | b | 309 | CHL | O2A-C1-C2-C3 |
| 21 | 8 | 611 | CLA | C5-C6-C7-C8 |
| 21 | b | 311 | CLA | O1D-CGD-O2D-CED |
| 29 | a | 609 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 817 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 807 | CLA | C15-C16-C17-C18 |
| 21 | B | 836 | CLA | C5-C6-C7-C8 |
| 23 | 1 | 301 | LHG | C2-C3-O3-P |
| 23 | 2 | 619 | LHG | C2-C3-O3-P |
| 23 | 4 | 618 | LHG | C5-C4-O6-P |
| 24 | B | 844 | BCR | C7-C8-C9-C34 |
| 24 | B | 844 | BCR | C36-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | J | 101 | BCR | C36-C18-C19-C20 |
| 24 | M | 101 | BCR | C7-C8-C9-C34 |
| 24 | M | 101 | BCR | C37-C22-C23-C24 |
| 24 | 3 | 419 | BCR | C7-C8-C9-C34 |
| 24 | 7 | 418 | BCR | C7-C8-C9-C34 |
| 30 | 5 | 615 | LUT | C11-C12-C13-C20 |
| 30 | 6 | 616 | LUT | C7-C8-C9-C19 |
| 31 | 9 | 616 | XAT | C27-C28-C29-C39 |
| 24 | A | 849 | BCR | C21-C22-C23-C24 |
| 24 | J | 101 | BCR | C17-C18-C19-C20 |
| 24 | M | 101 | BCR | C21-C22-C23-C24 |
| 24 | 3 | 419 | BCR | C7-C8-C9-C10 |
| 24 | 7 | 418 | BCR | C7-C8-C9-C10 |
| 30 | 5 | 615 | LUT | C11-C12-C13-C14 |
| 30 | 6 | 616 | LUT | C7-C8-C9-C10 |
| 31 | 9 | 616 | XAT | C27-C28-C29-C30 |
| 21 | A | 828 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 813 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 837 | CLA | C2A-CAA-CBA-CGA |
| 29 | a | 608 | CHL | C2A-CAA-CBA-CGA |
| 29 | c | 605 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 829 | CLA | C13-C15-C16-C17 |
| 21 | A | 829 | CLA | C15-C16-C17-C18 |
| 21 | B | 825 | CLA | C5-C6-C7-C8 |
| 21 | B | 831 | CLA | C5-C6-C7-C8 |
| 21 | B | 808 | CLA | C16-C17-C18-C19 |
| 21 | B | 808 | CLA | C16-C17-C18-C20 |
| 21 | 2 | 608 | CLA | C6-C7-C8-C9 |
| 21 | a | 602 | CLA | C11-C12-C13-C15 |
| 21 | c | 603 | CLA | C6-C7-C8-C10 |
| 21 | A | 824 | CLA | O1D-CGD-O2D-CED |
| 29 | 8 | 605 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 807 | CLA | O1A-CGA-O2A-C1 |
| 29 | 2 | 601 | CHL | O1A-CGA-O2A-C1 |
| 21 | A | 831 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 612 | CLA | C3-C5-C6-C7 |
| 21 | B | 808 | CLA | C13-C15-C16-C17 |
| 24 | 8 | 616 | BCR | C20-C21-C22-C23 |
| 21 | b | 315 | CLA | O1D-CGD-O2D-CED |
| 23 | a | 617 | LHG | O7-C5-C6-O8 |
| 21 | A | 806 | CLA | O1D-CGD-O2D-CED |
| 21 | 5 | 602 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 801 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 815 | CLA | CBD-CGD-O2D-CED |
| 29 | 5 | 606 | CHL | CBD-CGD-O2D-CED |
| 29 | c | 601 | CHL | CBD-CGD-O2D-CED |
| 23 | 8 | 617 | LHG | C23-C24-C25-C26 |
| 21 | A | 821 | CLA | C16-C17-C18-C20 |
| 21 | A | 824 | CLA | C6-C7-C8-C9 |
| 21 | A | 828 | CLA | C11-C12-C13-C15 |
| 21 | B | 817 | CLA | C16-C17-C18-C20 |
| 21 | c | 603 | CLA | C6-C7-C8-C9 |
| 21 | 1 | 305 | CLA | O1A-CGA-O2A-C1 |
| 21 | 3 | 409 | CLA | O1A-CGA-O2A-C1 |
| 21 | 3 | 402 | CLA | O1D-CGD-O2D-CED |
| 29 | 4 | 614 | CHL | O1D-CGD-O2D-CED |
| 29 | 9 | 605 | CHL | CBD-CGD-O2D-CED |
| 26 | A | 856 | LMU | C2-C3-C4-C5 |
| 29 | 6 | 614 | CHL | O1D-CGD-O2D-CED |
| 21 | B | 827 | CLA | CBA-CGA-O2A-C1 |
| 21 | 8 | 604 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 834 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 852 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 817 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 604 | CLA | O1D-CGD-O2D-CED |
| 21 | 1 | 313 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 403 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 607 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 411 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | b | 315 | CLA | C4B-C3B-CAB-CBB |
| 21 | c | 602 | CLA | C4B-C3B-CAB-CBB |
| 23 | a | 617 | LHG | C23-C24-C25-C26 |
| 21 | 2 | 608 | CLA | C6-C7-C8-C10 |
| 21 | 6 | 608 | CLA | C2A-CAA-CBA-CGA |
| 29 | 8 | 606 | CHL | C2A-CAA-CBA-CGA |
| 29 | b | 306 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 806 | CLA | C10-C11-C12-C13 |
| 21 | B | 802 | CLA | C11-C10-C8-C7 |
| 21 | B | 805 | CLA | C11-C10-C8-C7 |
| 21 | B | 812 | CLA | C11-C12-C13-C15 |
| 21 | c | 611 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | 2 | 619 | LHG | O2-C2-C3-O3 |
| 21 | c | 611 | CLA | C5-C6-C7-C8 |
| 26 | b | 301 | LMU | C3-C4-C5-C6 |
| 21 | A | 804 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 833 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 837 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 841 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 802 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 807 | CLA | C3A-C2A-CAA-CBA |
| 21 | 3 | 403 | CLA | C3A-C2A-CAA-CBA |
| 21 | 4 | 611 | CLA | C3A-C2A-CAA-CBA |
| 21 | 8 | 604 | CLA | C3A-C2A-CAA-CBA |
| 21 | 8 | 610 | CLA | C3A-C2A-CAA-CBA |
| 21 | 9 | 603 | CLA | C3A-C2A-CAA-CBA |
| 29 | 9 | 606 | CHL | C3A-C2A-CAA-CBA |
| 21 | B | 826 | CLA | O1D-CGD-O2D-CED |
| 21 | 2 | 604 | CLA | O1D-CGD-O2D-CED |
| 21 | 1 | 305 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 809 | CLA | C5-C6-C7-C8 |
| 21 | A | 841 | CLA | C15-C16-C17-C18 |
| 21 | a | 602 | CLA | C8-C10-C11-C12 |
| 24 | B | 844 | BCR | C19-C20-C21-C22 |
| 21 | A | 824 | CLA | C6-C7-C8-C10 |
| 21 | A | 828 | CLA | C11-C12-C13-C14 |
| 27 | B | 847 | DGD | CAA-CBA-CCA-CDA |
| 29 | 6 | 606 | CHL | CBD-CGD-O2D-CED |
| 23 | 2 | 619 | LHG | C4-C5-C6-O8 |
| 21 | A | 827 | CLA | C10-C11-C12-C13 |
| 21 | B | 823 | CLA | C10-C11-C12-C13 |
| 21 | b | 311 | CLA | C5-C6-C7-C8 |
| 21 | B | 828 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 817 | CLA | C16-C17-C18-C19 |
| 21 | 8 | 611 | CLA | C6-C7-C8-C10 |
| 21 | A | 802 | CLA | C2B-C3B-CAB-CBB |
| 21 | H | 201 | CLA | C2B-C3B-CAB-CBB |
| 21 | K | 204 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 313 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 403 | CLA | C2B-C3B-CAB-CBB |
| 21 | 4 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 605 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 607 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 603 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 7 | 401 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 402 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 410 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 411 | CLA | C2B-C3B-CAB-CBB |
| 21 | 8 | 610 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | b | 315 | CLA | C2B-C3B-CAB-CBB |
| 24 | A | 846 | BCR | C23-C24-C25-C26 |
| 24 | A | 846 | BCR | C23-C24-C25-C30 |
| 24 | B | 845 | BCR | C23-C24-C25-C30 |
| 24 | I | 101 | BCR | C1-C6-C7-C8 |
| 24 | I | 101 | BCR | C5-C6-C7-C8 |
| 24 | J | 101 | BCR | C1-C6-C7-C8 |
| 24 | J | 101 | BCR | C5-C6-C7-C8 |
| 24 | J | 103 | BCR | C1-C6-C7-C8 |
| 24 | J | 103 | BCR | C5-C6-C7-C8 |
| 24 | L | 306 | BCR | C23-C24-C25-C26 |
| 24 | L | 306 | BCR | C23-C24-C25-C30 |
| 24 | M | 101 | BCR | C23-C24-C25-C26 |
| 24 | M | 101 | BCR | C23-C24-C25-C30 |
| 24 | 2 | 618 | BCR | C23-C24-C25-C26 |
| 24 | 2 | 618 | BCR | C23-C24-C25-C30 |
| 24 | 6 | 618 | BCR | C1-C6-C7-C8 |
| 24 | 6 | 618 | BCR | C23-C24-C25-C26 |
| 24 | 6 | 618 | BCR | C23-C24-C25-C30 |
| 30 | 2 | 616 | LUT | C1-C6-C7-C8 |
| 30 | 2 | 616 | LUT | C5-C6-C7-C8 |
| 21 | c | 611 | CLA | C3-C5-C6-C7 |
| 21 | B | 822 | CLA | O1D-CGD-O2D-CED |
| 27 | B | 847 | DGD | C4A-C5A-C6A-C7A |
| 21 | A | 852 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 826 | CLA | C2A-CAA-CBA-CGA |
| 21 | 1 | 303 | CLA | C2A-CAA-CBA-CGA |
| 21 | 2 | 603 | CLA | C2A-CAA-CBA-CGA |
| 21 | 8 | 601 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 801 | CLA | O1A-CGA-O2A-C1 |
| 27 | B | 847 | DGD | O1B-C1B-O2G-C2G |
| 21 | B | 805 | CLA | C15-C16-C17-C18 |
| 21 | B | 836 | CLA | C2-C3-C5-C6 |
| 21 | 8 | 611 | CLA | C2-C3-C5-C6 |
| 28 | G | 206 | LMG | C10-C11-C12-C13 |
| 21 | A | 830 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 5 | 602 | CLA | CBA-CGA-O2A-C1 |
| 21 | 7 | 411 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 805 | CLA | C10-C11-C12-C13 |
| 27 | B | 847 | DGD | C9A-CAA-CBA-CCA |
| 28 | G | 206 | LMG | C2-C1-O1-C7 |
| 21 | c | 613 | CLA | C15-C16-C17-C18 |
| 21 | B | 827 | CLA | O1A-CGA-O2A-C1 |
| 26 | b | 301 | LMU | C7-C8-C9-C10 |
| 21 | 3 | 412 | CLA | C6-C7-C8-C9 |
| 21 | a | 602 | CLA | C11-C12-C13-C14 |
| 29 | 2 | 605 | CHL | CBD-CGD-O2D-CED |
| 21 | A | 841 | CLA | O1D-CGD-O2D-CED |
| 26 | A | 856 | LMU | O1'-C1-C2-C3 |
| 23 | A | 844 | LHG | C23-C24-C25-C26 |
| 21 | A | 807 | CLA | C3-C5-C6-C7 |
| 21 | A | 803 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 829 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 830 | CLA | C3-C5-C6-C7 |
| 21 | 6 | 612 | CLA | C2A-CAA-CBA-CGA |
| 29 | b | 309 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 840 | CLA | C16-C17-C18-C20 |
| 21 | 3 | 412 | CLA | C6-C7-C8-C10 |
| 21 | 8 | 611 | CLA | C6-C7-C8-C9 |
| 21 | L | 304 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 828 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 304 | CLA | CBD-CGD-O2D-CED |
| 21 | B | 803 | CLA | C3-C5-C6-C7 |
| 21 | B | 802 | CLA | C5-C6-C7-C8 |
| 21 | F | 302 | CLA | C5-C6-C7-C8 |
| 29 | c | 606 | CHL | O1D-CGD-O2D-CED |
| 28 | J | 105 | LMG | O6-C5-C6-O5 |
| 29 | 8 | 606 | CHL | CBD-CGD-O2D-CED |
| 26 | 3 | 420 | LMU | O1'-C1-C2-C3 |
| 21 | A | 827 | CLA | C8-C10-C11-C12 |
| 21 | B | 817 | CLA | C8-C10-C11-C12 |
| 21 | A | 828 | CLA | O1D-CGD-O2D-CED |
| 21 | K | 203 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 823 | CLA | C3-C5-C6-C7 |
| 23 | 4 | 619 | LHG | C9-C10-C11-C12 |
| 21 | A | 831 | CLA | C5-C6-C7-C8 |
| 21 | B | 825 | CLA | C2-C3-C5-C6 |
| 21 | A | 823 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 830 | CLA | C2A-CAA-CBA-CGA |
| 21 | 2 | 612 | CLA | C2A-CAA-CBA-CGA |
| 21 | 4 | 602 | CLA | C2A-CAA-CBA-CGA |
| 21 | 9 | 613 | CLA | C2A-CAA-CBA-CGA |
| 29 | 6 | 602 | CHL | C2A-CAA-CBA-CGA |
| 29 | b | 308 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 819 | CLA | O1D-CGD-O2D-CED |
| 28 | 6 | 615 | LMG | O6-C5-C6-O5 |
| 21 | B | 812 | CLA | C2C-C3C-CAC-CBC |
| 21 | b | 304 | CLA | O1D-CGD-O2D-CED |
| 29 | b | 306 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 840 | CLA | C13-C15-C16-C17 |
| 21 | 1 | 309 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 825 | CLA | C16-C17-C18-C20 |
| 21 | 4 | 612 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 840 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 830 | CLA | O1A-CGA-O2A-C1 |
| 21 | 8 | 611 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 805 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 811 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 818 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 826 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 828 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 830 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 833 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 835 | CLA | C1A-C2A-CAA-CBA |
| 21 | O | 203 | CLA | C1A-C2A-CAA-CBA |
| 21 | 1 | 303 | CLA | C1A-C2A-CAA-CBA |
| 21 | 1 | 310 | CLA | C1A-C2A-CAA-CBA |
| 21 | 3 | 403 | CLA | C1A-C2A-CAA-CBA |
| 21 | 4 | 602 | CLA | C1A-C2A-CAA-CBA |
| 21 | 4 | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 4 | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | 4 | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | 5 | 602 | CLA | C1A-C2A-CAA-CBA |
| 21 | 5 | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 6 | 608 | CLA | C1A-C2A-CAA-CBA |
| 21 | 7 | 407 | CLA | C1A-C2A-CAA-CBA |
| 21 | 8 | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | 9 | 602 | CLA | C1A-C2A-CAA-CBA |
| 21 | 9 | 603 | CLA | C1A-C2A-CAA-CBA |
| 21 | 9 | 604 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | a | 602 | CLA | C1A-C2A-CAA-CBA |
| 21 | a | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | b | 311 | CLA | C1A-C2A-CAA-CBA |
| 21 | c | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | c | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | c | 614 | CLA | C1A-C2A-CAA-CBA |
| 23 | 9 | 618 | LHG | C33-C34-C35-C36 |
| 21 | B | 802 | CLA | C13-C15-C16-C17 |
| 28 | 2 | 615 | LMG | O6-C5-C6-O5 |
| 21 | A | 825 | CLA | C12-C13-C15-C16 |
| 21 | A | 826 | CLA | C12-C13-C15-C16 |
| 21 | A | 827 | CLA | C11-C10-C8-C7 |
| 21 | B | 802 | CLA | C11-C12-C13-C15 |
| 21 | B | 805 | CLA | C12-C13-C15-C16 |
| 21 | B | 807 | CLA | C6-C7-C8-C10 |
| 21 | B | 808 | CLA | C11-C10-C8-C7 |
| 21 | B | 817 | CLA | C11-C10-C8-C7 |
| 21 | B | 827 | CLA | C11-C10-C8-C7 |
| 21 | B | 836 | CLA | C12-C13-C15-C16 |
| 21 | 1 | 303 | CLA | C11-C10-C8-C7 |
| 21 | 3 | 402 | CLA | C6-C7-C8-C10 |
| 21 | 5 | 602 | CLA | C11-C12-C13-C15 |
| 21 | c | 613 | CLA | C16-C17-C18-C20 |
| 21 | B | 805 | CLA | C5-C6-C7-C8 |
| 21 | O | 204 | CLA | C3A-C2A-CAA-CBA |
| 29 | 2 | 602 | CHL | CBD-CGD-O2D-CED |
| 21 | B | 812 | CLA | C8-C10-C11-C12 |
| 21 | B | 835 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 602 | CLA | O1A-CGA-O2A-C1 |
| 21 | 7 | 411 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 825 | CLA | C8-C10-C11-C12 |
| 21 | A | 818 | CLA | C2A-CAA-CBA-CGA |
| 21 | G | 202 | CLA | C2A-CAA-CBA-CGA |
| 21 | 1 | 313 | CLA | C2A-CAA-CBA-CGA |
| 21 | 3 | 412 | CLA | C2A-CAA-CBA-CGA |
| 21 | 8 | 609 | CLA | C2A-CAA-CBA-CGA |
| 21 | b | 305 | CLA | C2A-CAA-CBA-CGA |
| 21 | c | 602 | CLA | C2A-CAA-CBA-CGA |
| 29 | 2 | 602 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 819 | CLA | C11-C12-C13-C14 |
| 21 | A | 819 | CLA | C14-C13-C15-C16 |
| 21 | A | 826 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 829 | CLA | C14-C13-C15-C16 |
| 21 | B | 801 | CLA | C6-C7-C8-C9 |
| 21 | B | 805 | CLA | C14-C13-C15-C16 |
| 21 | B | 808 | CLA | C11-C10-C8-C9 |
| 21 | 1 | 303 | CLA | C11-C10-C8-C9 |
| 21 | 5 | 602 | CLA | C11-C12-C13-C14 |
| 21 | B | 831 | CLA | C11-C10-C8-C9 |
| 23 | A | 844 | LHG | C4-C5-C6-O8 |
| 23 | 1 | 301 | LHG | C4-C5-C6-O8 |
| 23 | 4 | 618 | LHG | C24-C25-C26-C27 |
| 29 | b | 302 | CHL | O1D-CGD-O2D-CED |
| 21 | O | 203 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 840 | CLA | C16-C17-C18-C19 |
| 29 | 2 | 602 | CHL | CHA-CBD-CGD-O1D |
| 29 | 2 | 602 | CHL | CHA-CBD-CGD-O2D |
| 29 | 2 | 607 | CHL | CHA-CBD-CGD-O2D |
| 29 | 8 | 607 | CHL | CHA-CBD-CGD-O1D |
| 29 | 8 | 607 | CHL | CHA-CBD-CGD-O2D |
| 29 | 9 | 605 | CHL | CHA-CBD-CGD-O1D |
| 29 | 9 | 605 | CHL | CHA-CBD-CGD-O2D |
| 29 | a | 609 | CHL | CHA-CBD-CGD-O1D |
| 30 | 5 | 615 | LUT | C11-C10-C9-C19 |
| 21 | 3 | 408 | CLA | C8-C10-C11-C12 |
| 21 | B | 821 | CLA | C3-C5-C6-C7 |
| 26 | O | 206 | LMU | O5'-C5'-C6'-O6' |
| 21 | B | 825 | CLA | C4-C3-C5-C6 |
| 21 | B | 835 | CLA | C4-C3-C5-C6 |
| 24 | B | 844 | BCR | C37-C22-C23-C24 |
| 21 | B | 811 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 816 | CLA | C2A-CAA-CBA-CGA |
| 21 | 5 | 602 | CLA | C2A-CAA-CBA-CGA |
| 29 | 2 | 614 | CHL | C2A-CAA-CBA-CGA |
| 29 | 6 | 602 | CHL | C3C-C2C-CMC-OMC |
| 29 | 9 | 607 | CHL | C3C-C2C-CMC-OMC |
| 21 | A | 817 | CLA | C2C-C3C-CAC-CBC |
| 21 | c | 613 | CLA | C16-C17-C18-C19 |
| 28 | G | 206 | LMG | C40-C41-C42-C43 |
| 29 | 4 | 605 | CHL | O1D-CGD-O2D-CED |
| 21 | 2 | 608 | CLA | C5-C6-C7-C8 |
| 21 | 5 | 605 | CLA | C2C-C3C-CAC-CBC |
| 21 | b | 311 | CLA | C4-C3-C5-C6 |
| 21 | a | 613 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 5 | 605 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 824 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 809 | CLA | C11-C12-C13-C14 |
| 29 | 6 | 602 | CHL | C1C-C2C-CMC-OMC |
| 21 | A | 821 | CLA | C13-C15-C16-C17 |
| 21 | 3 | 412 | CLA | C5-C6-C7-C8 |
| 21 | A | 803 | CLA | C4-C3-C5-C6 |
| 26 | O | 206 | LMU | C2-C1-O1'-C1' |
| 21 | A | 812 | CLA | C11-C12-C13-C14 |
| 21 | A | 827 | CLA | C11-C10-C8-C9 |
| 21 | A | 828 | CLA | C11-C10-C8-C9 |
| 21 | A | 833 | CLA | C11-C10-C8-C9 |
| 21 | B | 802 | CLA | C11-C12-C13-C14 |
| 21 | B | 806 | CLA | C6-C7-C8-C9 |
| 21 | B | 814 | CLA | C6-C7-C8-C9 |
| 21 | B | 817 | CLA | C6-C7-C8-C9 |
| 21 | 3 | 402 | CLA | C6-C7-C8-C9 |
| 21 | F | 305 | CLA | O1D-CGD-O2D-CED |
| 23 | 4 | 618 | LHG | C2-C3-O3-P |
| 21 | A | 837 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 840 | CLA | C4B-C3B-CAB-CBB |
| 21 | H | 201 | CLA | C4B-C3B-CAB-CBB |
| 21 | K | 204 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 305 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 604 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 605 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 410 | CLA | C4B-C3B-CAB-CBB |
| 21 | a | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | b | 313 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 806 | CLA | C11-C10-C8-C7 |
| 21 | A | 809 | CLA | C6-C7-C8-C10 |
| 21 | A | 812 | CLA | C11-C12-C13-C15 |
| 21 | A | 819 | CLA | C11-C12-C13-C15 |
| 21 | A | 825 | CLA | C11-C12-C13-C15 |
| 21 | A | 826 | CLA | C6-C7-C8-C10 |
| 21 | A | 829 | CLA | C12-C13-C15-C16 |
| 21 | A | 833 | CLA | C11-C10-C8-C7 |
| 21 | A | 842 | CLA | C6-C7-C8-C10 |
| 21 | B | 801 | CLA | C6-C7-C8-C10 |
| 21 | B | 814 | CLA | C6-C7-C8-C10 |
| 21 | B | 817 | CLA | C6-C7-C8-C10 |
| 21 | B | 824 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 830 | CLA | C6-C7-C8-C10 |
| 21 | 1 | 303 | CLA | C11-C12-C13-C15 |
| 21 | 4 | 602 | CLA | C11-C10-C8-C7 |
| 21 | c | 613 | CLA | C11-C12-C13-C15 |
| 21 | B | 801 | CLA | C8-C10-C11-C12 |
| 29 | 5 | 606 | CHL | O1D-CGD-O2D-CED |
| 23 | 9 | 618 | LHG | C23-C24-C25-C26 |
| 21 | A | 842 | CLA | C5-C6-C7-C8 |
| 21 | O | 203 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 842 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 811 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 832 | CLA | C3A-C2A-CAA-CBA |
| 21 | F | 302 | CLA | C4-C3-C5-C6 |
| 21 | L | 302 | CLA | C3A-C2A-CAA-CBA |
| 21 | L | 303 | CLA | C3A-C2A-CAA-CBA |
| 21 | 9 | 613 | CLA | C3A-C2A-CAA-CBA |
| 29 | 1 | 302 | CHL | C3A-C2A-CAA-CBA |
| 29 | 6 | 601 | CHL | C3A-C2A-CAA-CBA |
| 29 | b | 302 | CHL | C3A-C2A-CAA-CBA |
| 21 | A | 838 | CLA | C15-C16-C17-C18 |
| 29 | c | 601 | CHL | O1D-CGD-O2D-CED |
| 21 | 4 | 612 | CLA | C4C-C3C-CAC-CBC |
| 27 | B | 847 | DGD | C6B-C7B-C8B-C9B |
| 21 | B | 805 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 809 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 843 | BCR | C15-C16-C17-C18 |
| 24 | B | 844 | BCR | C9-C10-C11-C12 |
| 24 | J | 104 | BCR | C19-C20-C21-C22 |
| 29 | 9 | 605 | CHL | O1D-CGD-O2D-CED |
| 24 | B | 843 | BCR | C17-C18-C19-C20 |
| 31 | 6 | 617 | XAT | C11-C12-C13-C14 |
| 21 | a | 604 | CLA | O2A-C1-C2-C3 |
| 21 | a | 604 | CLA | C2A-CAA-CBA-CGA |
| 29 | 2 | 601 | CHL | C2A-CAA-CBA-CGA |
| 29 | 2 | 601 | CHL | C3-C5-C6-C7 |
| 21 | B | 807 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 837 | CLA | C13-C15-C16-C17 |
| 23 | 6 | 619 | LHG | C4-C5-C6-O8 |
| 21 | 3 | 412 | CLA | C3-C5-C6-C7 |
| 21 | b | 311 | CLA | C3-C5-C6-C7 |
| 29 | 4 | 607 | CHL | C1A-C2A-CAA-CBA |
| 21 | 3 | 412 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 824 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 803 | CLA | C2-C3-C5-C6 |
| 21 | F | 302 | CLA | C2-C3-C5-C6 |
| 21 | 3 | 412 | CLA | C2-C3-C5-C6 |
| 21 | 7 | 411 | CLA | C2-C3-C5-C6 |
| 21 | 2 | 609 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 815 | CLA | O1D-CGD-O2D-CED |
| 28 | G | 206 | LMG | C32-C33-C34-C35 |
| 21 | B | 814 | CLA | C11-C12-C13-C15 |
| 21 | B | 825 | CLA | C16-C17-C18-C19 |
| 21 | A | 837 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 604 | CLA | C2B-C3B-CAB-CBB |
| 21 | a | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | b | 313 | CLA | C2B-C3B-CAB-CBB |
| 24 | A | 846 | BCR | C1-C6-C7-C8 |
| 24 | B | 843 | BCR | C23-C24-C25-C30 |
| 24 | J | 101 | BCR | C23-C24-C25-C30 |
| 24 | 3 | 418 | BCR | C23-C24-C25-C30 |
| 24 | 3 | 419 | BCR | C1-C6-C7-C8 |
| 24 | 3 | 419 | BCR | C23-C24-C25-C30 |
| 24 | 4 | 617 | BCR | C23-C24-C25-C30 |
| 24 | 7 | 418 | BCR | C1-C6-C7-C8 |
| 30 | 3 | 416 | LUT | C1-C6-C7-C8 |
| 30 | 5 | 615 | LUT | C1-C6-C7-C8 |
| 21 | A | 803 | CLA | CBD-CGD-O2D-CED |
| 29 | 6 | 606 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 817 | CLA | C16-C17-C18-C19 |
| 21 | B | 812 | CLA | C16-C17-C18-C20 |
| 23 | 1 | 301 | LHG | O7-C5-C6-O8 |
| 23 | 9 | 618 | LHG | O7-C5-C6-O8 |
| 21 | A | 840 | CLA | C10-C11-C12-C13 |
| 21 | a | 602 | CLA | C10-C11-C12-C13 |
| 26 | A | 856 | LMU | C1-C2-C3-C4 |
| 21 | 7 | 411 | CLA | C4-C3-C5-C6 |
| 21 | A | 813 | CLA | C5-C6-C7-C8 |
| 21 | A | 821 | CLA | C16-C17-C18-C19 |
| 21 | B | 827 | CLA | C10-C11-C12-C13 |
| 21 | 1 | 305 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 829 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 836 | CLA | C3-C5-C6-C7 |
| 21 | A | 841 | CLA | C14-C13-C15-C16 |
| 21 | B | 801 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 806 | CLA | C11-C12-C13-C14 |
| 21 | B | 817 | CLA | C11-C12-C13-C14 |
| 21 | B | 838 | CLA | C11-C10-C8-C9 |
| 21 | 4 | 602 | CLA | C11-C10-C8-C9 |
| 21 | b | 303 | CLA | C6-C7-C8-C9 |
| 29 | 2 | 605 | CHL | O1D-CGD-O2D-CED |
| 21 | B | 812 | CLA | C16-C17-C18-C19 |
| 29 | 8 | 606 | CHL | O1D-CGD-O2D-CED |
| 21 | b | 303 | CLA | C11-C12-C13-C14 |
| 21 | L | 304 | CLA | C1A-C2A-CAA-CBA |
| 21 | 2 | 613 | CLA | C1A-C2A-CAA-CBA |
| 21 | 6 | 613 | CLA | C1A-C2A-CAA-CBA |
| 21 | 7 | 404 | CLA | C1A-C2A-CAA-CBA |
| 21 | L | 304 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 817 | CLA | C4C-C3C-CAC-CBC |
| 24 | K | 205 | BCR | C19-C20-C21-C22 |
| 21 | B | 825 | CLA | C16-C17-C18-C20 |
| 21 | 9 | 610 | CLA | C6-C7-C8-C9 |
| 27 | B | 847 | DGD | C7B-C8B-C9B-CAB |
| 30 | 7 | 415 | LUT | C11-C10-C9-C19 |
| 31 | 6 | 617 | XAT | C20-C13-C14-C15 |
| 31 | a | 618 | XAT | C11-C10-C9-C19 |
| 21 | 9 | 611 | CLA | CBA-CGA-O2A-C1 |
| 23 | 8 | 617 | LHG | O6-C4-C5-C6 |
| 29 | a | 601 | CHL | CBD-CGD-O2D-CED |
| 21 | B | 802 | CLA | C8-C10-C11-C12 |
| 24 | B | 843 | BCR | C37-C22-C23-C24 |
| 21 | A | 807 | CLA | C11-C12-C13-C15 |
| 21 | A | 841 | CLA | C12-C13-C15-C16 |
| 21 | B | 801 | CLA | C11-C10-C8-C7 |
| 21 | B | 817 | CLA | C11-C12-C13-C15 |
| 21 | B | 823 | CLA | C11-C12-C13-C15 |
| 21 | B | 827 | CLA | C6-C7-C8-C10 |
| 21 | B | 836 | CLA | C6-C7-C8-C10 |
| 21 | B | 837 | CLA | C6-C7-C8-C10 |
| 21 | B | 838 | CLA | C11-C10-C8-C7 |
| 21 | b | 303 | CLA | C6-C7-C8-C10 |
| 21 | A | 804 | CLA | C13-C15-C16-C17 |
| 24 | B | 843 | BCR | C21-C22-C23-C24 |
| 24 | B | 844 | BCR | C21-C22-C23-C24 |
| 21 | 3 | 412 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 824 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 1 | 309 | CLA | C4C-C3C-CAC-CBC |
| 21 | B | 806 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 832 | CLA | C2A-CAA-CBA-CGA |
| 29 | a | 609 | CHL | C2A-CAA-CBA-CGA |
| 21 | B | 815 | CLA | C6-C7-C8-C10 |
| 21 | 8 | 601 | CLA | CBD-CGD-O2D-CED |
| 21 | 1 | 304 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 824 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 809 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 806 | CLA | C8-C10-C11-C12 |
| 21 | A | 806 | CLA | O2A-C1-C2-C3 |
| 21 | A | 825 | CLA | C16-C17-C18-C19 |
| 21 | 8 | 602 | CLA | CBA-CGA-O2A-C1 |
| 30 | 5 | 615 | LUT | C11-C10-C9-C8 |
| 23 | a | 617 | LHG | C4-C5-C6-O8 |
| 21 | B | 831 | CLA | C4C-C3C-CAC-CBC |
| 28 | G | 206 | LMG | C11-C10-O7-C8 |
| 27 | B | 847 | DGD | C1A-C2A-C3A-C4A |
| 21 | A | 838 | CLA | C13-C15-C16-C17 |
| 21 | 7 | 403 | CLA | C2A-CAA-CBA-CGA |
| 23 | A | 844 | LHG | C13-C14-C15-C16 |
| 23 | 6 | 619 | LHG | O7-C5-C6-O8 |
| 21 | A | 821 | CLA | C8-C10-C11-C12 |
| 21 | B | 836 | CLA | C6-C7-C8-C9 |
| 21 | B | 837 | CLA | C6-C7-C8-C9 |
| 21 | c | 613 | CLA | C11-C12-C13-C14 |
| 23 | 9 | 618 | LHG | C29-C30-C31-C32 |
| 21 | A | 829 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 838 | CLA | C3-C5-C6-C7 |
| 21 | b | 314 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 825 | CLA | C10-C11-C12-C13 |
| 21 | B | 812 | CLA | C15-C16-C17-C18 |
| 21 | a | 602 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 804 | CLA | C16-C17-C18-C19 |
| 21 | B | 814 | CLA | C11-C12-C13-C14 |
| 21 | 9 | 611 | CLA | O1A-CGA-O2A-C1 |
| 21 | b | 311 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 817 | CLA | C16-C17-C18-C20 |
| 21 | B | 815 | CLA | C3-C5-C6-C7 |
| 21 | B | 812 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 820 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 823 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 824 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 824 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 833 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 842 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 801 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 802 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 807 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 809 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 826 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 831 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 833 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 835 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 838 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 839 | CLA | C4B-C3B-CAB-CBB |
| 21 | F | 302 | CLA | C4B-C3B-CAB-CBB |
| 21 | G | 203 | CLA | C4B-C3B-CAB-CBB |
| 21 | J | 102 | CLA | C4B-C3B-CAB-CBB |
| 21 | K | 201 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 308 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 315 | CLA | C4B-C3B-CAB-CBB |
| 21 | 2 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 410 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 412 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 413 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 414 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 412 | CLA | C4B-C3B-CAB-CBB |
| 21 | a | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | a | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | a | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | b | 312 | CLA | C4B-C3B-CAB-CBB |
| 21 | c | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | c | 612 | CLA | C4B-C3B-CAB-CBB |
| 29 | 1 | 302 | CHL | CBA-CGA-O2A-C1 |
| 21 | 4 | 602 | CLA | C2C-C3C-CAC-CBC |
| 21 | 3 | 412 | CLA | O1A-CGA-O2A-C1 |
| 21 | a | 610 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 813 | CLA | CBD-CGD-O2D-CED |
| 21 | 8 | 602 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 837 | CLA | C2-C3-C5-C6 |
| 21 | A | 821 | CLA | C11-C10-C8-C7 |
| 21 | A | 834 | CLA | C11-C12-C13-C15 |
| 21 | B | 802 | CLA | C12-C13-C15-C16 |
| 21 | B | 804 | CLA | C11-C10-C8-C7 |
| 21 | B | 840 | CLA | C11-C12-C13-C15 |
| 21 | 1 | 303 | CLA | C6-C7-C8-C10 |
| 29 | 2 | 602 | CHL | O1D-CGD-O2D-CED |
| 21 | 7 | 404 | CLA | C3A-C2A-CAA-CBA |
| 21 | A | 828 | CLA | C10-C11-C12-C13 |
| 21 | A | 815 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 815 | CLA | C6-C7-C8-C9 |
| 21 | A | 828 | CLA | C2-C3-C5-C6 |
| 21 | 1 | 303 | CLA | C2C-C3C-CAC-CBC |
| 23 | 8 | 617 | LHG | O6-C4-C5-O7 |
| 21 | A | 817 | CLA | C2A-CAA-CBA-CGA |
| 21 | 3 | 409 | CLA | C2A-CAA-CBA-CGA |
| 29 | 1 | 302 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 842 | CLA | C6-C7-C8-C9 |
| 21 | B | 804 | CLA | C11-C10-C8-C9 |
| 21 | B | 823 | CLA | C11-C12-C13-C14 |
| 21 | B | 824 | CLA | C14-C13-C15-C16 |
| 21 | B | 827 | CLA | C6-C7-C8-C9 |
| 21 | B | 830 | CLA | C6-C7-C8-C9 |
| 21 | A | 803 | CLA | O1D-CGD-O2D-CED |
| 21 | 8 | 601 | CLA | O1D-CGD-O2D-CED |
| 29 | a | 601 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 838 | CLA | C10-C11-C12-C13 |
| 21 | O | 204 | CLA | CAD-CBD-CGD-O1D |
| 21 | 1 | 305 | CLA | C1-C2-C3-C4 |
| 21 | 5 | 604 | CLA | C1-C2-C3-C4 |
| 21 | 5 | 613 | CLA | CAD-CBD-CGD-O1D |
| 21 | 7 | 411 | CLA | CAD-CBD-CGD-O1D |
| 21 | 7 | 414 | CLA | CAD-CBD-CGD-O1D |
| 21 | 8 | 603 | CLA | CAD-CBD-CGD-O1D |
| 21 | a | 604 | CLA | CAD-CBD-CGD-O1D |
| 21 | b | 314 | CLA | O1A-CGA-O2A-C1 |
| 23 | 2 | 619 | LHG | O7-C5-C6-O8 |
| 23 | b | 319 | LHG | O7-C5-C6-O8 |
| 21 | b | 303 | CLA | C10-C11-C12-C13 |
| 23 | 4 | 618 | LHG | C4-C5-C6-O8 |
| 23 | 9 | 618 | LHG | C4-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | F | 302 | CLA | CAD-CBD-CGD-O2D |
| 21 | 4 | 601 | CLA | CAD-CBD-CGD-O2D |
| 21 | 6 | 611 | CLA | CAD-CBD-CGD-O2D |
| 21 | b | 315 | CLA | CAD-CBD-CGD-O2D |
| 29 | 2 | 601 | CHL | CAD-CBD-CGD-O2D |
| 21 | b | 311 | CLA | O1A-CGA-O2A-C1 |
| 29 | 1 | 302 | CHL | O1A-CGA-O2A-C1 |
| 21 | B | 802 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 827 | CLA | C3-C5-C6-C7 |
| 21 | B | 815 | CLA | C2A-CAA-CBA-CGA |
| 21 | L | 303 | CLA | C2A-CAA-CBA-CGA |
| 21 | 4 | 610 | CLA | C2A-CAA-CBA-CGA |
| 29 | 9 | 607 | CHL | C2A-CAA-CBA-CGA |
| 21 | A | 834 | CLA | C13-C15-C16-C17 |
| 21 | A | 804 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 804 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 822 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 822 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 813 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 814 | CLA | CHA-CBD-CGD-O2D |
| 21 | F | 302 | CLA | CAD-CBD-CGD-O1D |
| 21 | K | 203 | CLA | CHA-CBD-CGD-O1D |
| 21 | K | 203 | CLA | CHA-CBD-CGD-O2D |
| 21 | O | 202 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 304 | CLA | CHA-CBD-CGD-O1D |
| 21 | 1 | 304 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 308 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 308 | CLA | CAD-CBD-CGD-O2D |
| 21 | 1 | 311 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 311 | CLA | CAD-CBD-CGD-O2D |
| 21 | 3 | 405 | CLA | CHA-CBD-CGD-O2D |
| 21 | 3 | 410 | CLA | CHA-CBD-CGD-O2D |
| 21 | 4 | 601 | CLA | CAD-CBD-CGD-O1D |
| 21 | 4 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 5 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 5 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 5 | 609 | CLA | CHA-CBD-CGD-O2D |
| 21 | 5 | 609 | CLA | CAD-CBD-CGD-O2D |
| 21 | 6 | 611 | CLA | CAD-CBD-CGD-O1D |
| 21 | 7 | 403 | CLA | CAD-CBD-CGD-O2D |
| 21 | 7 | 407 | CLA | CHA-CBD-CGD-O2D |
| 21 | 7 | 409 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 8 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 9 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 9 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 9 | 604 | CLA | CHA-CBD-CGD-O1D |
| 21 | 9 | 604 | CLA | CHA-CBD-CGD-O2D |
| 21 | b | 303 | CLA | CAD-CBD-CGD-O1D |
| 21 | b | 315 | CLA | CAD-CBD-CGD-O1D |
| 23 | A | 844 | LHG | C3-O3-P-O5 |
| 23 | A | 844 | LHG | C4-O6-P-O4 |
| 23 | A | 845 | LHG | C3-O3-P-O5 |
| 23 | 1 | 319 | LHG | C3-O3-P-O5 |
| 23 | 4 | 618 | LHG | C4-O6-P-O4 |
| 23 | 5 | 617 | LHG | C4-O6-P-O3 |
| 23 | 5 | 617 | LHG | C4-O6-P-O4 |
| 23 | b | 319 | LHG | C4-O6-P-O4 |
| 24 | B | 846 | BCR | C9-C10-C11-C12 |
| 29 | 1 | 302 | CHL | CHA-CBD-CGD-O1D |
| 29 | 1 | 302 | CHL | CHA-CBD-CGD-O2D |
| 29 | 2 | 601 | CHL | CAD-CBD-CGD-O1D |
| 29 | 2 | 607 | CHL | CHA-CBD-CGD-O1D |
| 29 | 6 | 602 | CHL | CHA-CBD-CGD-O1D |
| 29 | 6 | 602 | CHL | CHA-CBD-CGD-O2D |
| 29 | 6 | 606 | CHL | CHA-CBD-CGD-O2D |
| 29 | 9 | 607 | CHL | CHA-CBD-CGD-O1D |
| 29 | 9 | 607 | CHL | CHA-CBD-CGD-O2D |
| 29 | a | 605 | CHL | CHA-CBD-CGD-O2D |
| 29 | a | 608 | CHL | CHA-CBD-CGD-O1D |
| 29 | a | 608 | CHL | CHA-CBD-CGD-O2D |
| 29 | a | 609 | CHL | CHA-CBD-CGD-O2D |
| 29 | c | 601 | CHL | CHA-CBD-CGD-O1D |
| 29 | c | 601 | CHL | CHA-CBD-CGD-O2D |
| 29 | c | 608 | CHL | CHA-CBD-CGD-O2D |
| 21 | A | 806 | CLA | C4-C3-C5-C6 |
| 21 | A | 833 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 801 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 833 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 838 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 839 | CLA | C2B-C3B-CAB-CBB |
| 21 | K | 201 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 308 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 413 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 414 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 6 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 412 | CLA | C2B-C3B-CAB-CBB |
| 21 | a | 603 | CLA | C2B-C3B-CAB-CBB |
| 21 | a | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | b | 312 | CLA | C2B-C3B-CAB-CBB |
| 21 | c | 602 | CLA | C2B-C3B-CAB-CBB |
| 21 | c | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | c | 612 | CLA | C2B-C3B-CAB-CBB |
| 24 | G | 205 | BCR | C1-C6-C7-C8 |
| 23 | 4 | 619 | LHG | C28-C29-C30-C31 |
| 21 | B | 838 | CLA | C5-C6-C7-C8 |
| 21 | K | 201 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 802 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 843 | PQN | C25-C26-C27-C28 |
| 30 | 3 | 416 | LUT | C10-C11-C12-C13 |
| 21 | A | 804 | CLA | C16-C17-C18-C20 |
| 21 | A | 805 | CLA | C6-C7-C8-C10 |
| 21 | A | 810 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 821 | CLA | C6-C7-C8-C9 |
| 21 | A | 827 | CLA | C6-C7-C8-C9 |
| 21 | B | 812 | CLA | C14-C13-C15-C16 |
| 21 | B | 823 | CLA | C11-C10-C8-C9 |
| 21 | 1 | 303 | CLA | C11-C12-C13-C14 |
| 21 | a | 602 | CLA | C6-C7-C8-C9 |
| 21 | B | 827 | CLA | C8-C10-C11-C12 |
| 23 | a | 617 | LHG | C14-C15-C16-C17 |
| 21 | B | 802 | CLA | C4-C3-C5-C6 |
| 21 | b | 311 | CLA | C2-C3-C5-C6 |
| 21 | B | 809 | CLA | C2A-CAA-CBA-CGA |
| 21 | H | 201 | CLA | CBD-CGD-O2D-CED |
| 23 | A | 855 | LHG | C12-C13-C14-C15 |
| 21 | 7 | 401 | CLA | C2C-C3C-CAC-CBC |
| 21 | B | 801 | CLA | C4-C3-C5-C6 |
| 21 | B | 831 | CLA | C4-C3-C5-C6 |
| 21 | A | 801 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 821 | CLA | CBD-CGD-O2D-CED |
| 23 | b | 319 | LHG | C4-C5-C6-O8 |
| 21 | B | 831 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 813 | CLA | O1D-CGD-O2D-CED |
| 27 | B | 847 | DGD | C5D-C6D-O5D-C1E |
| 21 | 4 | 603 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 4 | 612 | CLA | C2A-CAA-CBA-CGA |
| 21 | c | 613 | CLA | C2A-CAA-CBA-CGA |
| 21 | b | 314 | CLA | C4-C3-C5-C6 |
| 26 | 3 | 420 | LMU | C2-C1-O1'-C1' |
| 21 | B | 840 | CLA | C11-C12-C13-C14 |
| 21 | 9 | 611 | CLA | C11-C10-C8-C9 |
| 21 | c | 611 | CLA | C6-C7-C8-C9 |
| 21 | B | 820 | CLA | C4B-C3B-CAB-CBB |
| 21 | 2 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 2 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 601 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 601 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 831 | CLA | C6-C7-C8-C10 |
| 21 | A | 827 | CLA | C4-C3-C5-C6 |
| 21 | A | 834 | CLA | C4-C3-C5-C6 |
| 21 | B | 810 | CLA | C4-C3-C5-C6 |
| 21 | B | 801 | CLA | C2-C3-C5-C6 |
| 21 | B | 802 | CLA | C2-C3-C5-C6 |
| 21 | 2 | 609 | CLA | CAA-CBA-CGA-O2A |
| 26 | b | 301 | LMU | C4-C5-C6-C7 |
| 21 | A | 810 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 804 | CLA | C12-C13-C15-C16 |
| 21 | A | 826 | CLA | C11-C10-C8-C7 |
| 21 | B | 805 | CLA | C11-C12-C13-C15 |
| 21 | B | 818 | CLA | C6-C7-C8-C10 |
| 21 | b | 315 | CLA | CAA-CBA-CGA-O2A |
| 29 | c | 607 | CHL | CAA-CBA-CGA-O2A |
| 21 | 9 | 610 | CLA | C5-C6-C7-C8 |
| 21 | A | 805 | CLA | C6-C7-C8-C9 |
| 21 | 4 | 602 | CLA | C4C-C3C-CAC-CBC |
| 21 | B | 818 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 835 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 839 | CLA | C3A-C2A-CAA-CBA |
| 21 | H | 201 | CLA | C3A-C2A-CAA-CBA |
| 21 | 8 | 601 | CLA | C3A-C2A-CAA-CBA |
| 21 | b | 305 | CLA | C3A-C2A-CAA-CBA |
| 21 | b | 315 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 831 | CLA | C2-C3-C5-C6 |
| 24 | A | 850 | BCR | C11-C10-C9-C34 |
| 24 | A | 850 | BCR | C16-C17-C18-C36 |
| 24 | L | 301 | BCR | C11-C10-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 1 | 317 | LUT | C20-C13-C14-C15 |
| 30 | 3 | 416 | LUT | C11-C10-C9-C19 |
| 30 | 4 | 615 | LUT | C20-C13-C14-C15 |
| 30 | 8 | 614 | LUT | C20-C13-C14-C15 |
| 31 | 9 | 616 | XAT | C40-C33-C34-C35 |
| 32 | 9 | 617 | NEX | C39-C29-C30-C31 |
| 32 | b | 318 | NEX | C39-C29-C30-C31 |
| 32 | c | 618 | NEX | C39-C29-C30-C31 |
| 21 | A | 804 | CLA | C15-C16-C17-C18 |
| 21 | A | 842 | CLA | C10-C11-C12-C13 |
| 29 | 4 | 606 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 832 | CLA | C2-C1-O2A-CGA |
| 24 | B | 844 | BCR | C13-C14-C15-C16 |
| 31 | 5 | 616 | XAT | C9-C10-C11-C12 |
| 21 | B | 815 | CLA | C5-C6-C7-C8 |
| 31 | 5 | 616 | XAT | C11-C12-C13-C20 |
| 21 | A | 832 | CLA | CAA-CBA-CGA-O1A |
| 29 | c | 607 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 837 | CLA | C4-C3-C5-C6 |
| 21 | 2 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | 4 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | 5 | 603 | CLA | CAA-CBA-CGA-O2A |
| 29 | 6 | 606 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 806 | CLA | C2-C3-C5-C6 |
| 21 | A | 802 | CLA | C2A-CAA-CBA-CGA |
| 21 | a | 613 | CLA | C2A-CAA-CBA-CGA |
| 29 | 5 | 606 | CHL | C2A-CAA-CBA-CGA |
| 21 | 6 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | b | 315 | CLA | CAA-CBA-CGA-O1A |
| 21 | B | 805 | CLA | C11-C12-C13-C14 |
| 21 | B | 818 | CLA | C6-C7-C8-C9 |
| 21 | B | 835 | CLA | C11-C12-C13-C14 |
| 21 | B | 839 | CLA | C14-C13-C15-C16 |
| 21 | 5 | 602 | CLA | C11-C10-C8-C9 |
| 21 | 8 | 602 | CLA | C11-C10-C8-C9 |
| 21 | B | 801 | CLA | CAA-CBA-CGA-O2A |
| 29 | 8 | 607 | CHL | C1A-C2A-CAA-CBA |
| 29 | c | 608 | CHL | C1A-C2A-CAA-CBA |
| 21 | 2 | 603 | CLA | CAA-CBA-CGA-O2A |
| 29 | 6 | 606 | CHL | CAA-CBA-CGA-O2A |
| 29 | 6 | 614 | CHL | CAA-CBA-CGA-O2A |
| 21 | H | 201 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | b | 303 | CLA | C2A-CAA-CBA-CGA |
| 21 | b | 315 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 815 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 812 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 828 | CLA | C1A-C2A-CAA-CBA |
| 21 | F | 302 | CLA | C1A-C2A-CAA-CBA |
| 21 | L | 303 | CLA | C1A-C2A-CAA-CBA |
| 21 | 8 | 601 | CLA | C1A-C2A-CAA-CBA |
| 21 | 9 | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | 9 | 613 | CLA | C1A-C2A-CAA-CBA |
| 24 | A | 850 | BCR | C11-C10-C9-C8 |
| 24 | A | 850 | BCR | C16-C17-C18-C19 |
| 24 | L | 301 | BCR | C11-C10-C9-C8 |
| 30 | 1 | 317 | LUT | C12-C13-C14-C15 |
| 30 | 3 | 416 | LUT | C11-C10-C9-C8 |
| 30 | 4 | 615 | LUT | C12-C13-C14-C15 |
| 30 | 8 | 614 | LUT | C12-C13-C14-C15 |
| 31 | 9 | 616 | XAT | C32-C33-C34-C35 |
| 32 | 9 | 617 | NEX | C28-C29-C30-C31 |
| 32 | c | 618 | NEX | C28-C29-C30-C31 |
| 27 | B | 847 | DGD | C2B-C3B-C4B-C5B |
| 21 | A | 832 | CLA | CAA-CBA-CGA-O2A |
| 21 | 8 | 603 | CLA | CAA-CBA-CGA-O2A |
| 29 | 4 | 606 | CHL | CAA-CBA-CGA-O2A |
| 29 | 6 | 614 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 820 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 823 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 824 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 840 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 807 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 809 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 820 | CLA | C2B-C3B-CAB-CBB |
| 21 | F | 302 | CLA | C2B-C3B-CAB-CBB |
| 21 | G | 203 | CLA | C2B-C3B-CAB-CBB |
| 21 | J | 102 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 305 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 315 | CLA | C2B-C3B-CAB-CBB |
| 21 | 2 | 603 | CLA | C2B-C3B-CAB-CBB |
| 21 | 2 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 410 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 412 | CLA | C2B-C3B-CAB-CBB |
| 21 | 4 | 612 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 5 | 603 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | a | 614 | CLA | C2B-C3B-CAB-CBB |
| 23 | A | 845 | LHG | O8-C23-C24-C25 |
| 24 | A | 846 | BCR | C5-C6-C7-C8 |
| 24 | A | 848 | BCR | C1-C6-C7-C8 |
| 24 | B | 843 | BCR | C23-C24-C25-C26 |
| 24 | B | 845 | BCR | C23-C24-C25-C26 |
| 24 | J | 101 | BCR | C23-C24-C25-C26 |
| 24 | L | 301 | BCR | C1-C6-C7-C8 |
| 24 | O | 205 | BCR | C1-C6-C7-C8 |
| 24 | 3 | 418 | BCR | C1-C6-C7-C8 |
| 24 | 3 | 418 | BCR | C23-C24-C25-C26 |
| 24 | 3 | 419 | BCR | C5-C6-C7-C8 |
| 24 | 3 | 419 | BCR | C23-C24-C25-C26 |
| 24 | 4 | 617 | BCR | C23-C24-C25-C26 |
| 24 | 7 | 417 | BCR | C1-C6-C7-C8 |
| 24 | 7 | 418 | BCR | C5-C6-C7-C8 |
| 24 | 8 | 616 | BCR | C1-C6-C7-C8 |
| 30 | 1 | 317 | LUT | C1-C6-C7-C8 |
| 30 | 3 | 416 | LUT | C5-C6-C7-C8 |
| 30 | 4 | 615 | LUT | C1-C6-C7-C8 |
| 30 | 5 | 615 | LUT | C5-C6-C7-C8 |
| 30 | 8 | 614 | LUT | C1-C6-C7-C8 |
| 30 | 9 | 614 | LUT | C1-C6-C7-C8 |
| 30 | b | 316 | LUT | C1-C6-C7-C8 |
| 30 | b | 317 | LUT | C1-C6-C7-C8 |
| 21 | A | 810 | CLA | CAA-CBA-CGA-O1A |
| 21 | 4 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 6 | 603 | CLA | CAA-CBA-CGA-O2A |
| 29 | 9 | 608 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 807 | CLA | C15-C16-C17-C18 |
| 21 | 9 | 604 | CLA | CAA-CBA-CGA-O1A |
| 21 | B | 828 | CLA | C4-C3-C5-C6 |
| 29 | 2 | 601 | CHL | C4-C3-C5-C6 |
| 21 | A | 834 | CLA | C2-C3-C5-C6 |
| 21 | A | 840 | CLA | C11-C12-C13-C15 |
| 21 | B | 806 | CLA | C12-C13-C15-C16 |
| 21 | B | 812 | CLA | C12-C13-C15-C16 |
| 21 | B | 823 | CLA | C12-C13-C15-C16 |
| 21 | a | 602 | CLA | C6-C7-C8-C10 |
| 21 | 3 | 402 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 838 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 804 | CLA | C2A-CAA-CBA-CGA |
| 21 | G | 204 | CLA | C2A-CAA-CBA-CGA |
| 21 | 7 | 411 | CLA | C2A-CAA-CBA-CGA |
| 21 | c | 604 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | a | 610 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 837 | CLA | C16-C17-C18-C19 |
| 27 | B | 847 | DGD | C4B-C5B-C6B-C7B |
| 21 | B | 831 | CLA | C11-C10-C8-C7 |
| 29 | a | 606 | CHL | CAA-CBA-CGA-O2A |
| 29 | a | 608 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 826 | CLA | C3-C5-C6-C7 |
| 21 | B | 809 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 827 | CLA | C2-C3-C5-C6 |
| 21 | B | 810 | CLA | C2-C3-C5-C6 |
| 29 | 2 | 601 | CHL | C2-C3-C5-C6 |
| 21 | c | 611 | CLA | C2-C1-O2A-CGA |
| 21 | 1 | 303 | CLA | C8-C10-C11-C12 |
| 21 | b | 313 | CLA | CAA-CBA-CGA-O2A |
| 29 | c | 608 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 841 | CLA | C16-C17-C18-C19 |
| 21 | B | 804 | CLA | C16-C17-C18-C19 |
| 21 | A | 805 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 826 | CLA | C3-C5-C6-C7 |
| 21 | A | 810 | CLA | CAA-CBA-CGA-O2A |
| 21 | 1 | 308 | CLA | CAA-CBA-CGA-O2A |
| 21 | 6 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | 8 | 608 | CLA | CAA-CBA-CGA-O1A |
| 29 | 8 | 606 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 821 | CLA | C11-C10-C8-C9 |
| 21 | A | 823 | CLA | C6-C7-C8-C9 |
| 21 | A | 838 | CLA | C11-C10-C8-C9 |
| 21 | B | 807 | CLA | C8-C10-C11-C12 |
| 28 | G | 206 | LMG | O9-C10-O7-C8 |
| 31 | 6 | 617 | XAT | C9-C10-C11-C12 |
| 21 | 5 | 603 | CLA | CAA-CBA-CGA-O1A |
| 29 | 9 | 608 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 821 | CLA | C4-C3-C5-C6 |
| 29 | a | 606 | CHL | CAA-CBA-CGA-O1A |
| 29 | a | 608 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 831 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 841 | CLA | C16-C17-C18-C20 |
| 21 | L | 302 | CLA | CAA-CBA-CGA-O1A |
| 21 | 7 | 401 | CLA | CAA-CBA-CGA-O2A |
| 21 | b | 305 | CLA | CAA-CBA-CGA-O2A |
| 21 | c | 604 | CLA | CAA-CBA-CGA-O2A |
| 29 | c | 605 | CHL | CAA-CBA-CGA-O2A |
| 21 | G | 204 | CLA | CAA-CBA-CGA-O2A |
| 21 | 4 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | 7 | 402 | CLA | CAA-CBA-CGA-O2A |
| 29 | 5 | 601 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 841 | CLA | C8-C10-C11-C12 |
| 21 | B | 828 | CLA | CBA-CGA-O2A-C1 |
| 21 | 1 | 312 | CLA | CAA-CBA-CGA-O2A |
| 21 | b | 312 | CLA | CAA-CBA-CGA-O2A |
| 29 | 2 | 606 | CHL | CAA-CBA-CGA-O2A |
| 21 | B | 840 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 836 | CLA | C8-C10-C11-C12 |
| 21 | 2 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 408 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 608 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 604 | CLA | CAA-CBA-CGA-O2A |
| 21 | a | 610 | CLA | CAA-CBA-CGA-O1A |
| 29 | 6 | 601 | CHL | CAA-CBA-CGA-O2A |
| 21 | B | 822 | CLA | CAA-CBA-CGA-O2A |
| 29 | 9 | 607 | CHL | CAA-CBA-CGA-O2A |
| 23 | A | 855 | LHG | C29-C30-C31-C32 |
| 21 | 1 | 310 | CLA | CAA-CBA-CGA-O2A |
| 21 | b | 313 | CLA | CAA-CBA-CGA-O1A |
| 21 | c | 610 | CLA | CAA-CBA-CGA-O2A |
| 29 | 8 | 606 | CHL | CAA-CBA-CGA-O1A |
| 21 | b | 314 | CLA | C2-C3-C5-C6 |
| 21 | A | 805 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 804 | CLA | C8-C10-C11-C12 |
| 21 | B | 817 | CLA | C10-C11-C12-C13 |
| 21 | A | 838 | CLA | C11-C10-C8-C7 |
| 23 | c | 619 | LHG | C17-C18-C19-C20 |
| 29 | a | 605 | CHL | CAA-CBA-CGA-O2A |
| 23 | A | 855 | LHG | C24-C25-C26-C27 |
| 24 | J | 104 | BCR | C13-C14-C15-C16 |
| 21 | B | 839 | CLA | CAA-CBA-CGA-O2A |
| 21 | 1 | 308 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 5 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | 8 | 608 | CLA | CAA-CBA-CGA-O2A |
| 29 | 9 | 609 | CHL | CAA-CBA-CGA-O2A |
| 29 | c | 608 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 817 | CLA | C6-C7-C8-C9 |
| 21 | A | 834 | CLA | C11-C12-C13-C14 |
| 21 | B | 805 | CLA | C11-C10-C8-C9 |
| 21 | B | 837 | CLA | C11-C10-C8-C9 |
| 21 | c | 602 | CLA | C6-C7-C8-C9 |
| 23 | A | 845 | LHG | O10-C23-C24-C25 |
| 21 | B | 828 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 821 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 834 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 801 | CLA | C2-C1-O2A-CGA |
| 21 | B | 809 | CLA | C2-C1-O2A-CGA |
| 29 | 6 | 602 | CHL | C2-C1-O2A-CGA |
| 23 | a | 617 | LHG | C24-C25-C26-C27 |
| 26 | O | 206 | LMU | C5'-C4'-O1B-C1B |
| 21 | 8 | 611 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 809 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 812 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 819 | CLA | C3A-C2A-CAA-CBA |
| 21 | 5 | 604 | CLA | C3A-C2A-CAA-CBA |
| 21 | 1 | 312 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 609 | CLA | CAA-CBA-CGA-O2A |
| 29 | 2 | 606 | CHL | CAA-CBA-CGA-O1A |
| 29 | 2 | 614 | CHL | CAA-CBA-CGA-O2A |
| 21 | 5 | 609 | CLA | CAA-CBA-CGA-O2A |
| 21 | 6 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 818 | CLA | CAA-CBA-CGA-O2A |
| 29 | 6 | 602 | CHL | O1D-CGD-O2D-CED |
| 28 | G | 206 | LMG | C7-C8-O7-C10 |
| 28 | G | 206 | LMG | C9-C8-O7-C10 |
| 21 | A | 836 | CLA | CAA-CBA-CGA-O2A |
| 21 | K | 204 | CLA | CAA-CBA-CGA-O2A |
| 21 | 4 | 611 | CLA | CAA-CBA-CGA-O1A |
| 21 | b | 305 | CLA | CAA-CBA-CGA-O1A |
| 21 | b | 312 | CLA | CAA-CBA-CGA-O1A |
| 29 | 5 | 601 | CHL | CAA-CBA-CGA-O1A |
| 29 | 9 | 607 | CHL | CAA-CBA-CGA-O1A |
| 29 | c | 609 | CHL | CAA-CBA-CGA-O2A |
| 21 | G | 204 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 5 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | 7 | 402 | CLA | CAA-CBA-CGA-O1A |
| 29 | 5 | 606 | CHL | CAA-CBA-CGA-O2A |
| 29 | c | 605 | CHL | CAA-CBA-CGA-O1A |
| 21 | c | 603 | CLA | C4-C3-C5-C6 |
| 21 | B | 822 | CLA | CAA-CBA-CGA-O1A |
| 21 | 7 | 401 | CLA | CAA-CBA-CGA-O1A |
| 29 | c | 606 | CHL | CAA-CBA-CGA-O1A |
| 27 | B | 847 | DGD | O6D-C5D-C6D-O5D |
| 31 | 9 | 616 | XAT | O24-C26-C27-C28 |
| 32 | b | 318 | NEX | C28-C29-C30-C31 |
| 21 | L | 302 | CLA | CAA-CBA-CGA-O2A |
| 21 | 5 | 614 | CLA | CAA-CBA-CGA-O1A |
| 29 | 6 | 601 | CHL | CAA-CBA-CGA-O1A |
| 29 | 9 | 606 | CHL | CAA-CBA-CGA-O2A |
| 29 | a | 605 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 808 | CLA | C8-C10-C11-C12 |
| 21 | 1 | 310 | CLA | CAA-CBA-CGA-O1A |
| 29 | 2 | 614 | CHL | CAA-CBA-CGA-O1A |
| 29 | a | 609 | CHL | CAA-CBA-CGA-O2A |
| 29 | c | 606 | CHL | CAA-CBA-CGA-O2A |
| 21 | c | 610 | CLA | CAA-CBA-CGA-O1A |
| 29 | 9 | 609 | CHL | CAA-CBA-CGA-O1A |
| 27 | B | 847 | DGD | C2A-C3A-C4A-C5A |
| 21 | B | 832 | CLA | C4-C3-C5-C6 |
| 21 | A | 814 | CLA | C16-C17-C18-C19 |
| 21 | A | 814 | CLA | C16-C17-C18-C20 |
| 21 | B | 804 | CLA | C16-C17-C18-C20 |
| 28 | G | 206 | LMG | C19-C20-C21-C22 |
| 21 | 5 | 609 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 610 | CLA | CAA-CBA-CGA-O1A |
| 29 | b | 307 | CHL | CAA-CBA-CGA-O2A |
| 26 | O | 206 | LMU | O5B-C1B-O1B-C4' |
| 21 | A | 836 | CLA | CAA-CBA-CGA-O1A |
| 21 | 5 | 611 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 610 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 807 | CLA | C11-C12-C13-C14 |
| 21 | B | 802 | CLA | C11-C10-C8-C9 |
| 21 | 8 | 609 | CLA | CAA-CBA-CGA-O1A |
| 29 | c | 609 | CHL | CAA-CBA-CGA-O1A |
| 24 | B | 844 | BCR | C17-C18-C19-C20 |
| 30 | a | 615 | LUT | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | K | 201 | CLA | O1A-CGA-O2A-C1 |
| 21 | B | 805 | CLA | O1A-CGA-O2A-C1 |
| 21 | 9 | 604 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 840 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 817 | CLA | C6-C7-C8-C10 |
| 21 | B | 804 | CLA | C11-C12-C13-C15 |
| 21 | B | 824 | CLA | C6-C7-C8-C10 |
| 21 | B | 837 | CLA | C11-C10-C8-C7 |
| 21 | c | 602 | CLA | C6-C7-C8-C10 |
| 26 | O | 206 | LMU | C3'-C4'-O1B-C1B |
| 21 | B | 814 | CLA | C8-C10-C11-C12 |
| 26 | 3 | 420 | LMU | C4'-C5'-C6'-O6' |
| 21 | B | 812 | CLA | C2B-C3B-CAB-CBB |
| 21 | 2 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 408 | CLA | C2B-C3B-CAB-CBB |
| 21 | 8 | 601 | CLA | C2B-C3B-CAB-CBB |
| 21 | a | 604 | CLA | C2B-C3B-CAB-CBB |
| 24 | L | 301 | BCR | C5-C6-C7-C8 |
| 24 | L | 305 | BCR | C23-C24-C25-C26 |
| 24 | L | 305 | BCR | C23-C24-C25-C30 |
| 24 | O | 205 | BCR | C5-C6-C7-C8 |
| 24 | 3 | 418 | BCR | C5-C6-C7-C8 |
| 24 | 7 | 417 | BCR | C5-C6-C7-C8 |
| 24 | 8 | 616 | BCR | C5-C6-C7-C8 |
| 30 | 4 | 615 | LUT | C5-C6-C7-C8 |
| 30 | 8 | 614 | LUT | C5-C6-C7-C8 |
| 30 | 9 | 614 | LUT | C5-C6-C7-C8 |
| 30 | 9 | 615 | LUT | C1-C6-C7-C8 |
| 30 | 9 | 615 | LUT | C5-C6-C7-C8 |
| 30 | b | 316 | LUT | C5-C6-C7-C8 |
| 30 | b | 317 | LUT | C5-C6-C7-C8 |
| 21 | A | 819 | CLA | C2-C1-O2A-CGA |
| 21 | A | 824 | CLA | C2-C1-O2A-CGA |
| 21 | B | 807 | CLA | C2-C1-O2A-CGA |
| 21 | A | 842 | CLA | C16-C17-C18-C19 |
| 21 | B | 824 | CLA | C10-C11-C12-C13 |
| 21 | A | 819 | CLA | C4-C3-C5-C6 |
| 21 | A | 819 | CLA | C2-C3-C5-C6 |
| 21 | 2 | 608 | CLA | C2-C3-C5-C6 |
| 21 | K | 204 | CLA | CAA-CBA-CGA-O1A |
| 29 | 9 | 606 | CHL | CAA-CBA-CGA-O1A |
| 21 | 9 | 604 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 823 | CLA | C5-C6-C7-C8 |
| 26 | b | 301 | LMU | C6-C7-C8-C9 |
| 21 | B | 805 | CLA | CBA-CGA-O2A-C1 |
| 21 | 1 | 303 | CLA | CAA-CBA-CGA-O2A |
| 21 | 9 | 613 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 806 | CLA | CAA-CBA-CGA-O2A |
| 21 | c | 603 | CLA | C2-C3-C5-C6 |
| 21 | a | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 837 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 808 | CLA | CAA-CBA-CGA-O2A |
| 29 | 5 | 606 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 827 | CLA | CAA-CBA-CGA-O2A |
| 21 | 9 | 613 | CLA | CBA-CGA-O2A-C1 |
| 21 | c | 603 | CLA | O1A-CGA-O2A-C1 |
| 21 | 2 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 807 | CLA | C6-C7-C8-C9 |
| 21 | B | 817 | CLA | C11-C10-C8-C9 |
| 23 | b | 319 | LHG | O2-C2-C3-O3 |
| 21 | A | 801 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 803 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 804 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 809 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 812 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 824 | CLA | C1A-C2A-CAA-CBA |
| 21 | H | 201 | CLA | C1A-C2A-CAA-CBA |
| 21 | 3 | 405 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | a | 604 | CLA | C4B-C3B-CAB-CBB |
| 21 | a | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | b | 305 | CLA | C1A-C2A-CAA-CBA |
| 21 | b | 315 | CLA | C1A-C2A-CAA-CBA |
| 29 | b | 306 | CHL | CAA-CBA-CGA-O2A |
| 21 | 2 | 608 | CLA | C4-C3-C5-C6 |
| 21 | c | 602 | CLA | CAA-CBA-CGA-O2A |
| 23 | A | 845 | LHG | O7-C7-C8-C9 |
| 29 | b | 307 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 824 | CLA | C8-C10-C11-C12 |
| 21 | c | 603 | CLA | CBA-CGA-O2A-C1 |
| 21 | B | 832 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 837 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 813 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 814 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 817 | CLA | C2A-CAA-CBA-CGA |
| 21 | b | 314 | CLA | C2A-CAA-CBA-CGA |
| 29 | c | 609 | CHL | C2A-CAA-CBA-CGA |
| 23 | a | 617 | LHG | C25-C26-C27-C28 |
| 21 | A | 814 | CLA | C2-C1-O2A-CGA |
| 21 | A | 841 | CLA | C2-C1-O2A-CGA |
| 21 | 2 | 608 | CLA | C2-C1-O2A-CGA |
| 29 | b | 309 | CHL | C2-C1-O2A-CGA |
| 21 | B | 805 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 805 | CLA | C6-C7-C8-C10 |
| 21 | B | 838 | CLA | C6-C7-C8-C10 |
| 29 | a | 609 | CHL | CAA-CBA-CGA-O1A |
| 21 | A | 827 | CLA | C16-C17-C18-C20 |
| 23 | A | 855 | LHG | C4-C5-O7-C7 |
| 23 | A | 855 | LHG | C6-C5-O7-C7 |
| 21 | 9 | 602 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 801 | CLA | C13-C15-C16-C17 |
| 29 | 6 | 607 | CHL | CAA-CBA-CGA-O2A |
| 21 | 5 | 602 | CLA | C8-C10-C11-C12 |
| 21 | F | 302 | CLA | C3A-C2A-CAA-CBA |
| 21 | K | 202 | CLA | C3A-C2A-CAA-CBA |
| 21 | 1 | 314 | CLA | CHA-CBD-CGD-O1D |
| 21 | 4 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 8 | 609 | CLA | C3A-C2A-CAA-CBA |
| 29 | c | 609 | CHL | C3A-C2A-CAA-CBA |
| 21 | a | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | 5 | 614 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 804 | CLA | C11-C12-C13-C14 |
| 21 | B | 806 | CLA | C14-C13-C15-C16 |
| 23 | 4 | 619 | LHG | C32-C33-C34-C35 |
| 24 | B | 843 | BCR | C19-C20-C21-C22 |
| 21 | A | 808 | CLA | CAA-CBA-CGA-O1A |
| 29 | 4 | 606 | CHL | O1D-CGD-O2D-CED |
| 21 | B | 828 | CLA | C2-C3-C5-C6 |
| 21 | G | 204 | CLA | CAD-CBD-CGD-O1D |
| 31 | 6 | 617 | XAT | C1-C6-C7-C8 |
| 29 | 6 | 602 | CHL | CBD-CGD-O2D-CED |
| 21 | K | 201 | CLA | CAA-CBA-CGA-O2A |
| 21 | 1 | 304 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 837 | CLA | C16-C17-C18-C20 |
| 29 | c | 601 | CHL | O1A-CGA-O2A-C1 |
| 21 | 2 | 610 | CLA | C2C-C3C-CAC-CBC |
| 21 | b | 304 | CLA | CAA-CBA-CGA-O2A |
| 27 | B | 847 | DGD | C3B-C4B-C5B-C6B |
| 21 | A | 806 | CLA | CAA-CBA-CGA-O1A |
| 21 | c | 602 | CLA | CAA-CBA-CGA-O1A |
| 23 | A | 845 | LHG | O9-C7-C8-C9 |
| 21 | B | 807 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 806 | CLA | C2A-CAA-CBA-CGA |
| 21 | 1 | 312 | CLA | C2A-CAA-CBA-CGA |
| 21 | 6 | 603 | CLA | C2A-CAA-CBA-CGA |
| 27 | B | 847 | DGD | C5A-C6A-C7A-C8A |
| 21 | 1 | 315 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 827 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 829 | CLA | C8-C10-C11-C12 |
| 21 | 2 | 612 | CLA | CAA-CBA-CGA-O1A |
| 29 | b | 306 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 805 | CLA | CAA-CBA-CGA-O1A |
| 21 | 1 | 303 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 801 | CLA | CAD-CBD-CGD-O2D |
| 21 | A | 815 | CLA | CAD-CBD-CGD-O2D |
| 21 | 7 | 410 | CLA | CAD-CBD-CGD-O2D |
| 21 | 8 | 612 | CLA | CAD-CBD-CGD-O2D |
| 21 | b | 303 | CLA | CAD-CBD-CGD-O2D |
| 29 | a | 607 | CHL | CAD-CBD-CGD-O2D |
| 29 | b | 306 | CHL | CAD-CBD-CGD-O2D |
| 22 | B | 841 | PQN | C23-C25-C26-C27 |
| 21 | 1 | 304 | CLA | O1A-CGA-O2A-C1 |
| 21 | 1 | 315 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 828 | CLA | C2-C1-O2A-CGA |
| 29 | 1 | 302 | CHL | C2-C1-O2A-CGA |
| 29 | b | 310 | CHL | C2-C1-O2A-CGA |
| 21 | K | 201 | CLA | CAA-CBA-CGA-O1A |
| 29 | 6 | 607 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 826 | CLA | CAA-CBA-CGA-O2A |
| 21 | 3 | 401 | CLA | C2C-C3C-CAC-CBC |
| 21 | B | 832 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 823 | CLA | CAA-CBA-CGA-O2A |
| 29 | 8 | 607 | CHL | CAA-CBA-CGA-O2A |
| 29 | a | 606 | CHL | O1D-CGD-O2D-CED |
| 21 | B | 829 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | a | 617 | LHG | C29-C30-C31-C32 |
| 21 | A | 825 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 841 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 830 | CLA | CAA-CBA-CGA-O2A |
| 21 | b | 303 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 837 | CLA | CAA-CBA-CGA-O1A |

There are no ring outliers.

307 monomers are involved in 867 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | A | 835 | CLA | 2 | 0 |
| 24 | I | 101 | BCR | 1 | 0 |
| 21 | A | 841 | CLA | 4 | 0 |
| 29 | c | 605 | CHL | 1 | 0 |
| 26 | O | 206 | LMU | 4 | 0 |
| 21 | b | 312 | CLA | 3 | 0 |
| 24 | B | 844 | BCR | 6 | 0 |
| 29 | 6 | 601 | CHL | 3 | 0 |
| 29 | 2 | 606 | CHL | 2 | 0 |
| 21 | G | 202 | CLA | 2 | 0 |
| 29 | 4 | 607 | CHL | 4 | 0 |
| 21 | 1 | 310 | CLA | 1 | 0 |
| 24 | B | 843 | BCR | 20 | 0 |
| 21 | b | 304 | CLA | 4 | 0 |
| 21 | 1 | 306 | CLA | 2 | 0 |
| 29 | 3 | 407 | CHL | 1 | 0 |
| 29 | c | 609 | CHL | 3 | 0 |
| 21 | B | 810 | CLA | 1 | 0 |
| 21 | A | 821 | CLA | 7 | 0 |
| 24 | A | 849 | BCR | 4 | 0 |
| 29 | b | 309 | CHL | 3 | 0 |
| 21 | B | 819 | CLA | 1 | 0 |
| 21 | 8 | 611 | CLA | 5 | 0 |
| 29 | 6 | 606 | CHL | 1 | 0 |
| 31 | 2 | 617 | XAT | 2 | 0 |
| 29 | 8 | 606 | CHL | 2 | 0 |
| 29 | 9 | 608 | CHL | 1 | 0 |
| 24 | G | 205 | BCR | 2 | 0 |
| 21 | A | 840 | CLA | 8 | 0 |
| 21 | b | 311 | CLA | 6 | 0 |
| 29 | a | 607 | CHL | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | a | 616 | LUT | 7 | 0 |
| 23 | c | 619 | LHG | 2 | 0 |
| 24 | B | 846 | BCR | 8 | 0 |
| 31 | 3 | 417 | XAT | 4 | 0 |
| 24 | L | 306 | BCR | 3 | 0 |
| 21 | K | 202 | CLA | 1 | 0 |
| 21 | A | 825 | CLA | 3 | 0 |
| 21 | 1 | 308 | CLA | 1 | 0 |
| 21 | F | 304 | CLA | 2 | 0 |
| 21 | 8 | 602 | CLA | 4 | 0 |
| 21 | B | 831 | CLA | 6 | 0 |
| 23 | b | 319 | LHG | 9 | 0 |
| 29 | 6 | 614 | CHL | 4 | 0 |
| 24 | G | 201 | BCR | 4 | 0 |
| 21 | 5 | 607 | CLA | 3 | 0 |
| 29 | 2 | 607 | CHL | 3 | 0 |
| 21 | A | 804 | CLA | 3 | 0 |
| 29 | a | 601 | CHL | 1 | 0 |
| 23 | 2 | 619 | LHG | 1 | 0 |
| 21 | B | 826 | CLA | 1 | 0 |
| 21 | c | 612 | CLA | 2 | 0 |
| 24 | A | 854 | BCR | 13 | 0 |
| 29 | 6 | 605 | CHL | 1 | 0 |
| 30 | 9 | 615 | LUT | 7 | 0 |
| 31 | 6 | 617 | XAT | 6 | 0 |
| 21 | O | 203 | CLA | 1 | 0 |
| 21 | B | 830 | CLA | 4 | 0 |
| 21 | 6 | 609 | CLA | 4 | 0 |
| 29 | 2 | 602 | CHL | 3 | 0 |
| 23 | 9 | 618 | LHG | 4 | 0 |
| 21 | A | 838 | CLA | 3 | 0 |
| 29 | 2 | 614 | CHL | 5 | 0 |
| 21 | A | 833 | CLA | 5 | 0 |
| 29 | a | 609 | CHL | 3 | 0 |
| 21 | b | 314 | CLA | 4 | 0 |
| 21 | 2 | 608 | CLA | 2 | 0 |
| 21 | 8 | 604 | CLA | 3 | 0 |
| 21 | A | 827 | CLA | 5 | 0 |
| 24 | 7 | 417 | BCR | 7 | 0 |
| 31 | 4 | 616 | XAT | 4 | 0 |
| 32 | 9 | 617 | NEX | 4 | 0 |
| 31 | 1 | 318 | XAT | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | a | 602 | CLA | 5 | 0 |
| 23 | 4 | 619 | LHG | 1 | 0 |
| 21 | A | 802 | CLA | 4 | 0 |
| 21 | L | 302 | CLA | 2 | 0 |
| 21 | A | 832 | CLA | 1 | 0 |
| 26 | b | 301 | LMU | 4 | 0 |
| 21 | 3 | 409 | CLA | 21 | 0 |
| 21 | A | 813 | CLA | 1 | 0 |
| 21 | c | 603 | CLA | 4 | 0 |
| 21 | 6 | 603 | CLA | 2 | 0 |
| 29 | 6 | 602 | CHL | 3 | 0 |
| 29 | b | 306 | CHL | 2 | 0 |
| 24 | J | 101 | BCR | 4 | 0 |
| 21 | A | 822 | CLA | 3 | 0 |
| 21 | 5 | 604 | CLA | 2 | 0 |
| 31 | 7 | 416 | XAT | 5 | 0 |
| 21 | A | 816 | CLA | 1 | 0 |
| 21 | 6 | 608 | CLA | 2 | 0 |
| 21 | A | 809 | CLA | 1 | 0 |
| 24 | J | 104 | BCR | 8 | 0 |
| 21 | A | 842 | CLA | 7 | 0 |
| 28 | 6 | 615 | LMG | 1 | 0 |
| 21 | A | 803 | CLA | 2 | 0 |
| 31 | 5 | 616 | XAT | 5 | 0 |
| 21 | 4 | 602 | CLA | 5 | 0 |
| 21 | 3 | 412 | CLA | 1 | 0 |
| 21 | 9 | 610 | CLA | 1 | 0 |
| 21 | B | 832 | CLA | 4 | 0 |
| 21 | c | 613 | CLA | 4 | 0 |
| 24 | 8 | 616 | BCR | 8 | 0 |
| 21 | 6 | 613 | CLA | 1 | 0 |
| 30 | c | 615 | LUT | 3 | 0 |
| 21 | 2 | 613 | CLA | 2 | 0 |
| 21 | B | 805 | CLA | 4 | 0 |
| 29 | 1 | 307 | CHL | 5 | 0 |
| 29 | 7 | 406 | CHL | 2 | 0 |
| 29 | 2 | 601 | CHL | 2 | 0 |
| 21 | B | 837 | CLA | 6 | 0 |
| 29 | c | 606 | CHL | 2 | 0 |
| 29 | c | 607 | CHL | 1 | 0 |
| 21 | 3 | 411 | CLA | 1 | 0 |
| 29 | a | 608 | CHL | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | B | 816 | CLA | 5 | 0 |
| 21 | 7 | 401 | CLA | 7 | 0 |
| 21 | 8 | 612 | CLA | 2 | 0 |
| 29 | 8 | 607 | CHL | 5 | 0 |
| 29 | 8 | 613 | CHL | 4 | 0 |
| 30 | a | 615 | LUT | 4 | 0 |
| 21 | 5 | 614 | CLA | 1 | 0 |
| 30 | 3 | 416 | LUT | 12 | 0 |
| 21 | a | 611 | CLA | 4 | 0 |
| 21 | 5 | 603 | CLA | 3 | 0 |
| 21 | 5 | 602 | CLA | 10 | 0 |
| 21 | 4 | 611 | CLA | 1 | 0 |
| 21 | B | 839 | CLA | 4 | 0 |
| 32 | b | 318 | NEX | 1 | 0 |
| 28 | G | 206 | LMG | 2 | 0 |
| 21 | 6 | 611 | CLA | 1 | 0 |
| 21 | B | 817 | CLA | 8 | 0 |
| 21 | 3 | 402 | CLA | 1 | 0 |
| 30 | c | 616 | LUT | 4 | 0 |
| 21 | 3 | 415 | CLA | 2 | 0 |
| 23 | A | 845 | LHG | 1 | 0 |
| 21 | 2 | 610 | CLA | 2 | 0 |
| 24 | L | 301 | BCR | 3 | 0 |
| 21 | A | 852 | CLA | 6 | 0 |
| 23 | 8 | 617 | LHG | 3 | 0 |
| 21 | A | 814 | CLA | 1 | 0 |
| 24 | O | 205 | BCR | 1 | 0 |
| 21 | A | 830 | CLA | 3 | 0 |
| 21 | B | 806 | CLA | 2 | 0 |
| 21 | b | 315 | CLA | 1 | 0 |
| 21 | 2 | 604 | CLA | 3 | 0 |
| 21 | a | 612 | CLA | 1 | 0 |
| 21 | a | 613 | CLA | 3 | 0 |
| 21 | B | 815 | CLA | 2 | 0 |
| 26 | 3 | 420 | LMU | 3 | 0 |
| 30 | 4 | 615 | LUT | 7 | 0 |
| 29 | 4 | 614 | CHL | 1 | 0 |
| 21 | a | 604 | CLA | 1 | 0 |
| 21 | 1 | 304 | CLA | 2 | 0 |
| 30 | b | 317 | LUT | 5 | 0 |
| 23 | 4 | 618 | LHG | 5 | 0 |
| 29 | 5 | 601 | CHL | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | A | 828 | CLA | 3 | 0 |
| 21 | B | 827 | CLA | 9 | 0 |
| 30 | b | 316 | LUT | 6 | 0 |
| 21 | 5 | 612 | CLA | 1 | 0 |
| 21 | 4 | 613 | CLA | 2 | 0 |
| 21 | B | 801 | CLA | 9 | 0 |
| 21 | B | 821 | CLA | 1 | 0 |
| 29 | 8 | 605 | CHL | 4 | 0 |
| 21 | 7 | 408 | CLA | 2 | 0 |
| 24 | A | 846 | BCR | 1 | 0 |
| 21 | 6 | 610 | CLA | 1 | 0 |
| 21 | 8 | 610 | CLA | 1 | 0 |
| 29 | 9 | 601 | CHL | 2 | 0 |
| 21 | B | 812 | CLA | 1 | 0 |
| 21 | A | 817 | CLA | 3 | 0 |
| 21 | B | 808 | CLA | 2 | 0 |
| 32 | c | 618 | NEX | 3 | 0 |
| 21 | 1 | 315 | CLA | 1 | 0 |
| 21 | B | 802 | CLA | 3 | 0 |
| 21 | B | 804 | CLA | 2 | 0 |
| 21 | 5 | 605 | CLA | 2 | 0 |
| 29 | b | 308 | CHL | 2 | 0 |
| 21 | A | 818 | CLA | 7 | 0 |
| 21 | A | 829 | CLA | 2 | 0 |
| 21 | 2 | 603 | CLA | 1 | 0 |
| 21 | A | 806 | CLA | 3 | 0 |
| 21 | B | 835 | CLA | 2 | 0 |
| 21 | B | 818 | CLA | 1 | 0 |
| 24 | F | 301 | BCR | 2 | 0 |
| 27 | B | 847 | DGD | 7 | 0 |
| 21 | L | 303 | CLA | 1 | 0 |
| 21 | H | 201 | CLA | 2 | 0 |
| 24 | B | 845 | BCR | 3 | 0 |
| 21 | 1 | 314 | CLA | 1 | 0 |
| 23 | A | 855 | LHG | 4 | 0 |
| 29 | 9 | 606 | CHL | 1 | 0 |
| 21 | c | 604 | CLA | 3 | 0 |
| 21 | 7 | 410 | CLA | 2 | 0 |
| 24 | 3 | 418 | BCR | 6 | 0 |
| 24 | L | 305 | BCR | 2 | 0 |
| 21 | A | 826 | CLA | 2 | 0 |
| 21 | F | 302 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | 3 | 408 | CLA | 5 | 0 |
| 30 | 9 | 614 | LUT | 3 | 0 |
| 21 | B | 840 | CLA | 1 | 0 |
| 21 | B | 809 | CLA | 4 | 0 |
| 21 | c | 610 | CLA | 2 | 0 |
| 21 | K | 204 | CLA | 1 | 0 |
| 21 | 8 | 618 | CLA | 2 | 0 |
| 21 | B | 825 | CLA | 2 | 0 |
| 21 | A | 819 | CLA | 6 | 0 |
| 21 | 5 | 609 | CLA | 2 | 0 |
| 23 | A | 844 | LHG | 3 | 0 |
| 21 | 1 | 312 | CLA | 1 | 0 |
| 21 | A | 824 | CLA | 3 | 0 |
| 21 | A | 807 | CLA | 2 | 0 |
| 21 | B | 807 | CLA | 5 | 0 |
| 29 | 5 | 606 | CHL | 3 | 0 |
| 21 | B | 803 | CLA | 2 | 0 |
| 24 | 3 | 419 | BCR | 1 | 0 |
| 21 | 1 | 313 | CLA | 1 | 0 |
| 22 | B | 841 | PQN | 3 | 0 |
| 30 | 6 | 616 | LUT | 6 | 0 |
| 21 | 9 | 612 | CLA | 1 | 0 |
| 29 | 9 | 607 | CHL | 1 | 0 |
| 24 | A | 850 | BCR | 1 | 0 |
| 21 | c | 614 | CLA | 2 | 0 |
| 21 | 6 | 612 | CLA | 2 | 0 |
| 21 | 7 | 407 | CLA | 18 | 0 |
| 23 | 5 | 617 | LHG | 1 | 0 |
| 31 | c | 617 | XAT | 3 | 0 |
| 21 | 4 | 601 | CLA | 2 | 0 |
| 21 | A | 820 | CLA | 1 | 0 |
| 21 | A | 805 | CLA | 4 | 0 |
| 24 | 7 | 418 | BCR | 4 | 0 |
| 29 | 4 | 606 | CHL | 1 | 0 |
| 21 | B | 838 | CLA | 1 | 0 |
| 21 | 9 | 611 | CLA | 5 | 0 |
| 21 | 4 | 612 | CLA | 1 | 0 |
| 21 | 1 | 309 | CLA | 10 | 0 |
| 21 | O | 202 | CLA | 1 | 0 |
| 29 | c | 608 | CHL | 3 | 0 |
| 21 | 8 | 608 | CLA | 2 | 0 |
| 24 | A | 847 | BCR | 3 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | 8 | 609 | CLA | 26 | 0 |
| 29 | b | 310 | CHL | 3 | 0 |
| 21 | G | 204 | CLA | 1 | 0 |
| 21 | B | 823 | CLA | 3 | 0 |
| 21 | A | 837 | CLA | 3 | 0 |
| 21 | 4 | 609 | CLA | 16 | 0 |
| 24 | M | 101 | BCR | 3 | 0 |
| 21 | A | 810 | CLA | 4 | 0 |
| 29 | b | 302 | CHL | 2 | 0 |
| 21 | 6 | 604 | CLA | 7 | 0 |
| 21 | B | 829 | CLA | 1 | 0 |
| 21 | a | 610 | CLA | 5 | 0 |
| 21 | A | 801 | CLA | 1 | 0 |
| 21 | 8 | 603 | CLA | 1 | 0 |
| 21 | K | 201 | CLA | 5 | 0 |
| 30 | 7 | 415 | LUT | 12 | 0 |
| 29 | 1 | 302 | CHL | 2 | 0 |
| 21 | A | 812 | CLA | 5 | 0 |
| 21 | A | 831 | CLA | 1 | 0 |
| 21 | A | 808 | CLA | 2 | 0 |
| 21 | 3 | 404 | CLA | 4 | 0 |
| 21 | B | 828 | CLA | 3 | 0 |
| 21 | A | 823 | CLA | 1 | 0 |
| 24 | 2 | 618 | BCR | 6 | 0 |
| 29 | 6 | 607 | CHL | 5 | 0 |
| 21 | B | 814 | CLA | 4 | 0 |
| 21 | A | 834 | CLA | 4 | 0 |
| 23 | 6 | 619 | LHG | 3 | 0 |
| 21 | 2 | 609 | CLA | 23 | 0 |
| 21 | B | 811 | CLA | 1 | 0 |
| 21 | B | 822 | CLA | 2 | 0 |
| 21 | 7 | 402 | CLA | 9 | 0 |
| 21 | a | 614 | CLA | 1 | 0 |
| 21 | K | 203 | CLA | 9 | 0 |
| 26 | A | 856 | LMU | 2 | 0 |
| 31 | a | 618 | XAT | 6 | 0 |
| 31 | 9 | 616 | XAT | 2 | 0 |
| 29 | a | 606 | CHL | 2 | 0 |
| 21 | c | 611 | CLA | 1 | 0 |
| 21 | B | 824 | CLA | 3 | 0 |
| 21 | 7 | 404 | CLA | 3 | 0 |
| 30 | 8 | 614 | LUT | 5 | 0 |

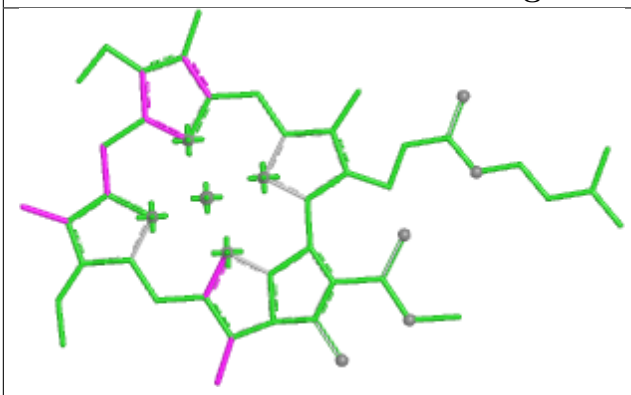
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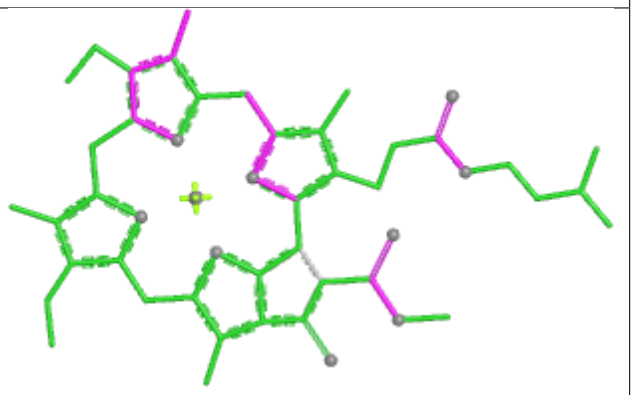
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 31 | 8 | 615 | XAT | 4 | 0 |
| 21 | 7 | 411 | CLA | 2 | 0 |
| 29 | b | 307 | CHL | 2 | 0 |
| 21 | 9 | 613 | CLA | 2 | 0 |
| 29 | 9 | 605 | CHL | 2 | 0 |
| 29 | 9 | 609 | CHL | 2 | 0 |
| 30 | 5 | 615 | LUT | 2 | 0 |
| 21 | B | 836 | CLA | 4 | 0 |
| 21 | c | 602 | CLA | 3 | 0 |
| 23 | a | 617 | LHG | 2 | 0 |
| 29 | a | 605 | CHL | 1 | 0 |
| 24 | 6 | 618 | BCR | 14 | 0 |
| 21 | 9 | 602 | CLA | 3 | 0 |
| 21 | 1 | 303 | CLA | 2 | 0 |
| 30 | 1 | 317 | LUT | 2 | 0 |
| 30 | 2 | 616 | LUT | 8 | 0 |
| 21 | A | 836 | CLA | 1 | 0 |
| 21 | B | 813 | CLA | 3 | 0 |
| 24 | J | 103 | BCR | 3 | 0 |
| 21 | b | 303 | CLA | 3 | 0 |
| 21 | 3 | 413 | CLA | 1 | 0 |
| 24 | B | 842 | BCR | 3 | 0 |
| 21 | 3 | 401 | CLA | 2 | 0 |
| 24 | K | 205 | BCR | 24 | 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.

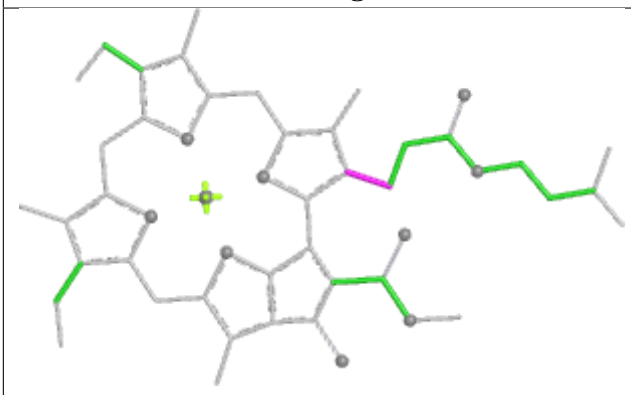
## Ligand CLA A 835



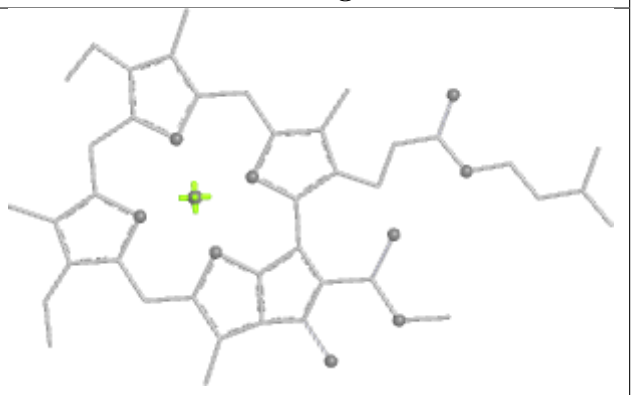
Bond lengths



Bond angles

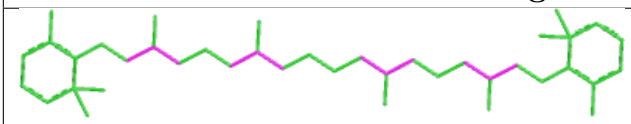


Torsions

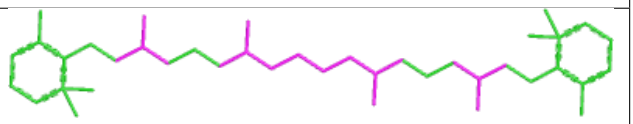


Rings

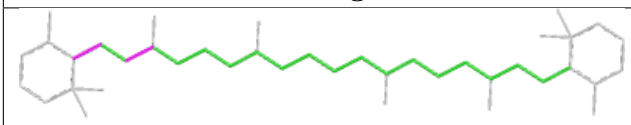
## Ligand BCR I 101



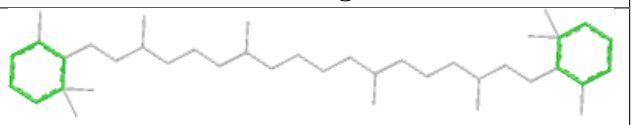
Bond lengths



Bond angles

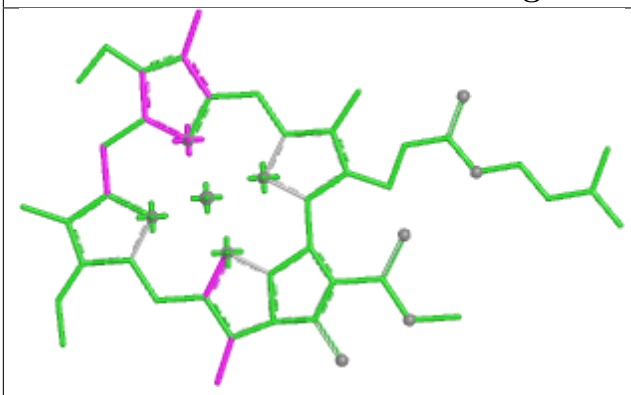


Torsions

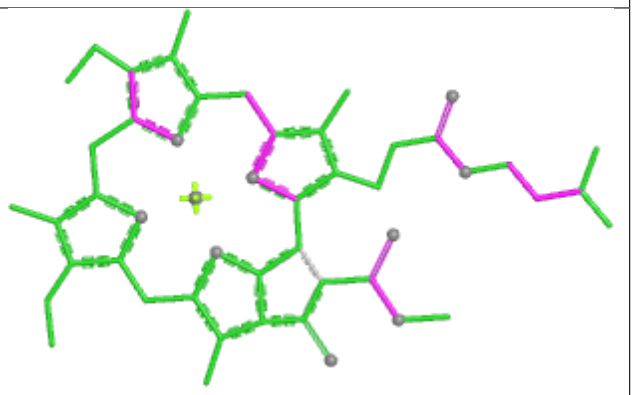


Rings

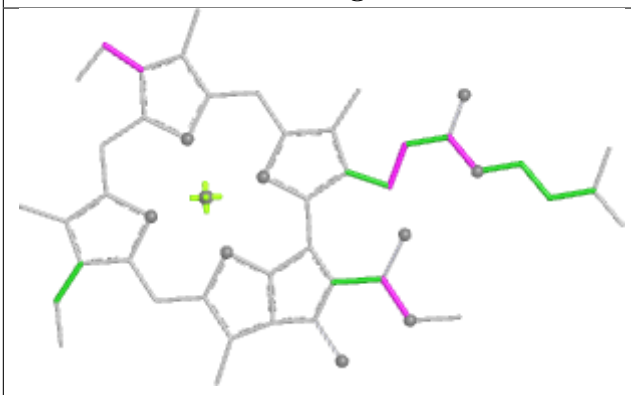
**Ligand CLA G 203**



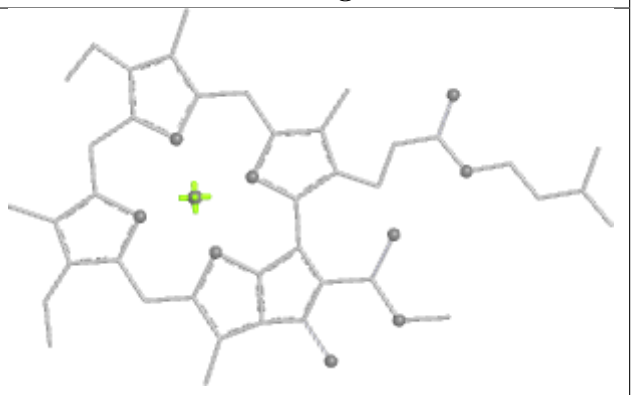
**Bond lengths**



**Bond angles**

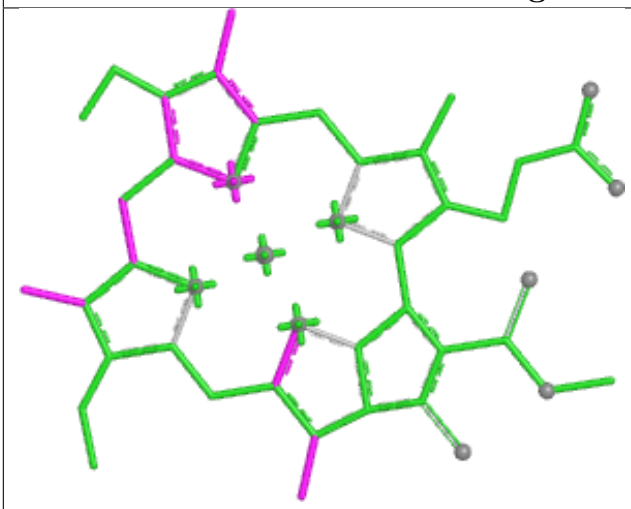


**Torsions**

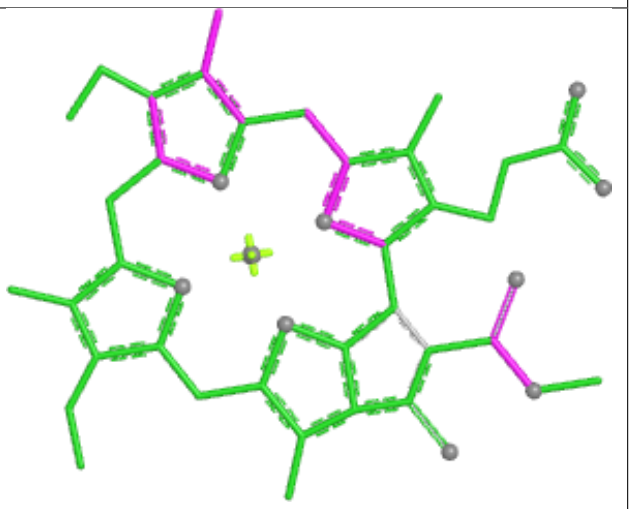


**Rings**

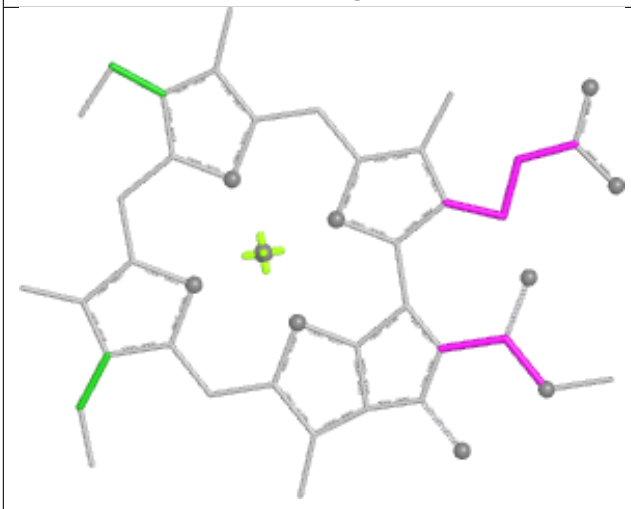
## Ligand CLA 9 604



Bond lengths



Bond angles

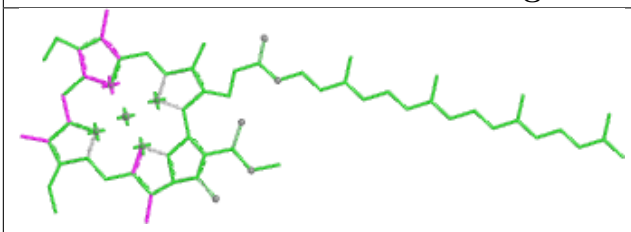


Torsions

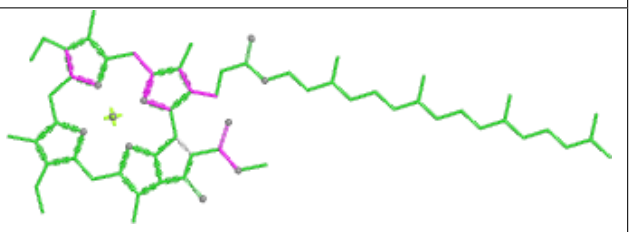


Rings

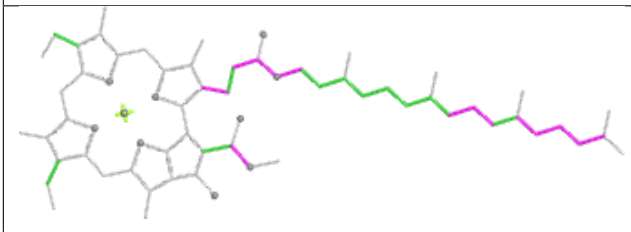
## Ligand CLA A 841



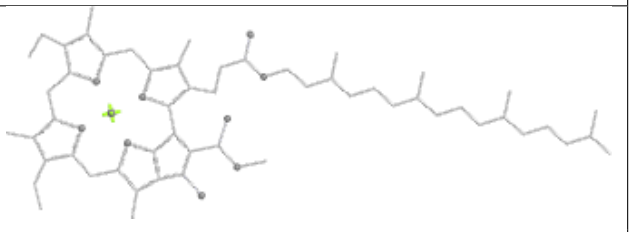
Bond lengths



Bond angles

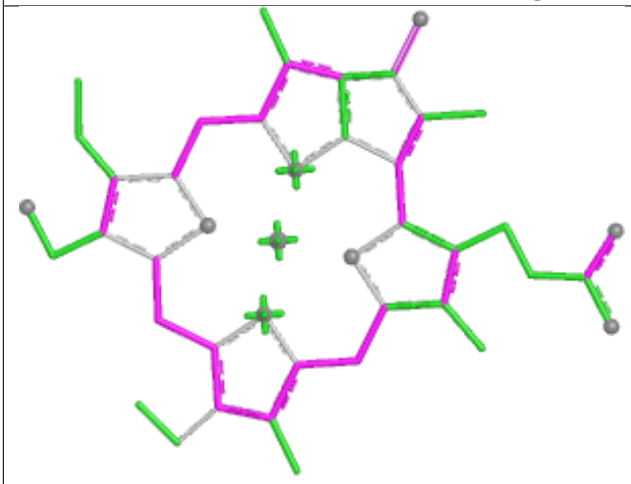


Torsions

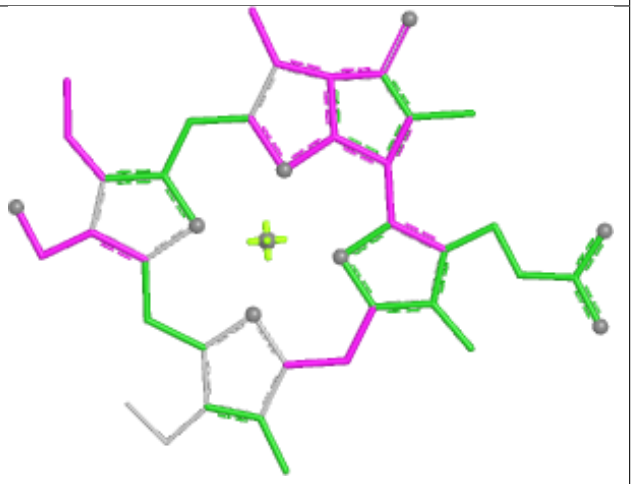


Rings

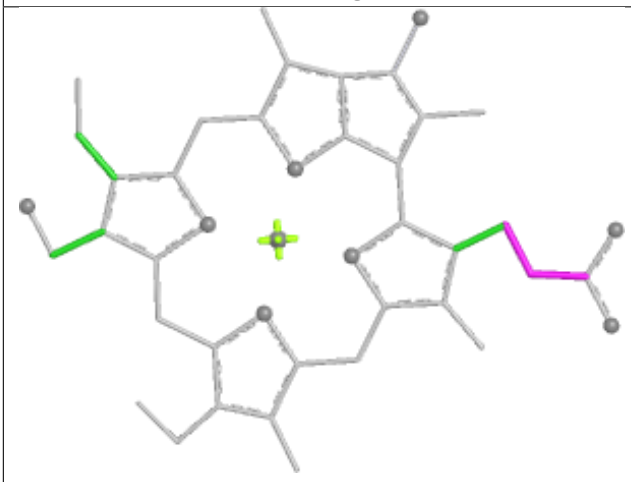
## Ligand CHL c 605



Bond lengths



Bond angles

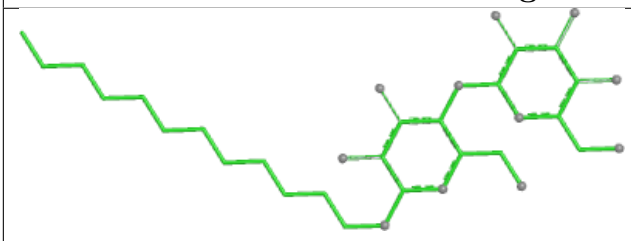


Torsions

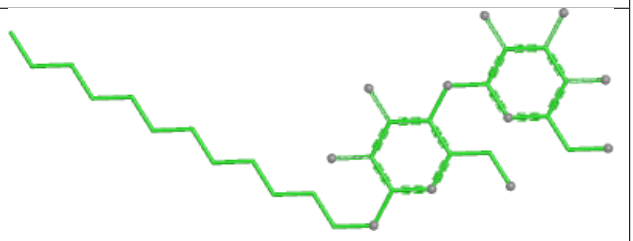


Rings

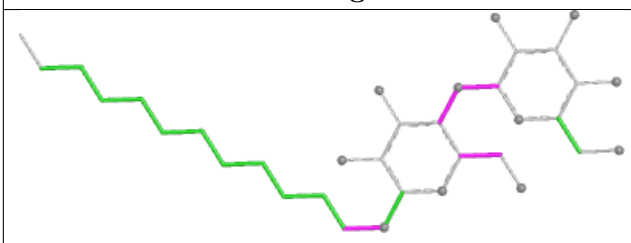
## Ligand LMU O 206



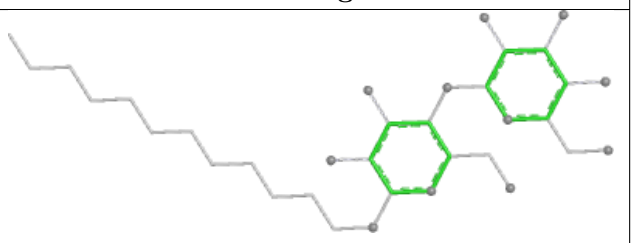
Bond lengths



Bond angles

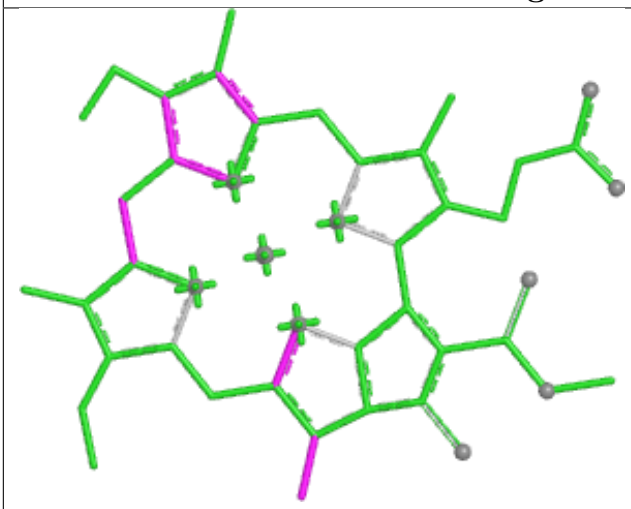


Torsions

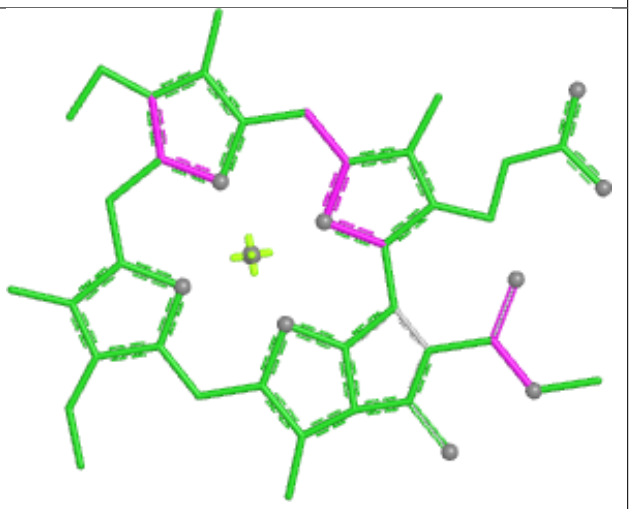


Rings

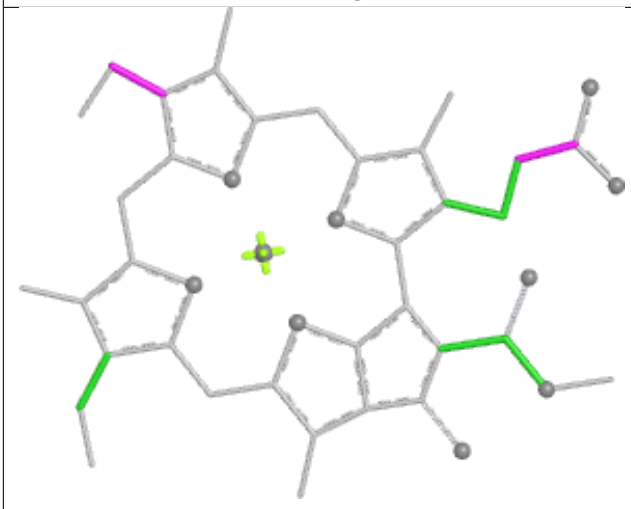
## Ligand CLA b 312



Bond lengths



Bond angles

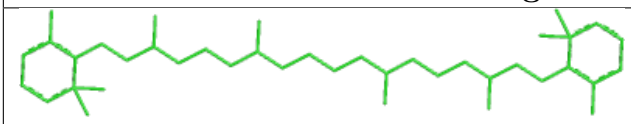


Torsions

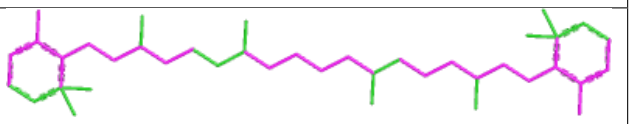


Rings

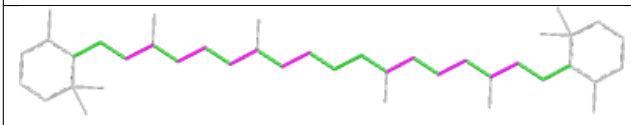
## Ligand BCR B 844



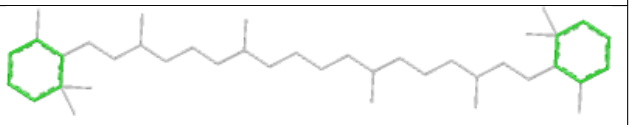
Bond lengths



Bond angles

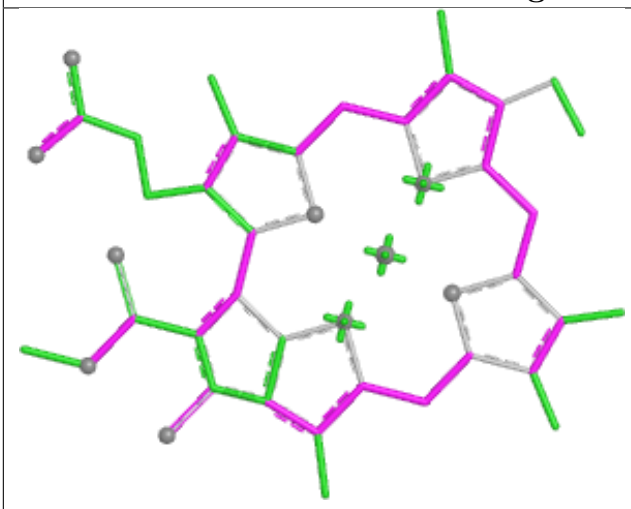


Torsions

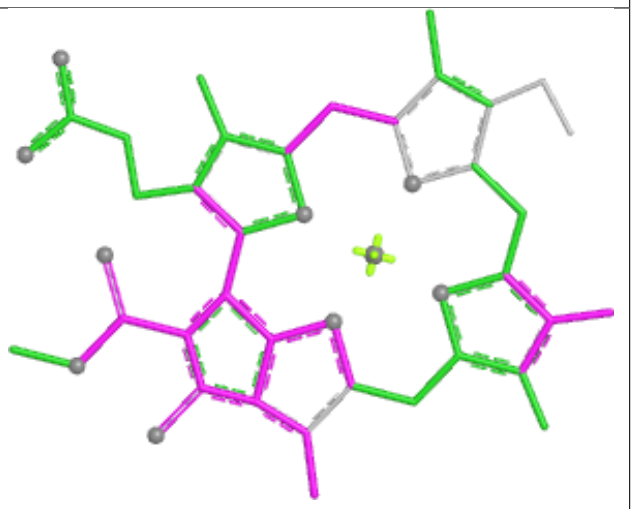


Rings

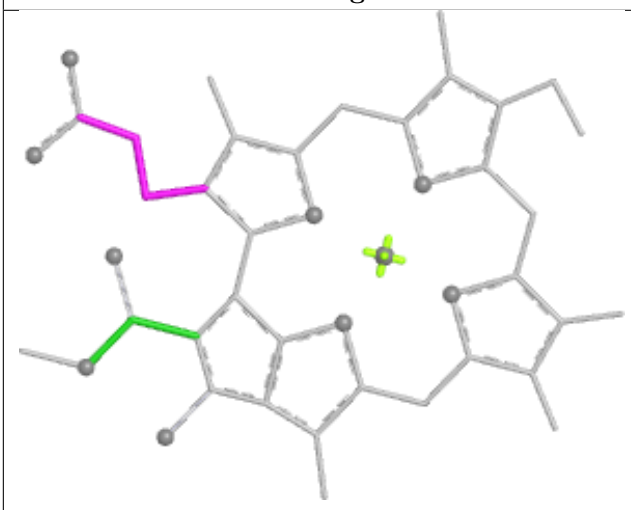
**Ligand CHL 6 601**



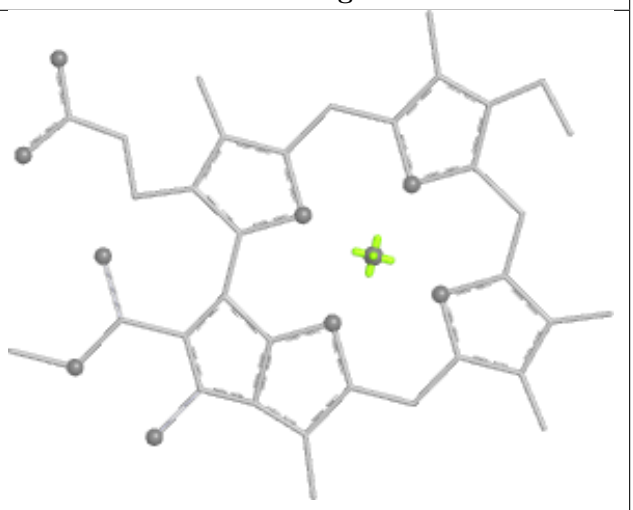
**Bond lengths**



**Bond angles**

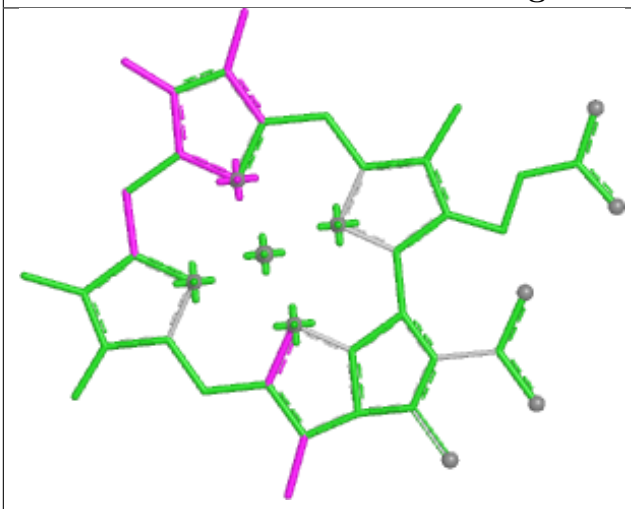


**Torsions**

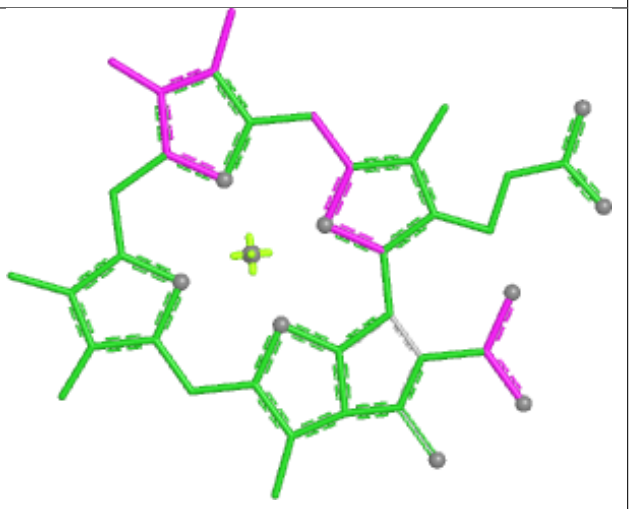


**Rings**

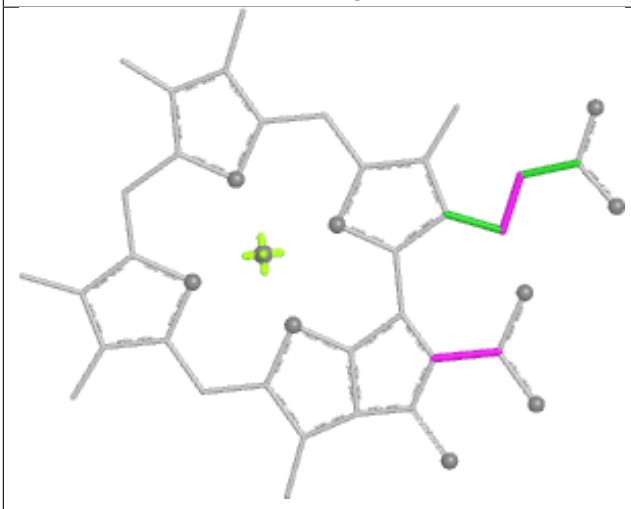
**Ligand CLA 7 403**



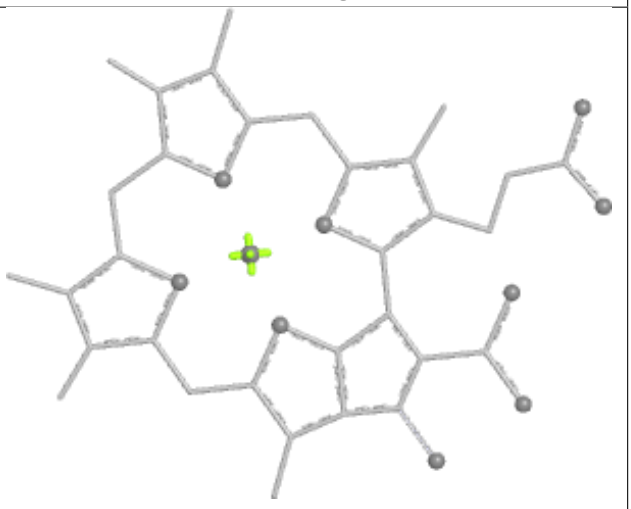
**Bond lengths**



**Bond angles**

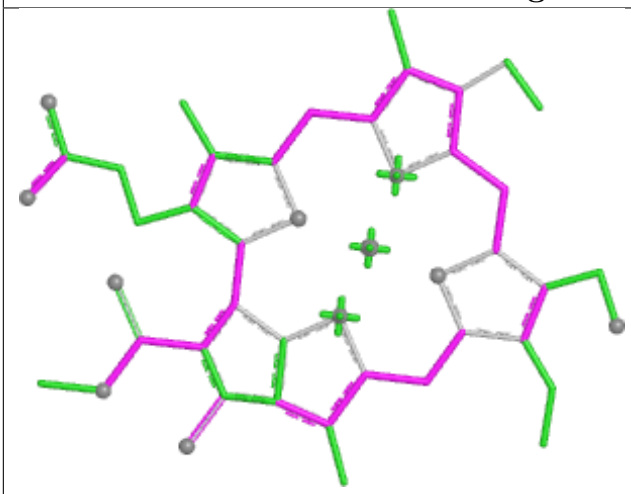


**Torsions**

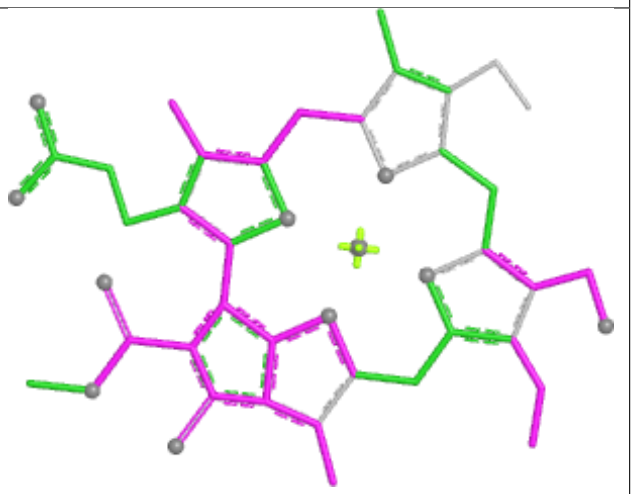


**Rings**

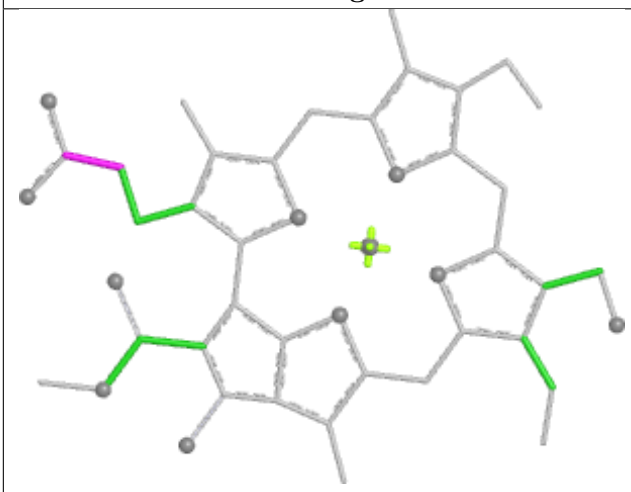
**Ligand CHL 2 606**



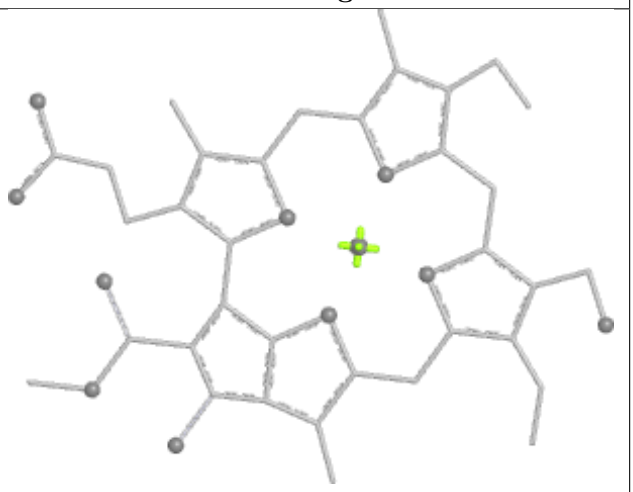
**Bond lengths**



**Bond angles**

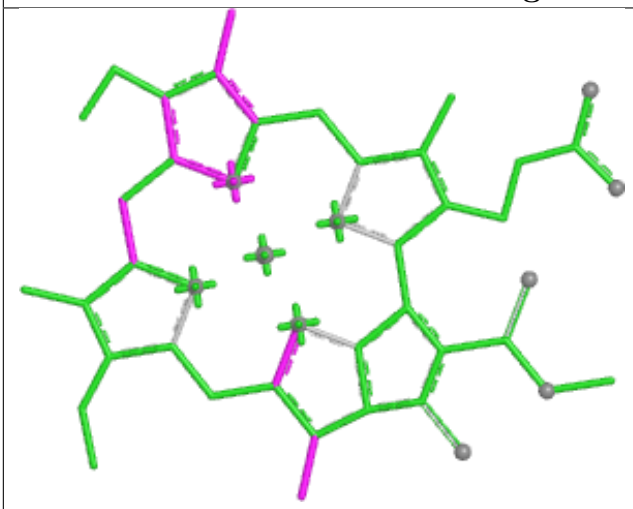


**Torsions**

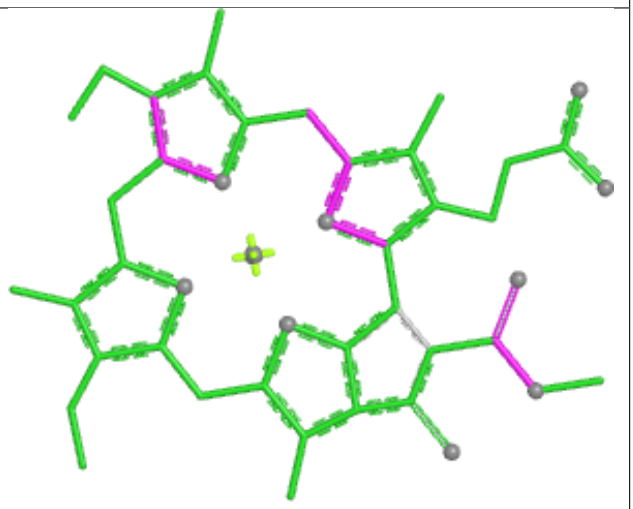


**Rings**

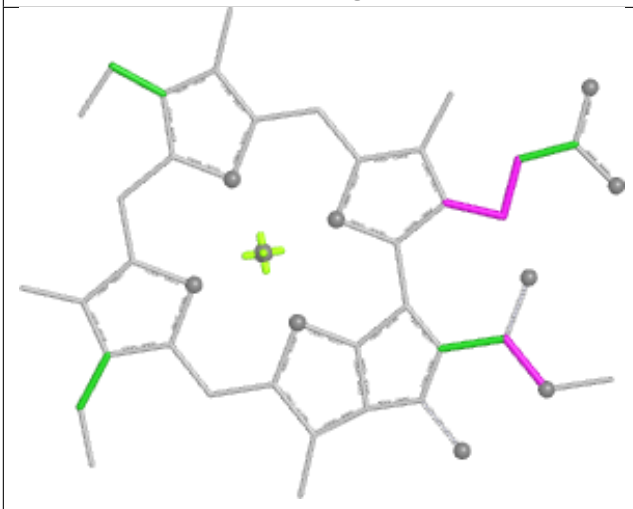
**Ligand CLA G 202**



**Bond lengths**



**Bond angles**

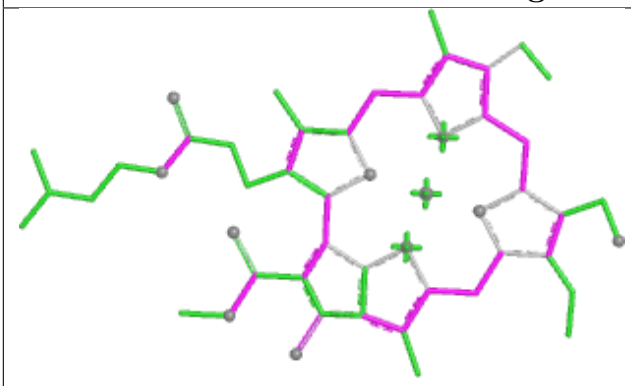


**Torsions**

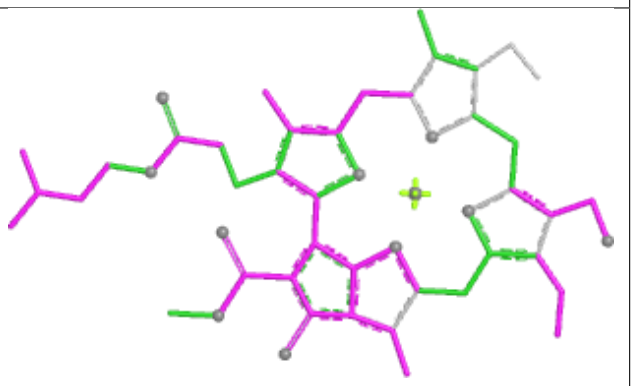


**Rings**

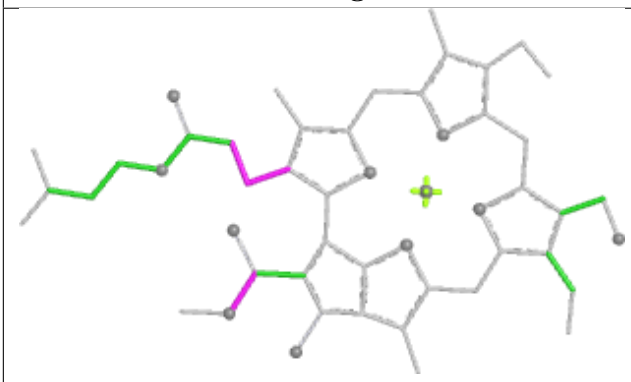
**Ligand CHL 4 607**



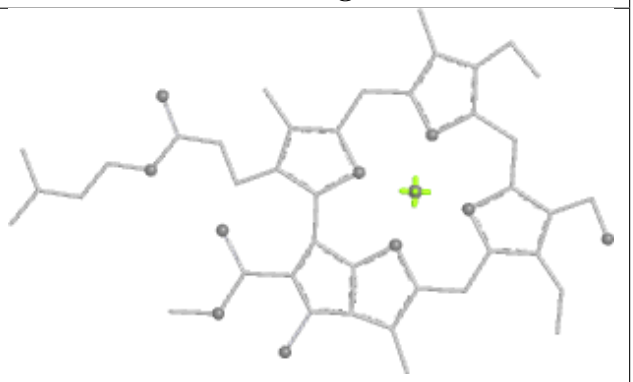
**Bond lengths**



**Bond angles**

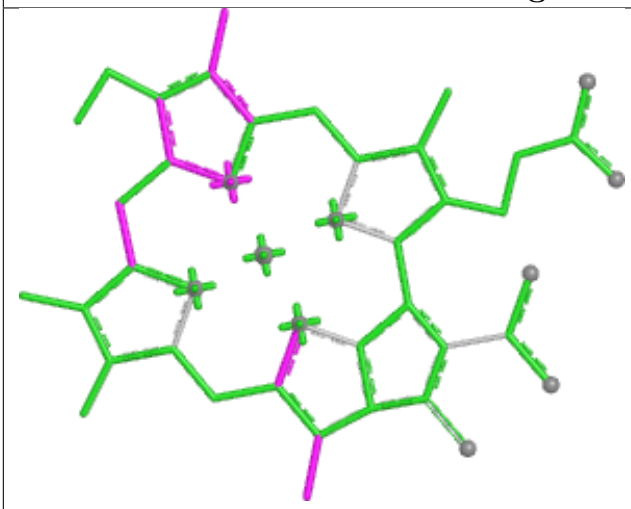


**Torsions**

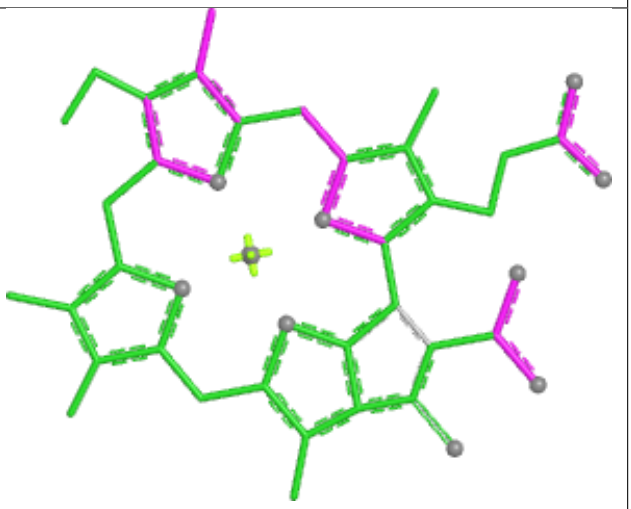


**Rings**

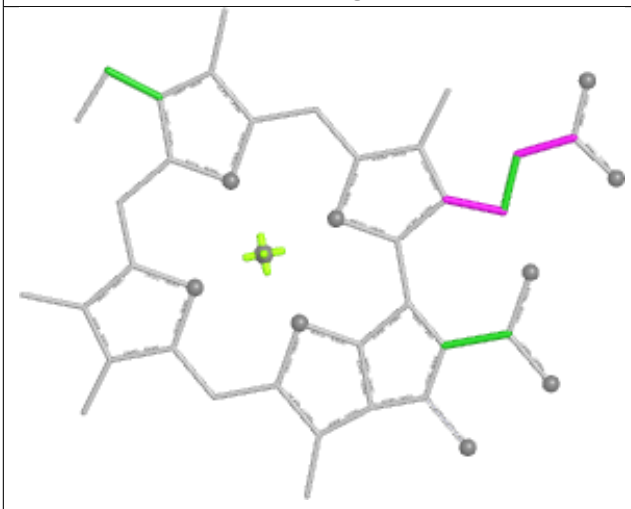
## Ligand CLA 1 310



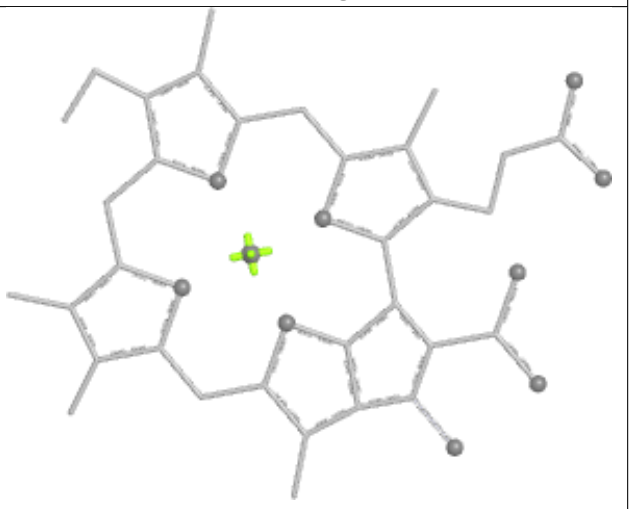
Bond lengths



Bond angles

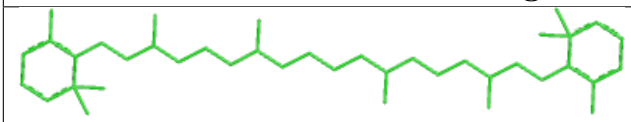


Torsions

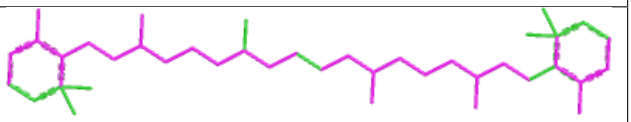


Rings

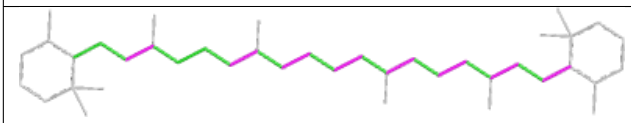
## Ligand BCR B 843



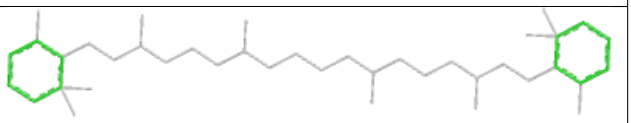
Bond lengths



Bond angles

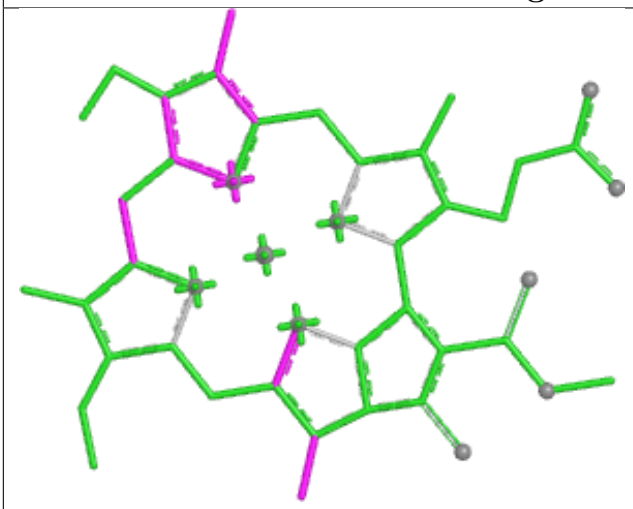


Torsions

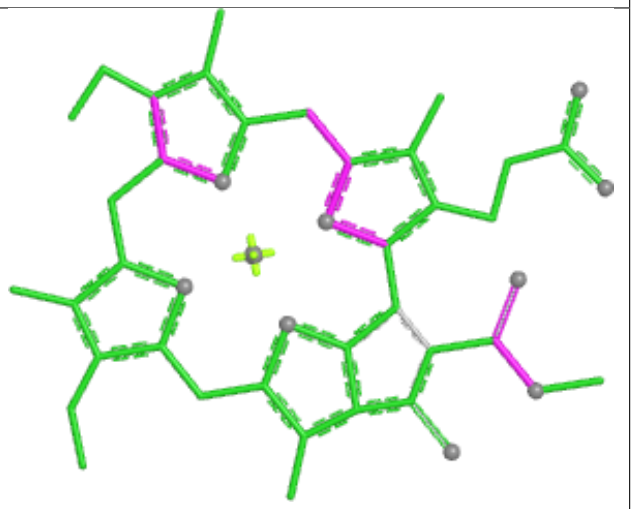


Rings

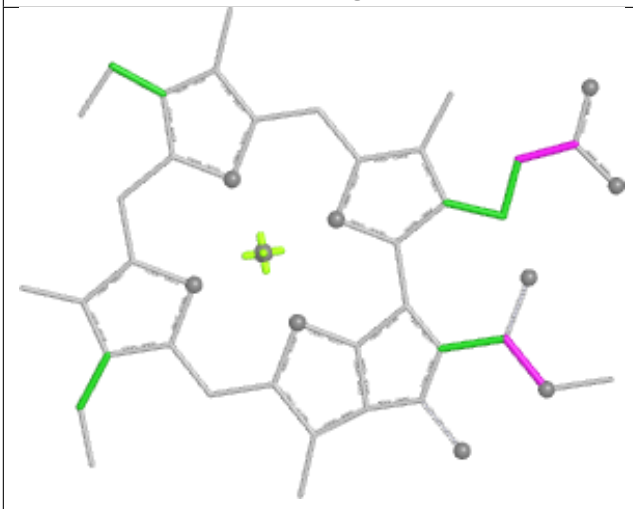
**Ligand CLA b 304**



**Bond lengths**



**Bond angles**

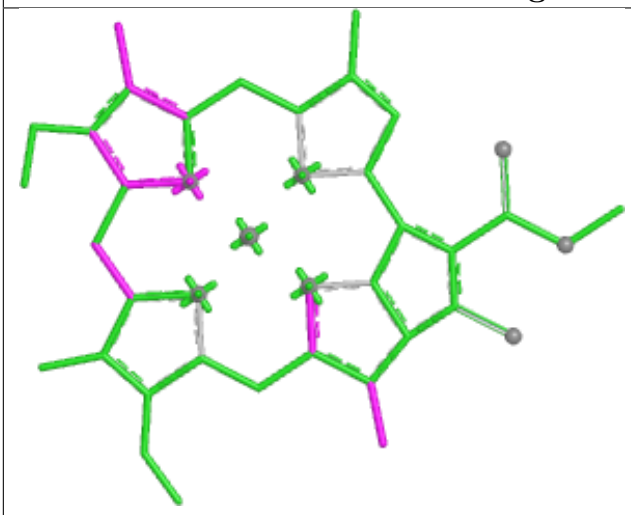


**Torsions**

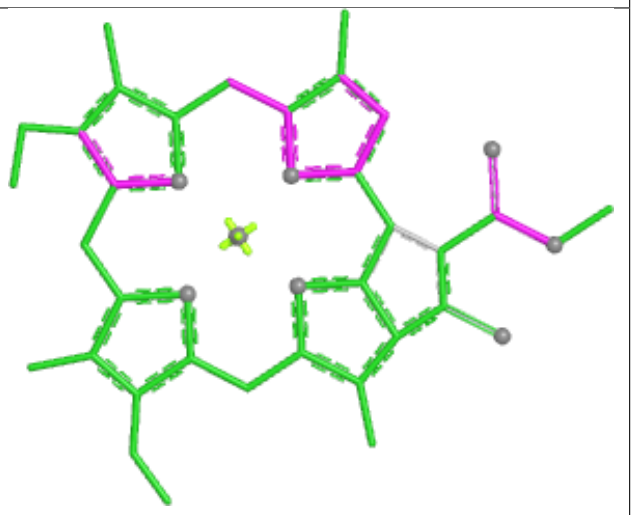


**Rings**

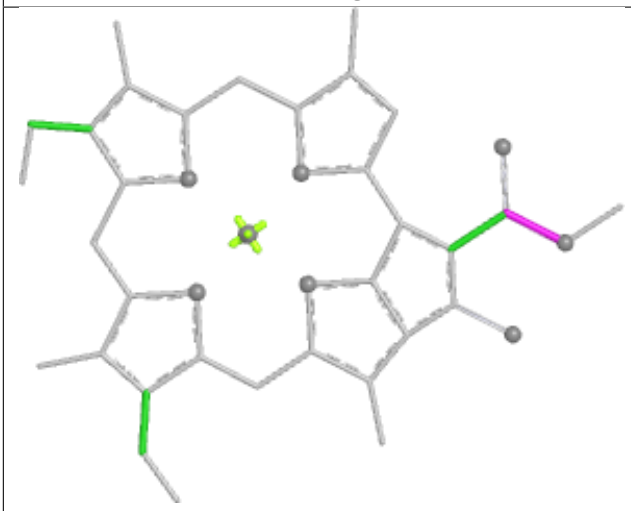
**Ligand CLA 1 306**



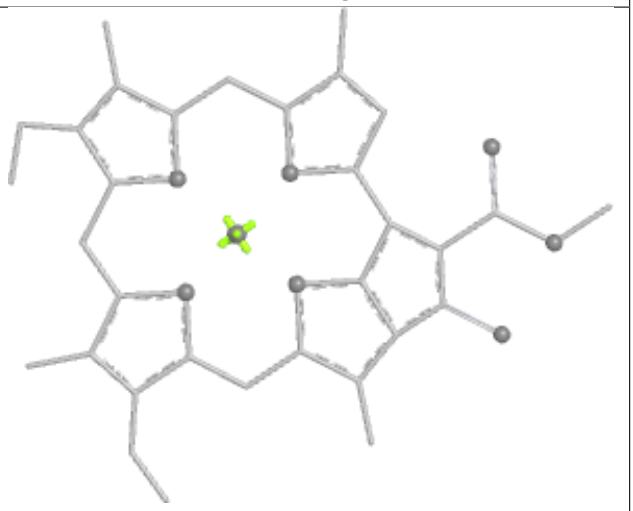
**Bond lengths**



**Bond angles**

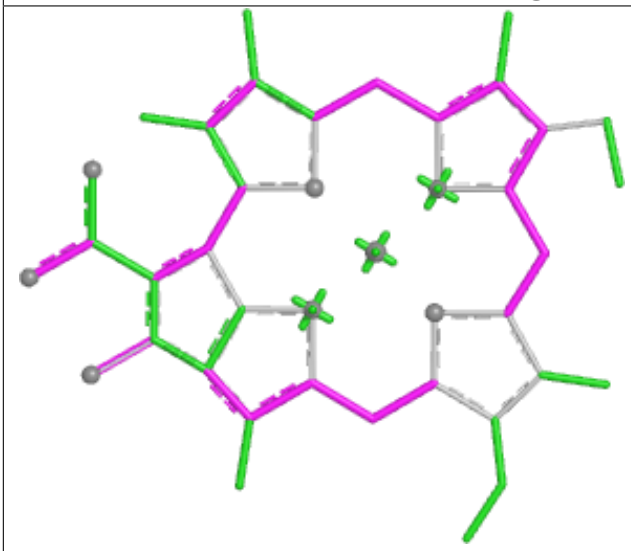


**Torsions**

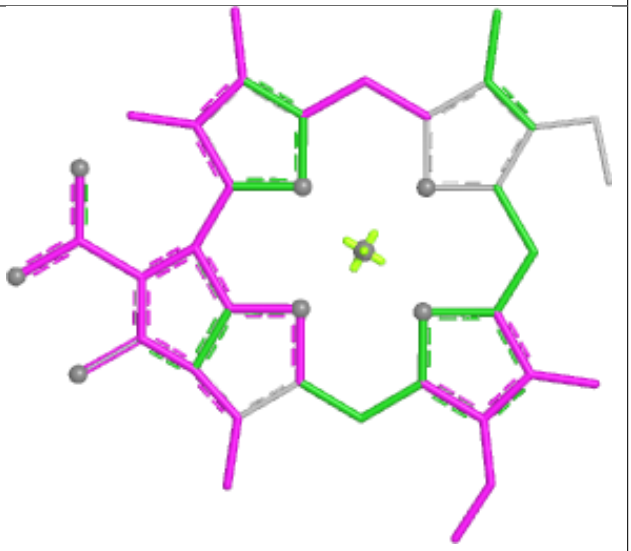


**Rings**

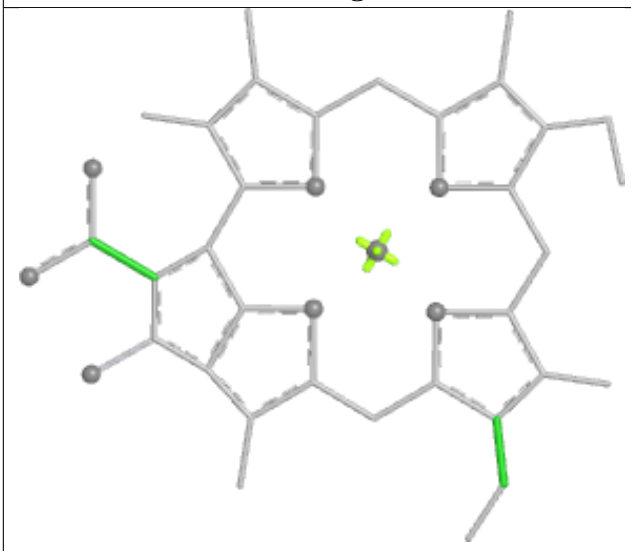
**Ligand CHL 3 407**



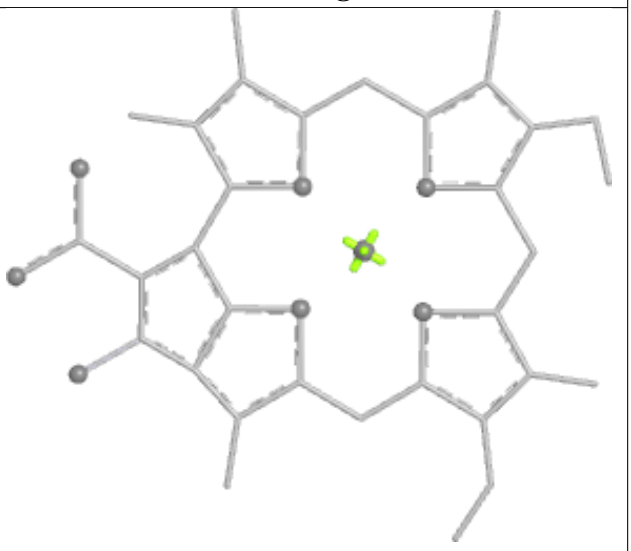
**Bond lengths**



**Bond angles**

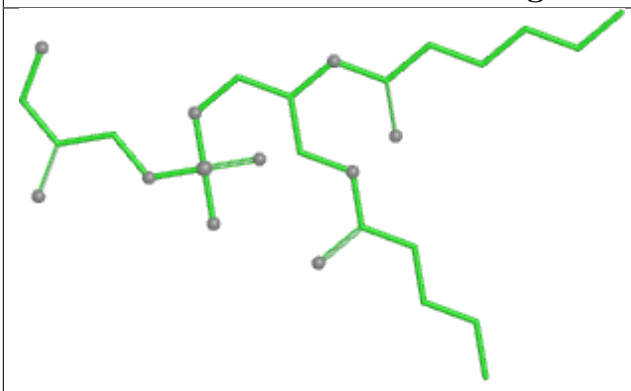


**Torsions**

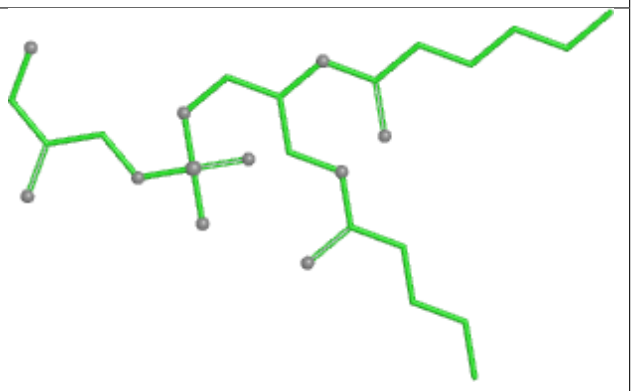


**Rings**

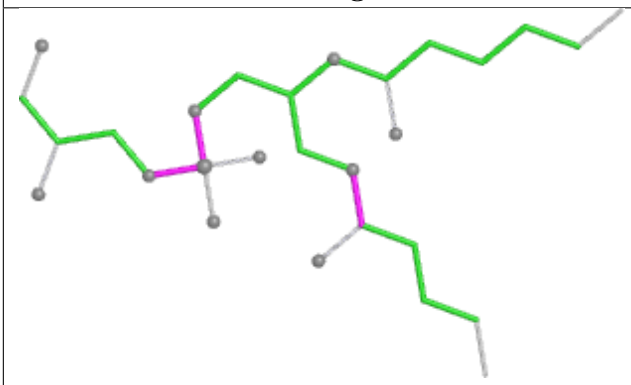
**Ligand LHG 1 319**



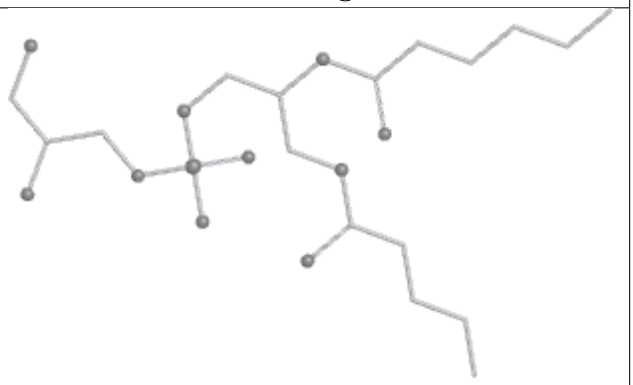
**Bond lengths**



**Bond angles**

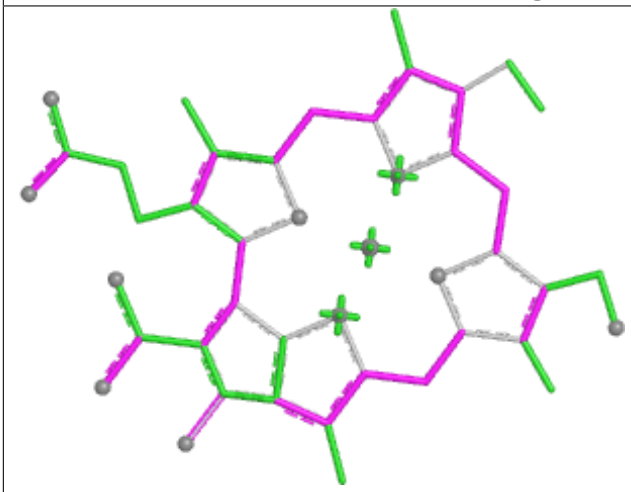


**Torsions**

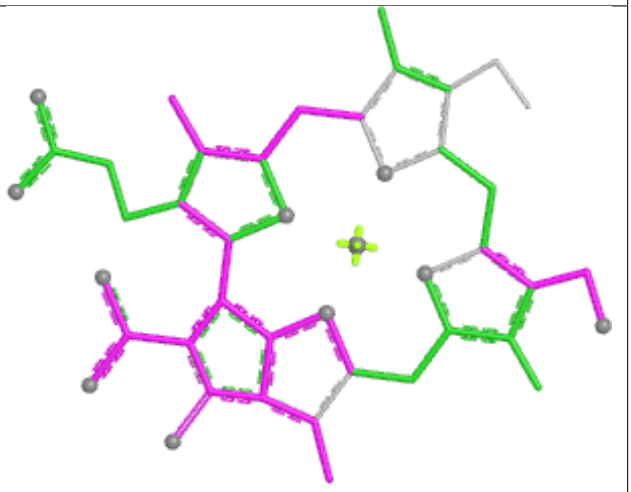


**Rings**

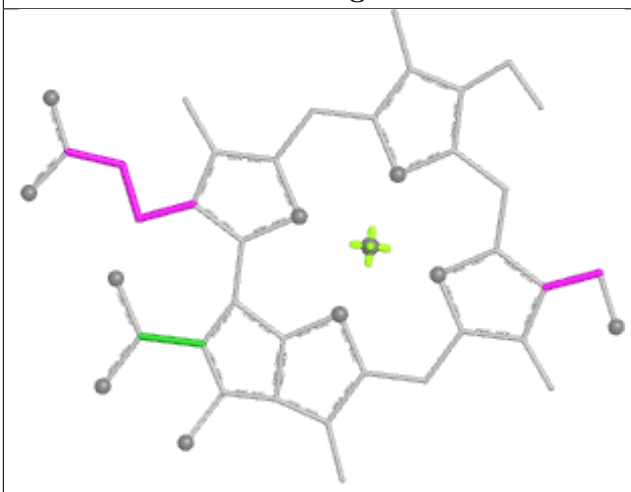
**Ligand CHL c 609**



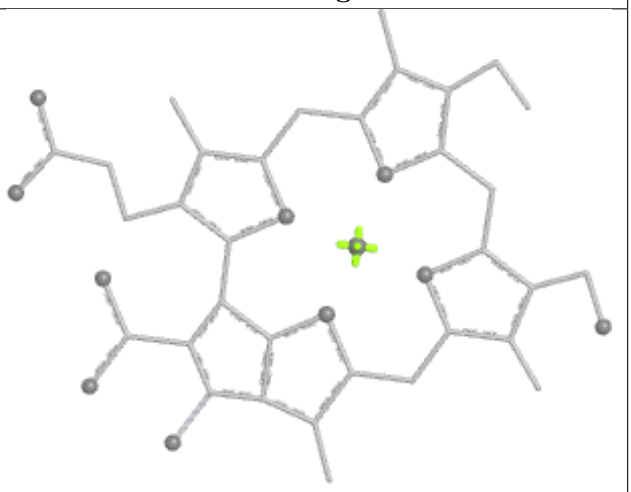
**Bond lengths**



**Bond angles**

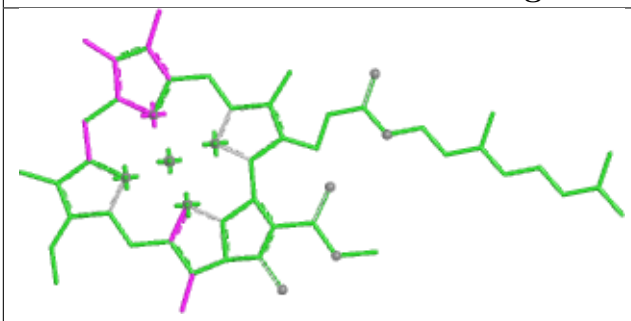


**Torsions**

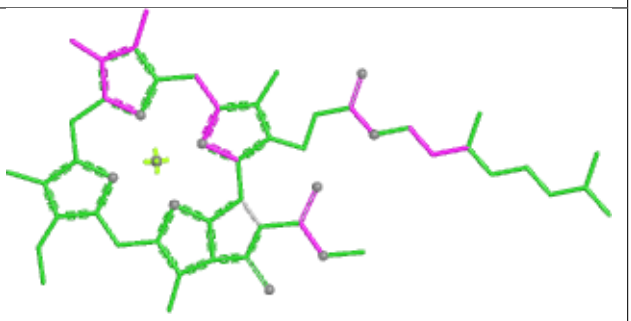


**Rings**

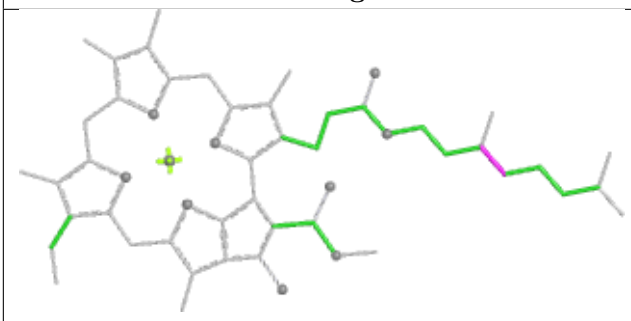
## Ligand CLA B 810



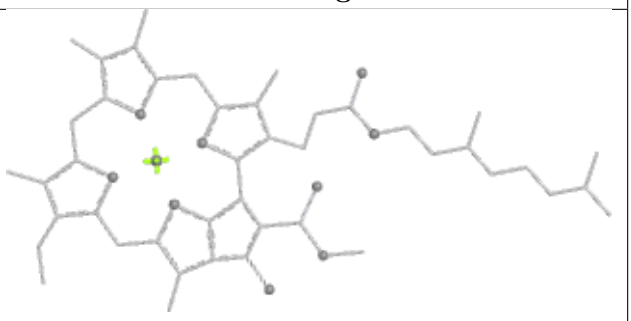
Bond lengths



Bond angles

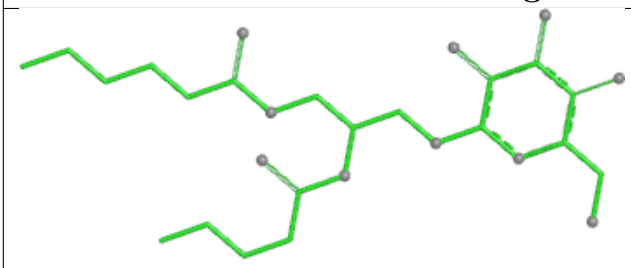


Torsions

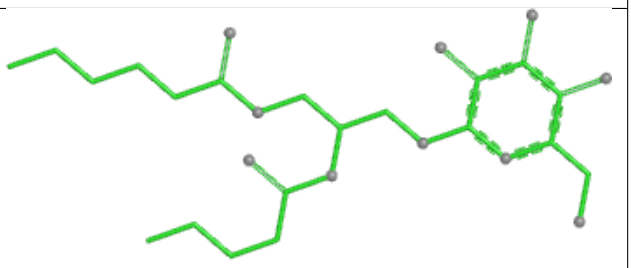


Rings

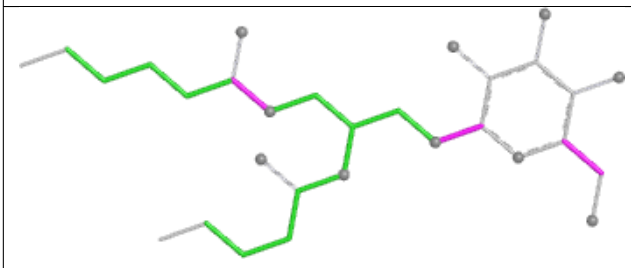
## Ligand LMG J 105



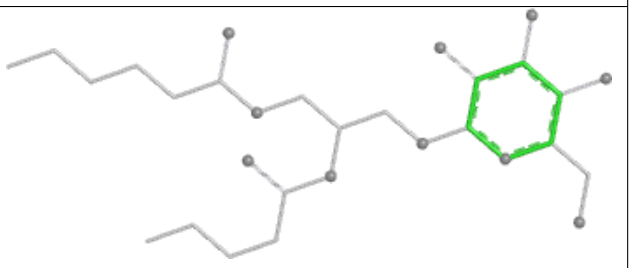
Bond lengths



Bond angles

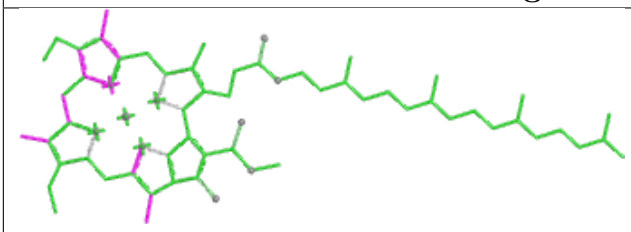


Torsions

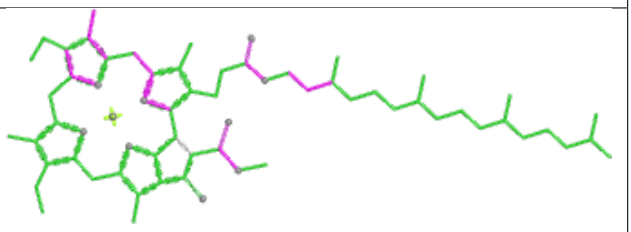


Rings

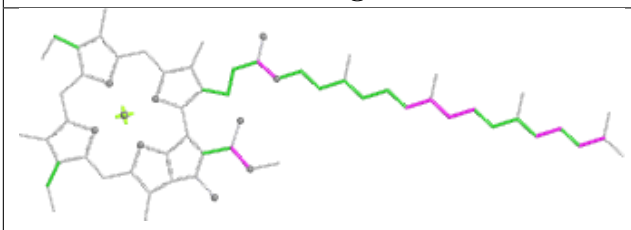
## Ligand CLA A 821



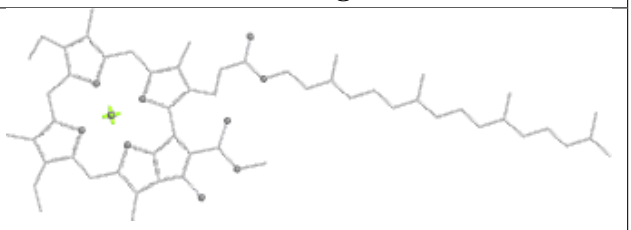
Bond lengths



Bond angles

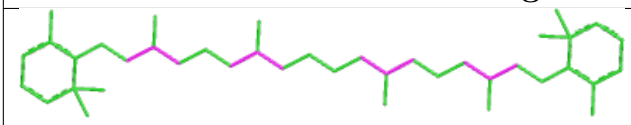


Torsions



Rings

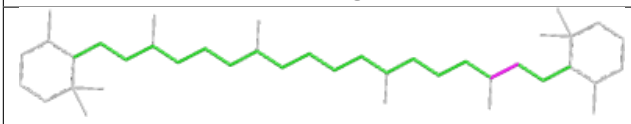
## Ligand BCR A 849



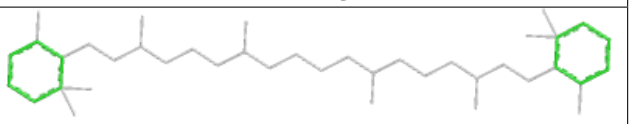
Bond lengths



Bond angles

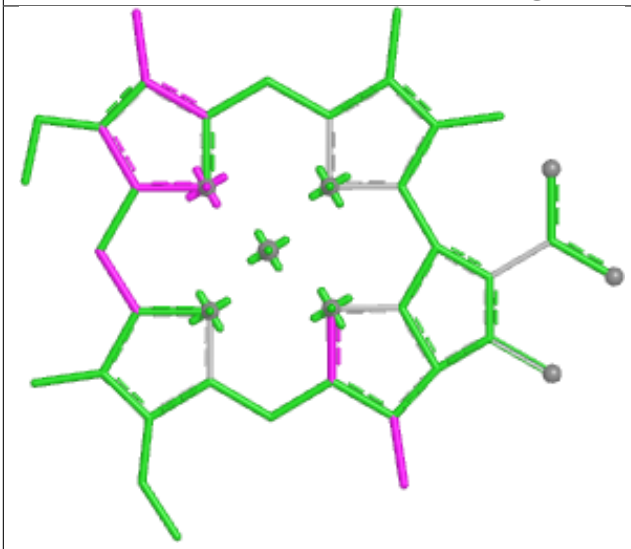


Torsions

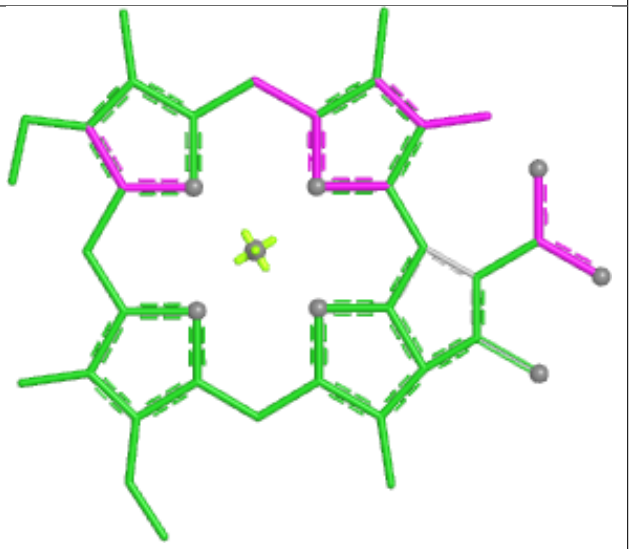


Rings

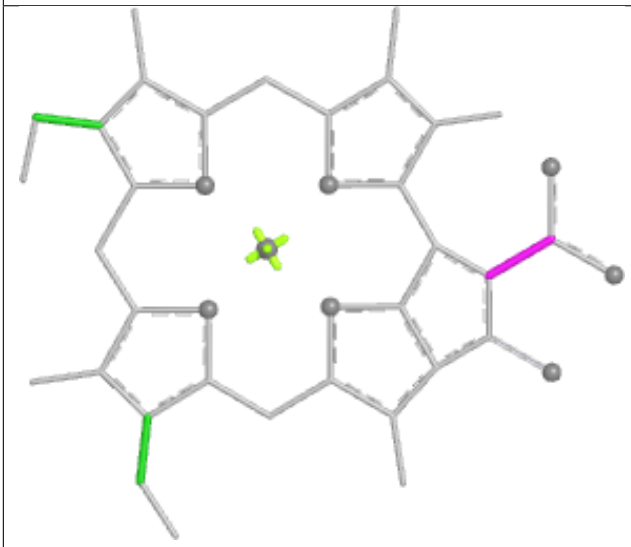
**Ligand CLA 7 409**



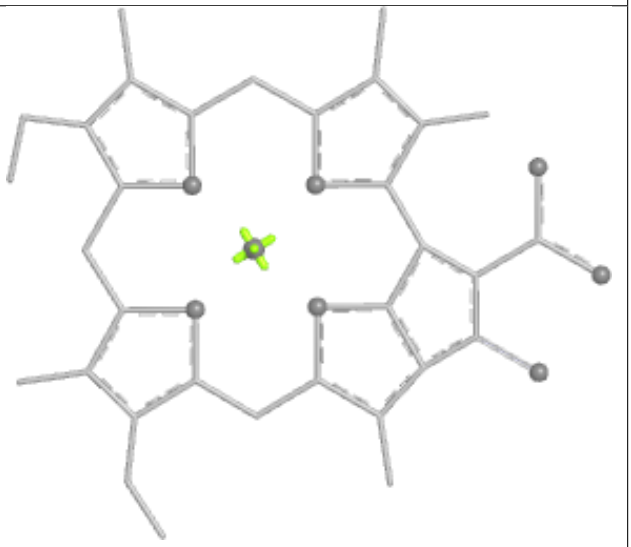
**Bond lengths**



**Bond angles**

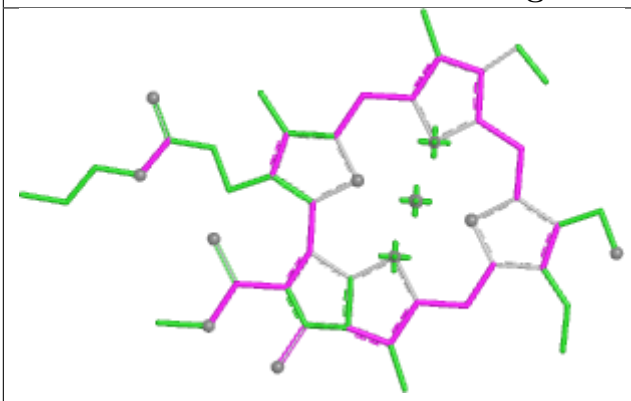


**Torsions**

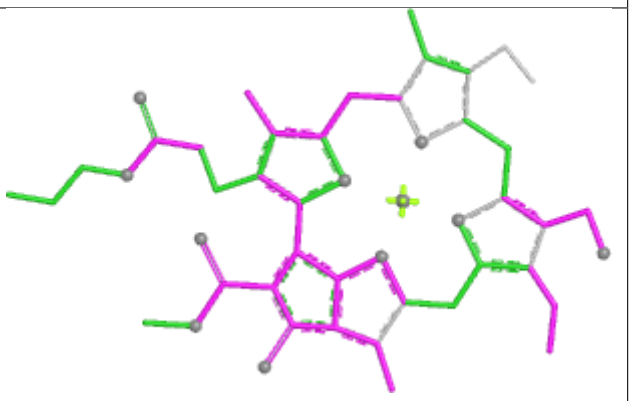


**Rings**

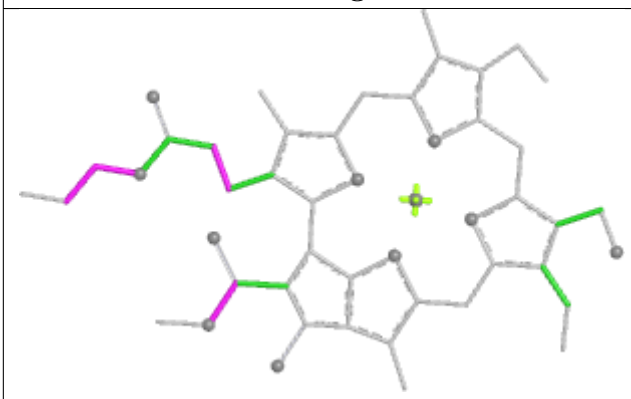
## Ligand CHL b 309



Bond lengths



Bond angles

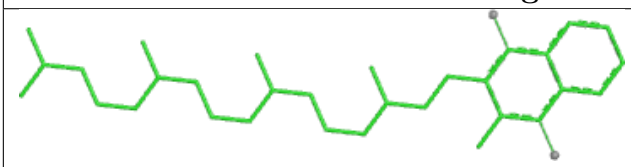


Torsions

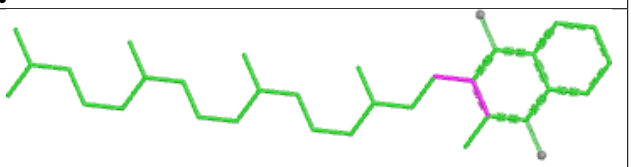


Rings

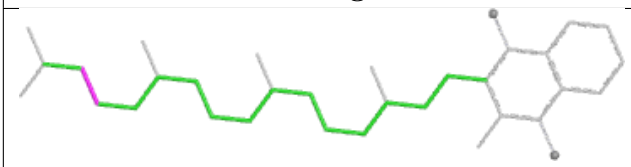
## Ligand PQN A 843



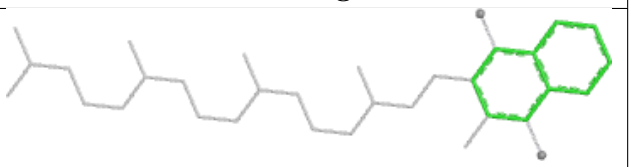
Bond lengths



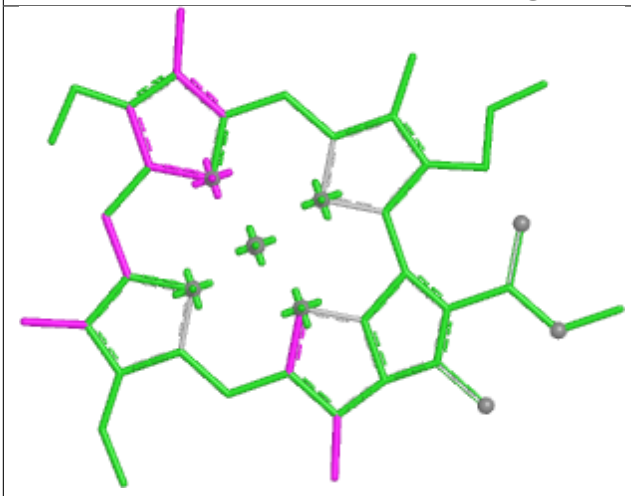
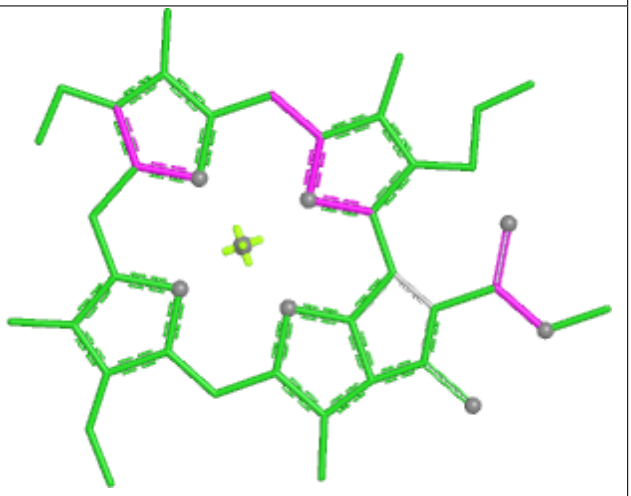
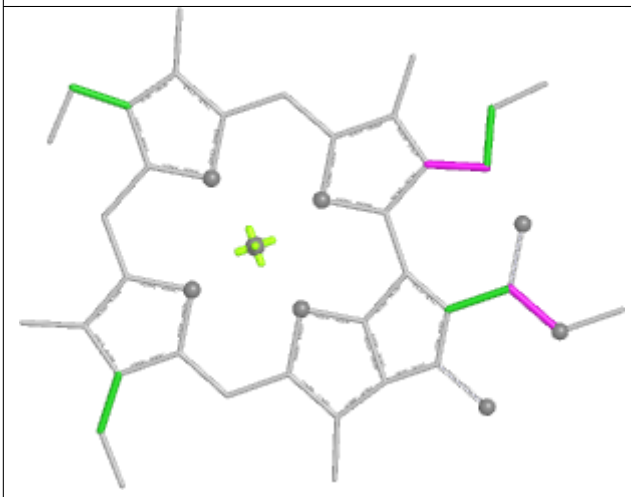
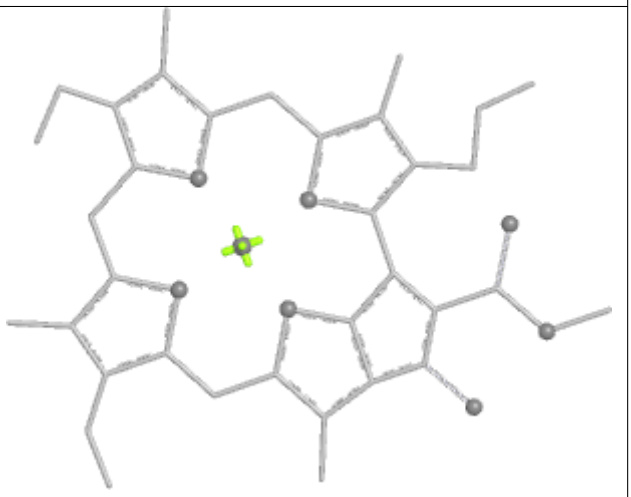
Bond angles



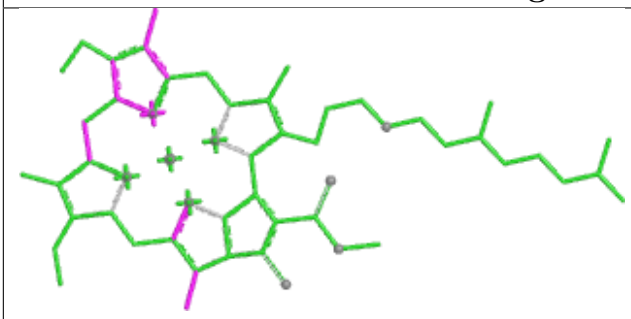
Torsions



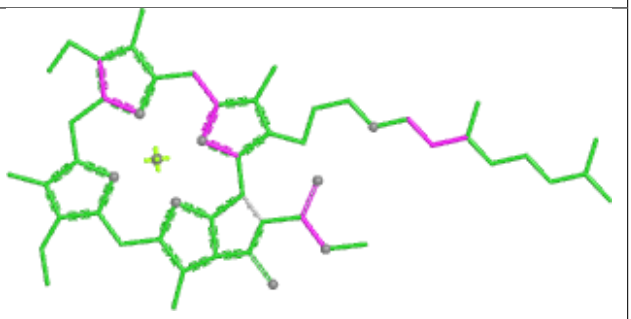
Rings

| Ligand CLA B 819 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

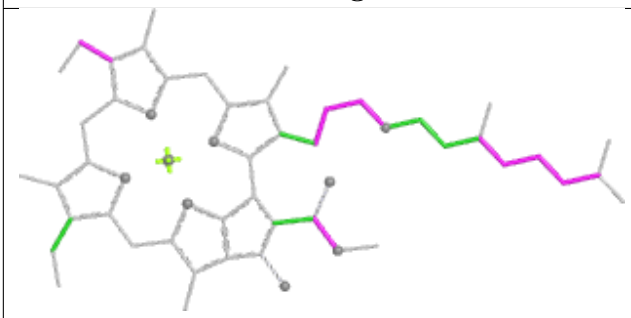
**Ligand CLA 8 611**



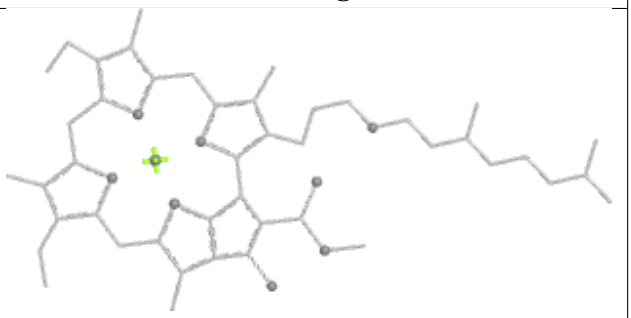
**Bond lengths**



**Bond angles**

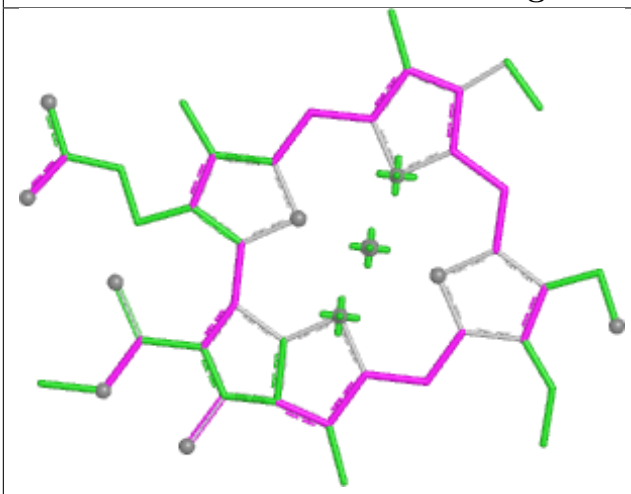


**Torsions**

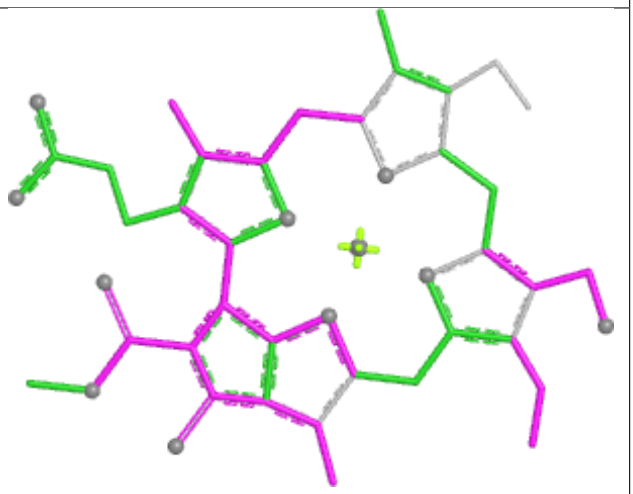


**Rings**

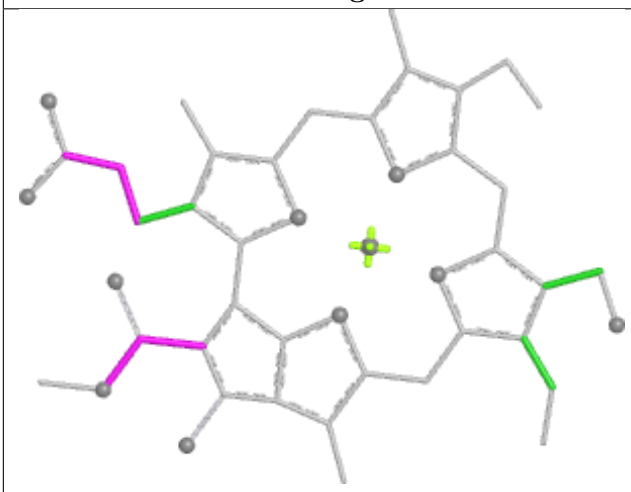
## Ligand CHL 6 606



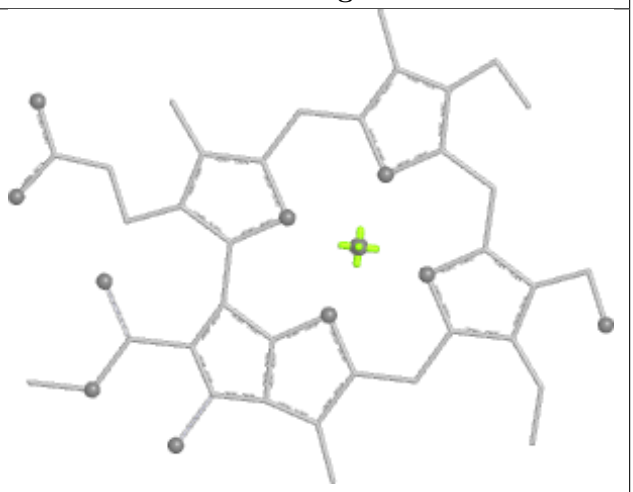
Bond lengths



Bond angles

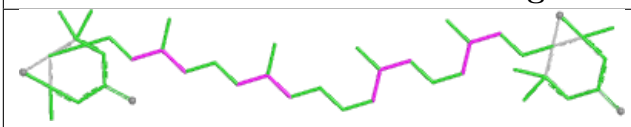


Torsions

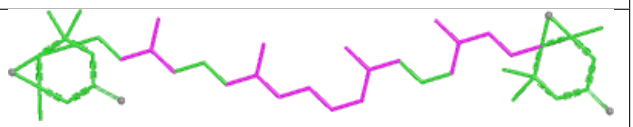


Rings

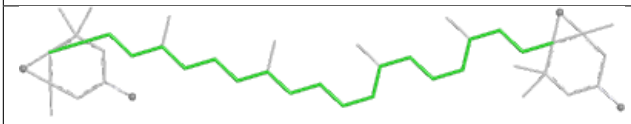
## Ligand XAT 2 617



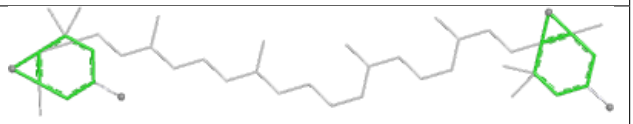
Bond lengths



Bond angles

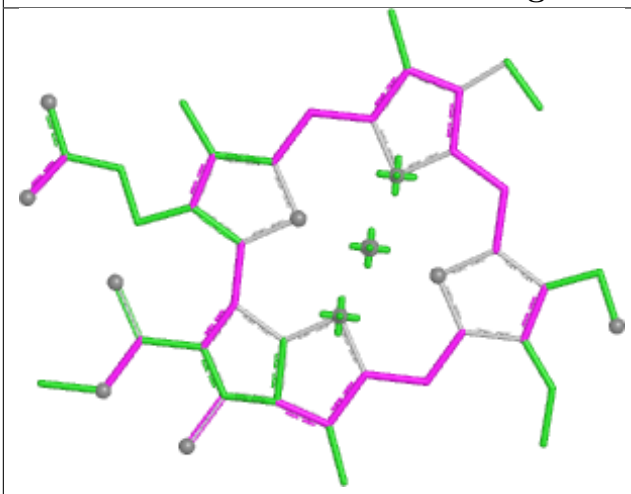


Torsions

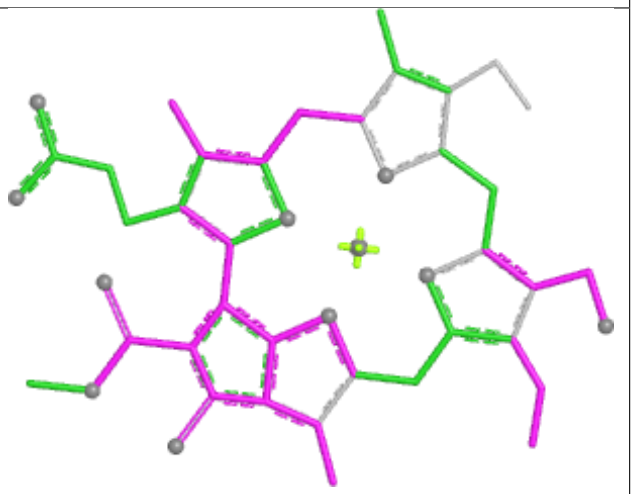


Rings

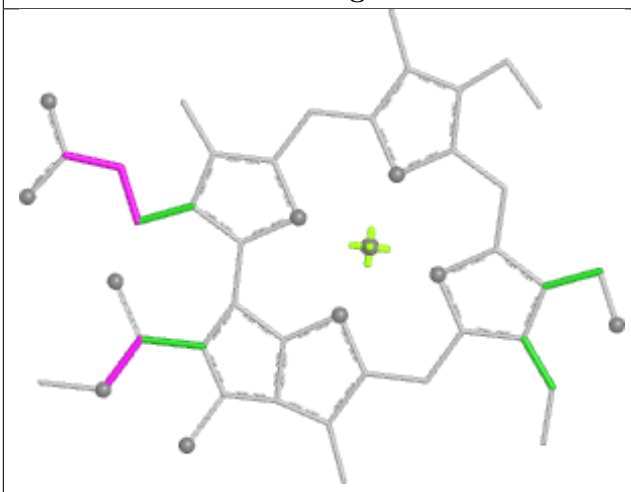
**Ligand CHL 8 606**



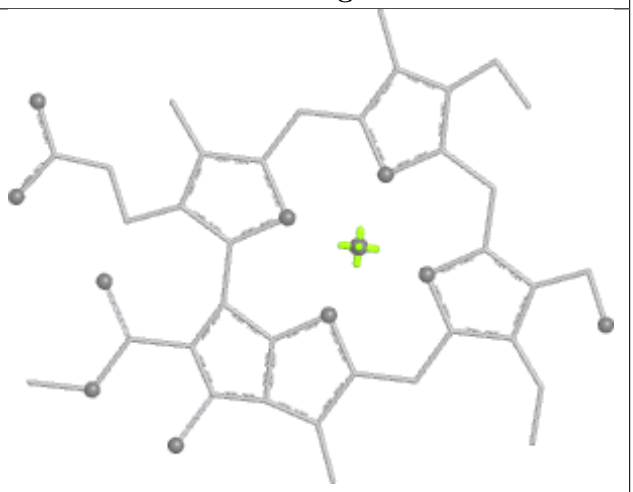
**Bond lengths**



**Bond angles**

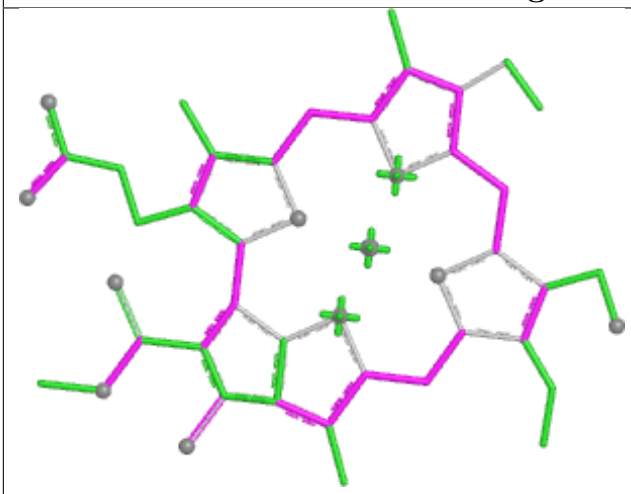


**Torsions**

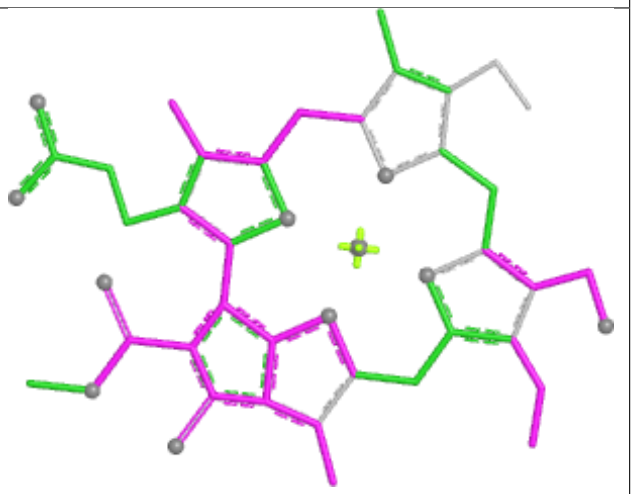


**Rings**

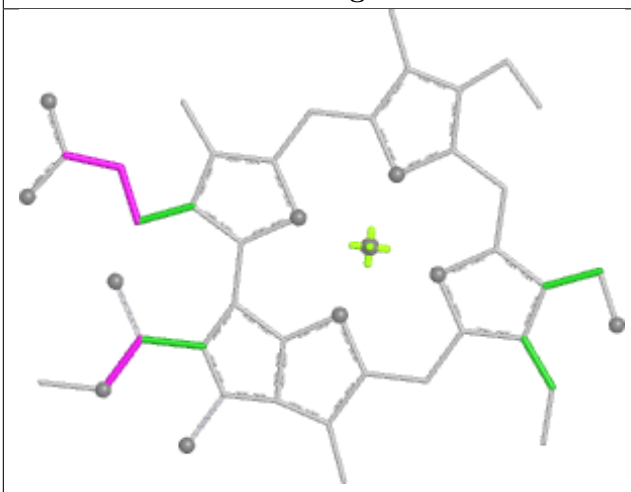
## Ligand CHL 9 608



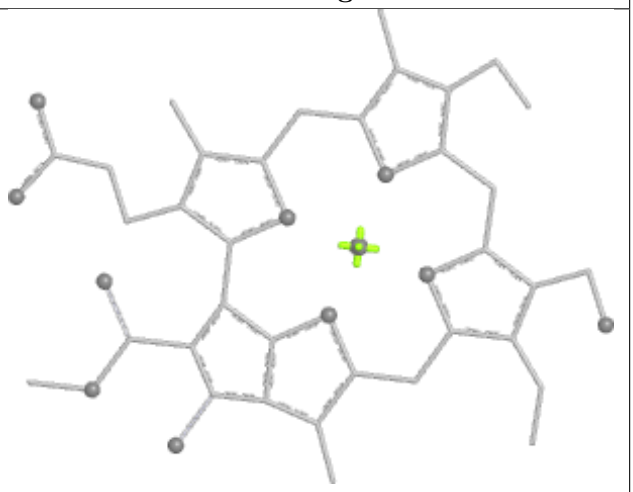
Bond lengths



Bond angles

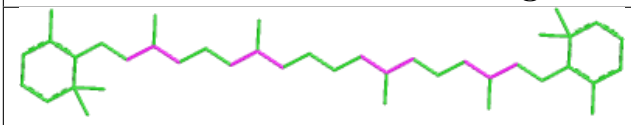


Torsions



Rings

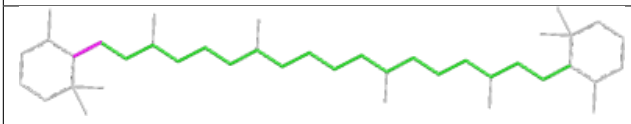
## Ligand BCR G 205



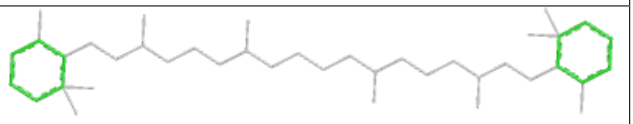
Bond lengths



Bond angles

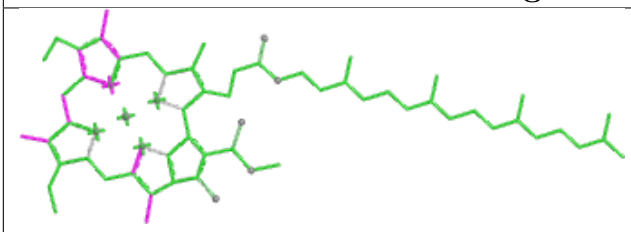


Torsions

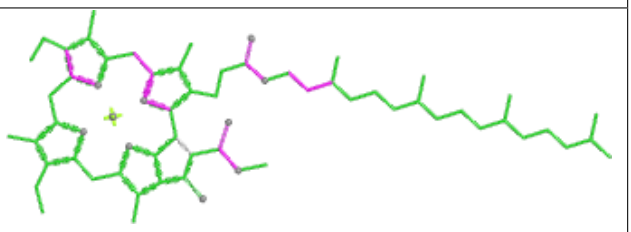


Rings

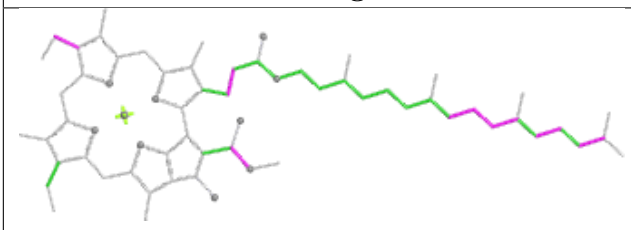
**Ligand CLA A 840**



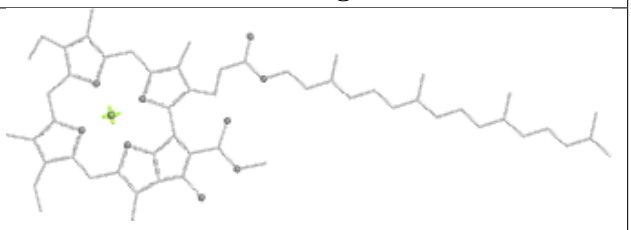
Bond lengths



Bond angles

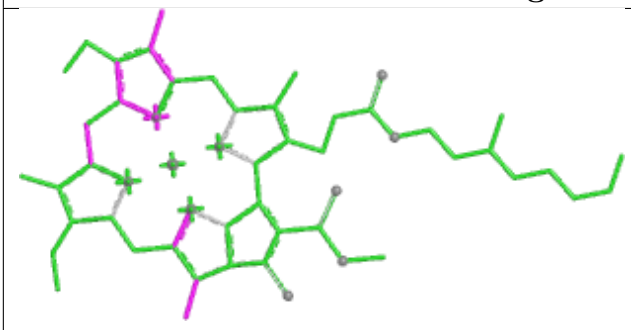


Torsions

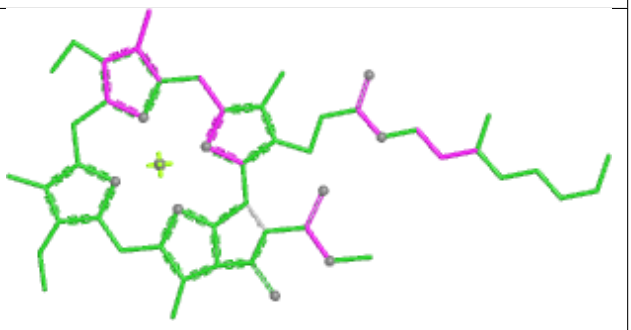


Rings

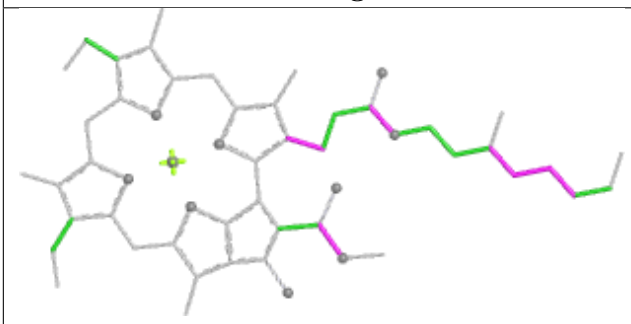
**Ligand CLA b 311**



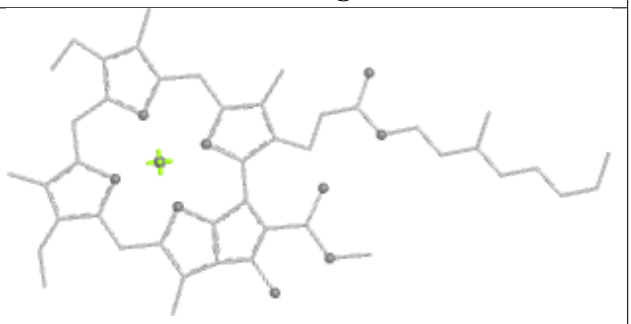
Bond lengths



Bond angles

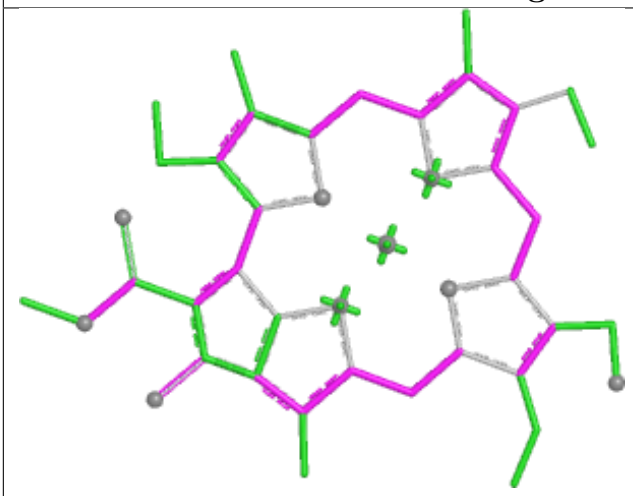


Torsions

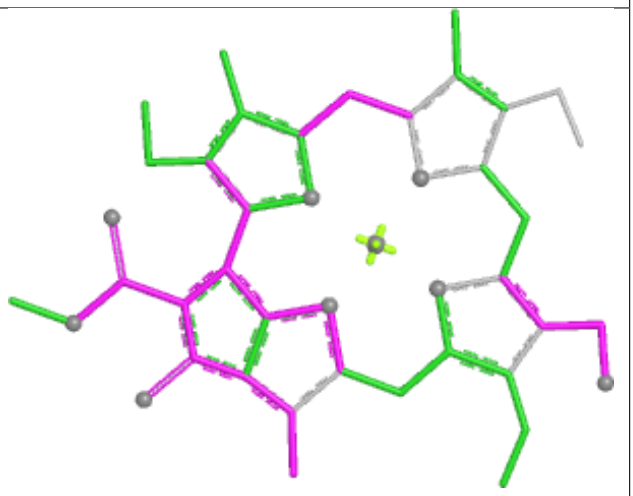


Rings

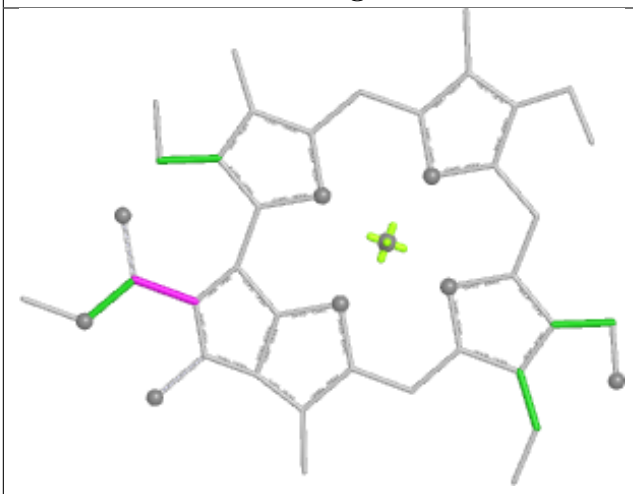
**Ligand CHL a 607**



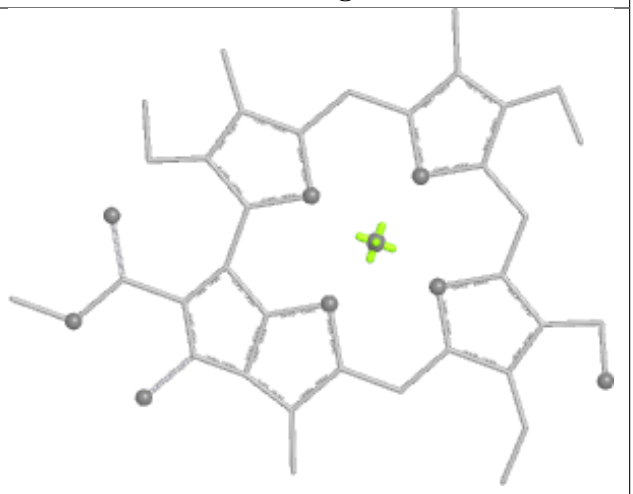
**Bond lengths**



**Bond angles**

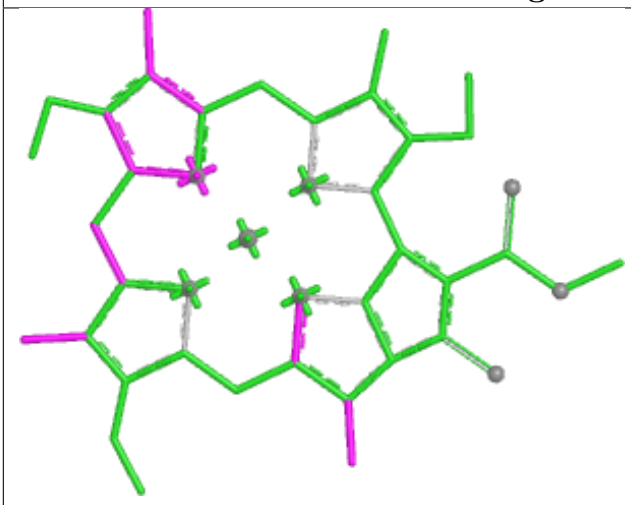


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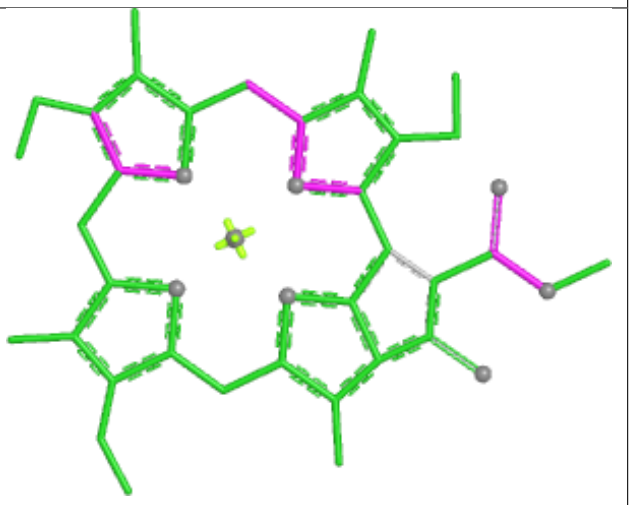


**Rings**

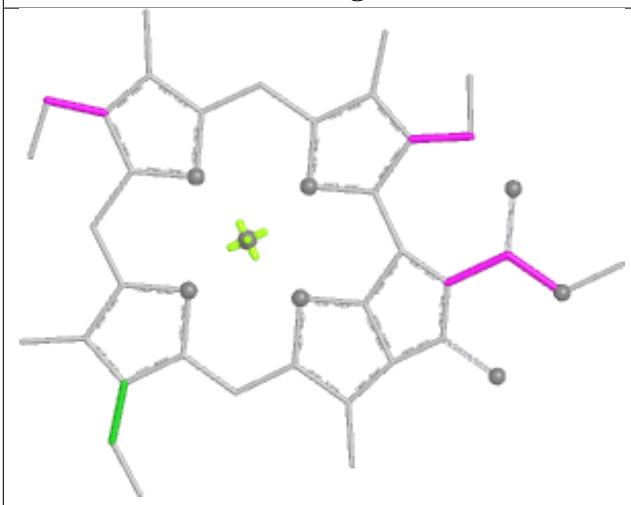
## Ligand CLA J 102



Bond lengths



Bond angles

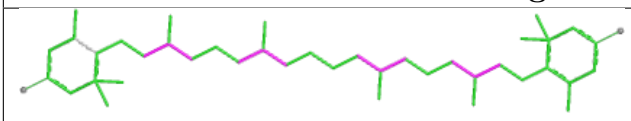


Torsions

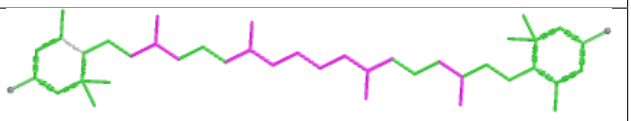


Rings

## Ligand LUT a 616



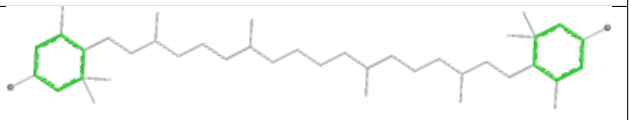
Bond lengths



Bond angles

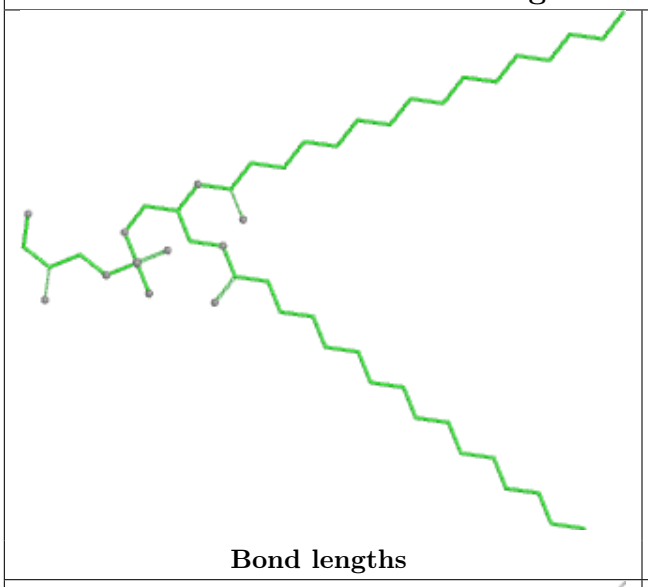


Torsions

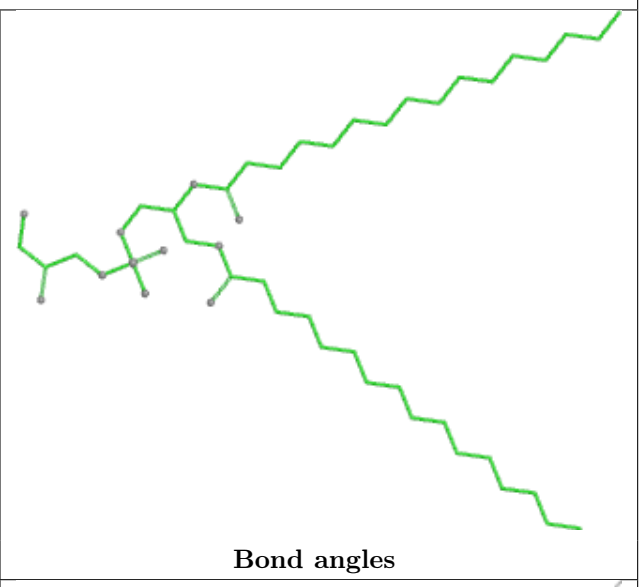


Rings

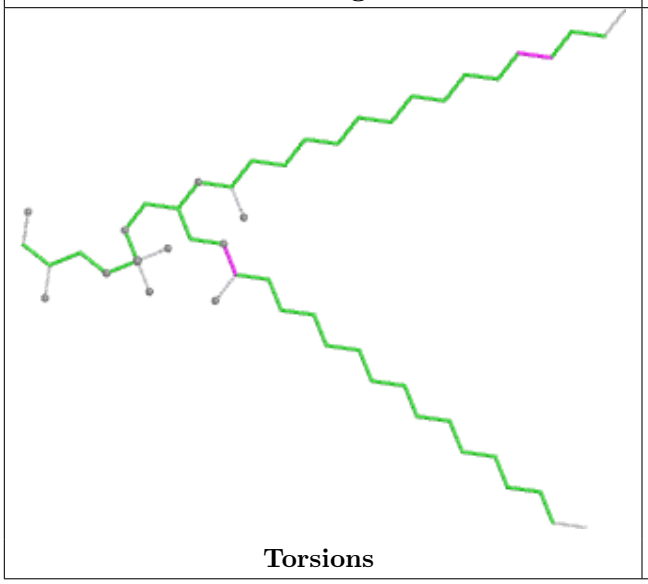
**Ligand LHG c 619**



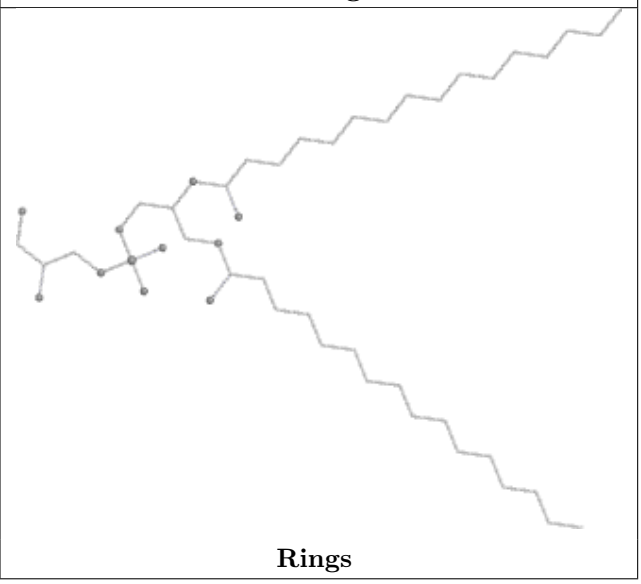
Bond lengths



Bond angles



Torsions

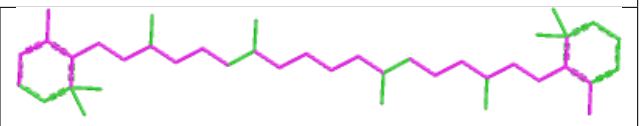


Rings

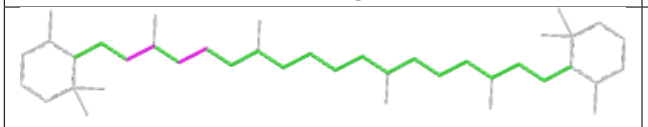
**Ligand BCR B 846**



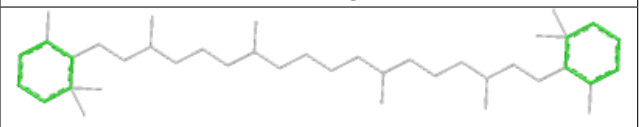
Bond lengths



Bond angles



Torsions

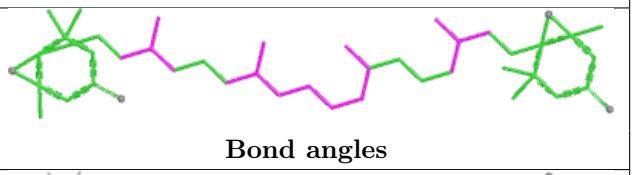


Rings

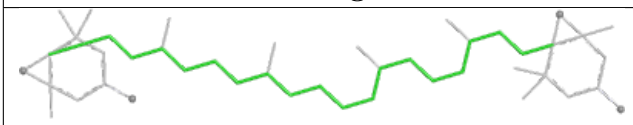
## Ligand XAT 3 417



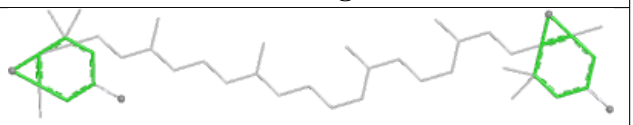
Bond lengths



Bond angles

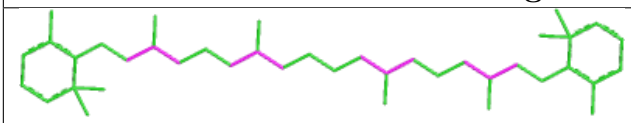


Torsions

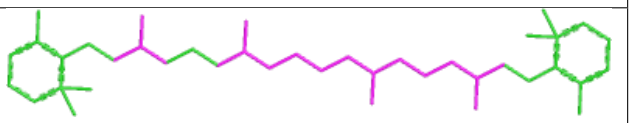


Rings

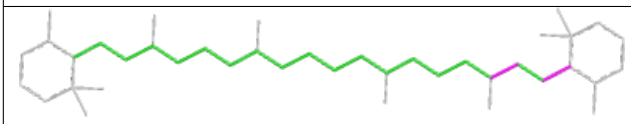
## Ligand BCR L 306



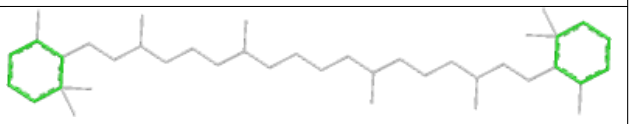
Bond lengths



Bond angles

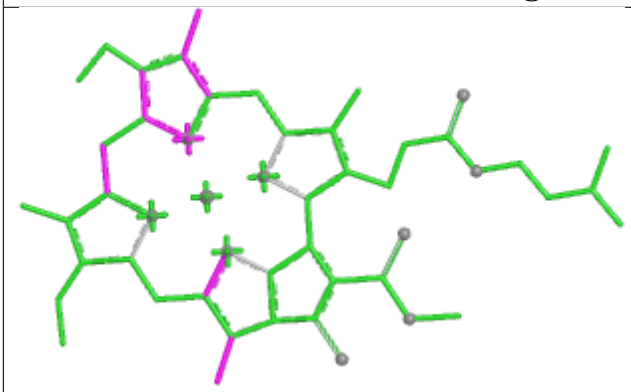


Torsions

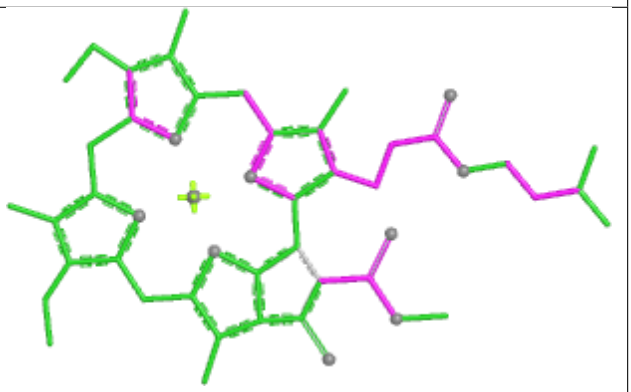


Rings

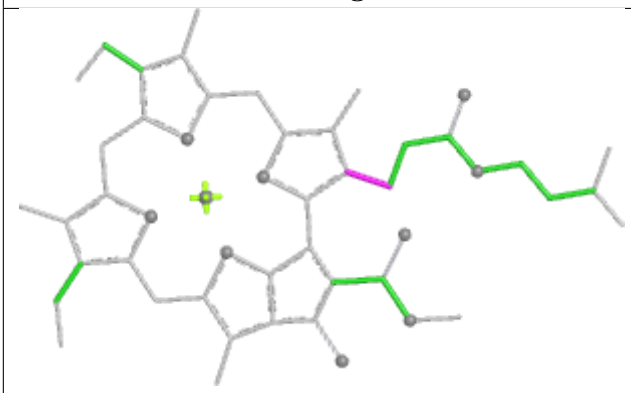
## Ligand CLA K 202



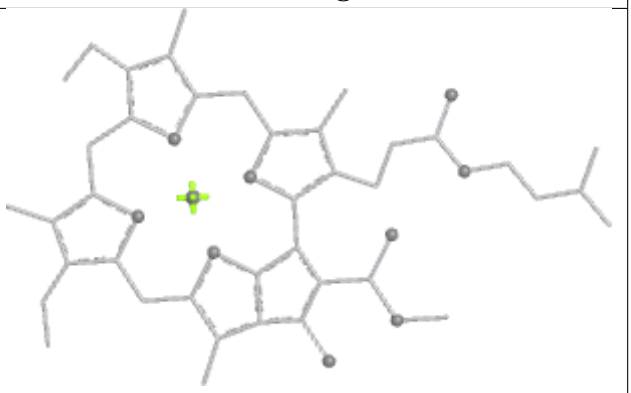
Bond lengths



Bond angles

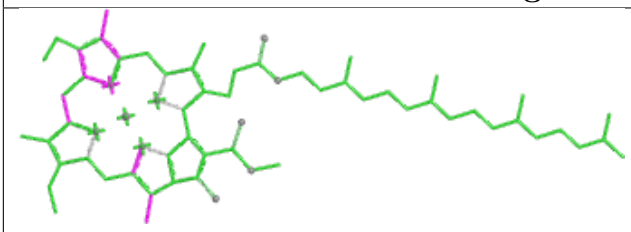


Torsions

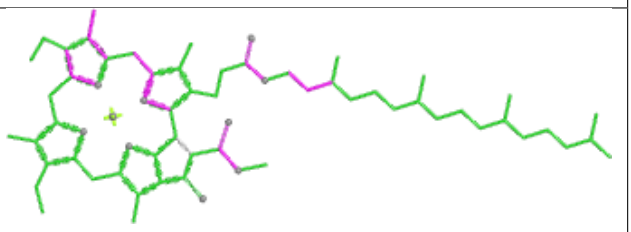


Rings

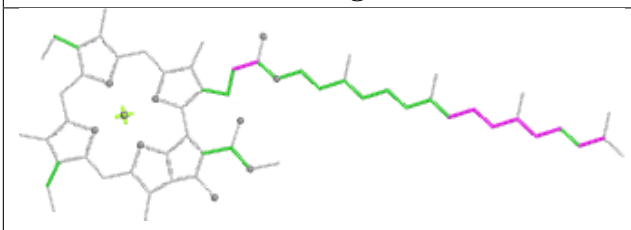
## Ligand CLA A 825



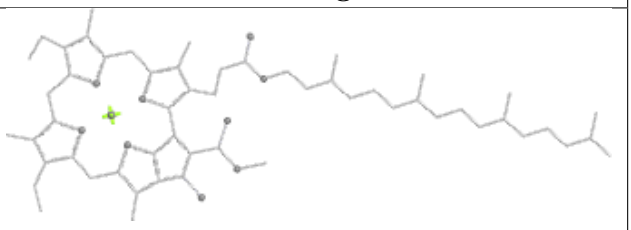
Bond lengths



Bond angles

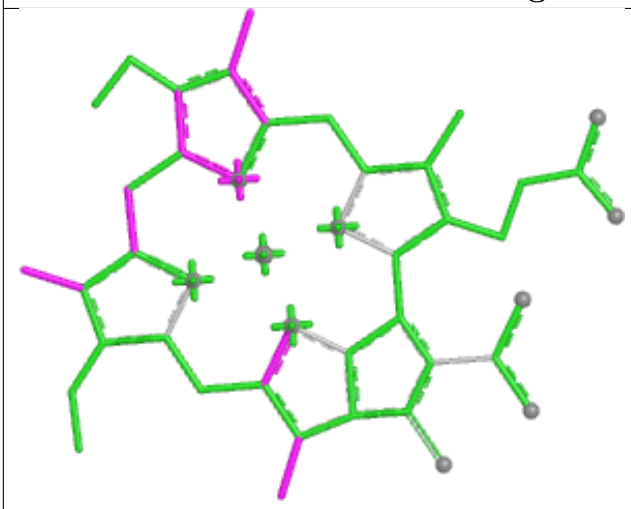


Torsions

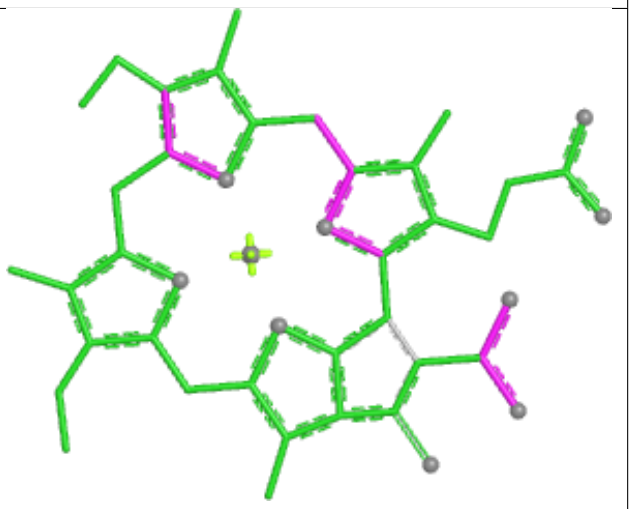


Rings

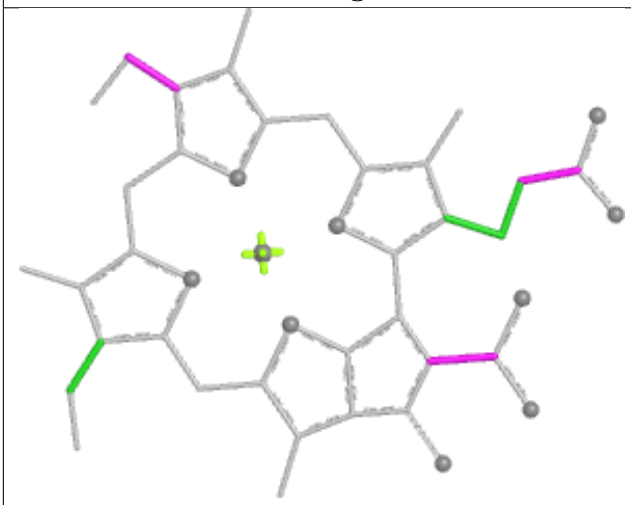
## Ligand CLA 1 308



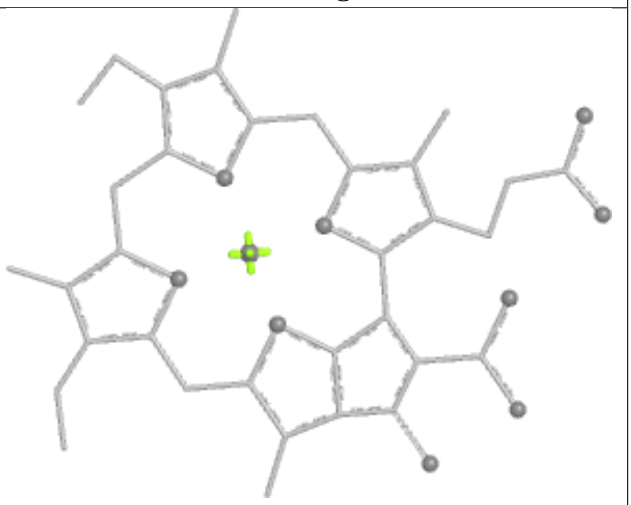
Bond lengths



Bond angles

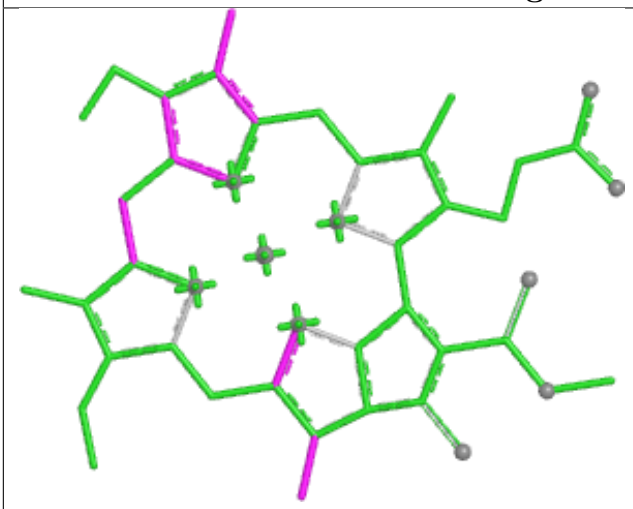


Torsions

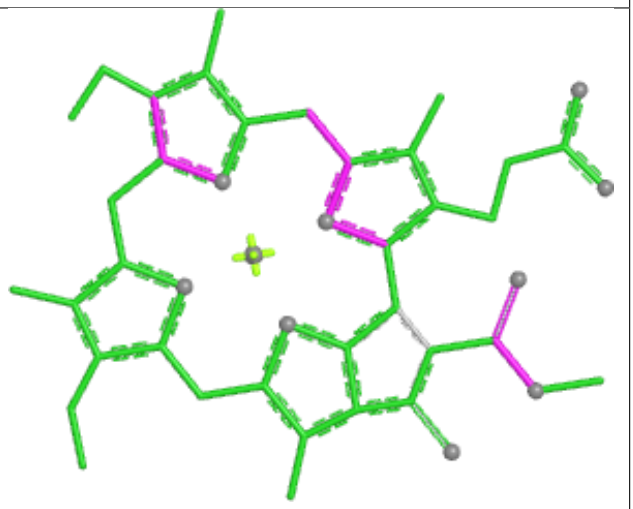


Rings

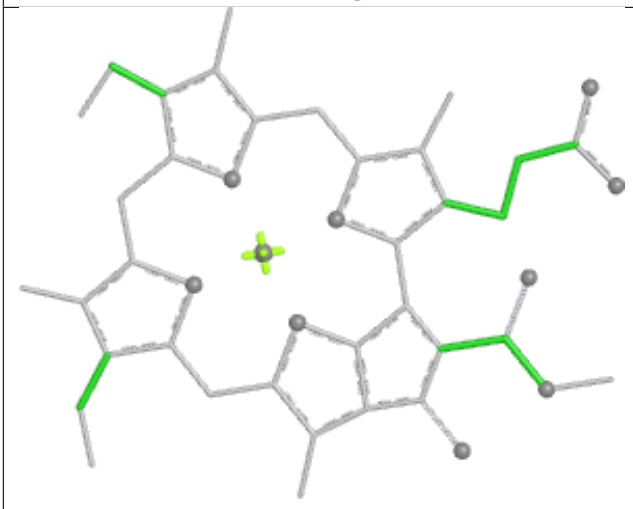
## Ligand CLA F 304



Bond lengths



Bond angles

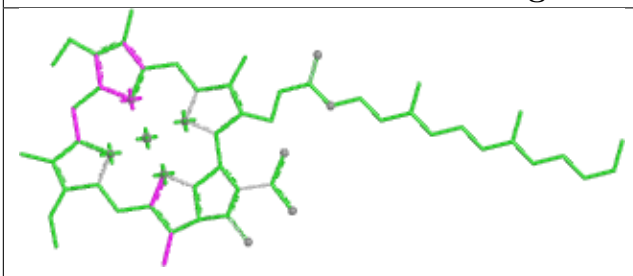


Torsions

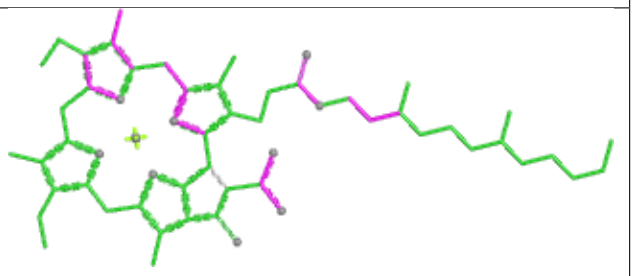


Rings

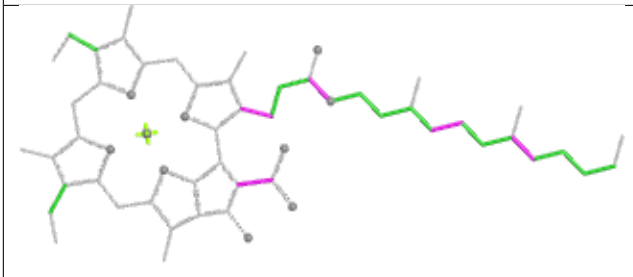
## Ligand CLA 8 602



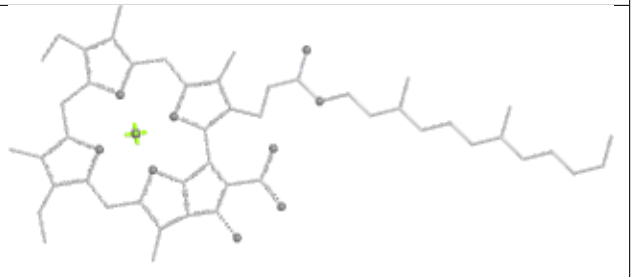
Bond lengths



Bond angles

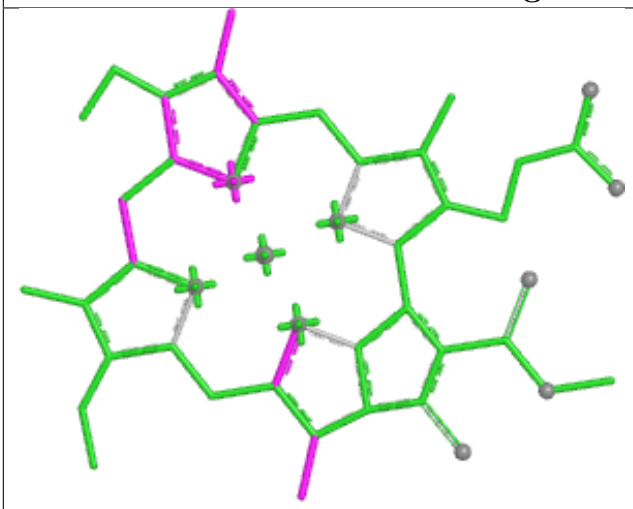


Torsions

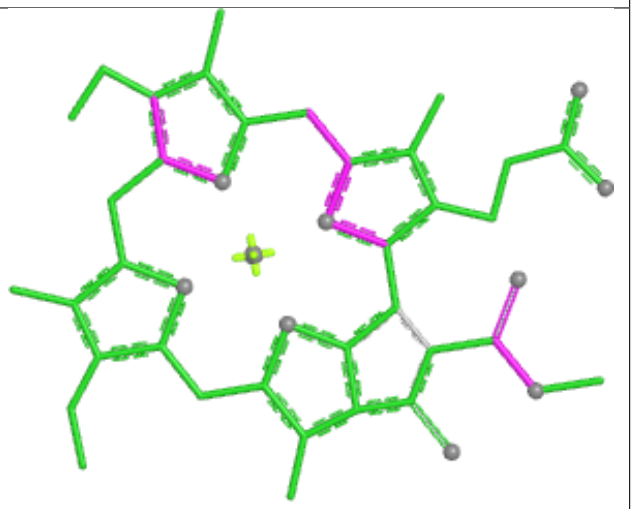


Rings

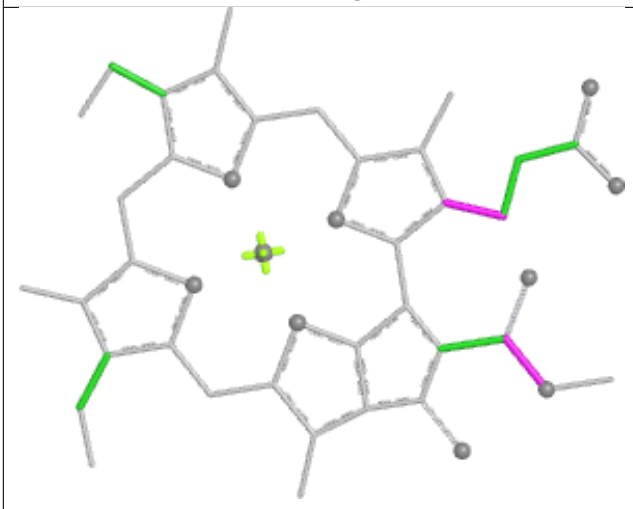
**Ligand CLA A 811**



**Bond lengths**



**Bond angles**

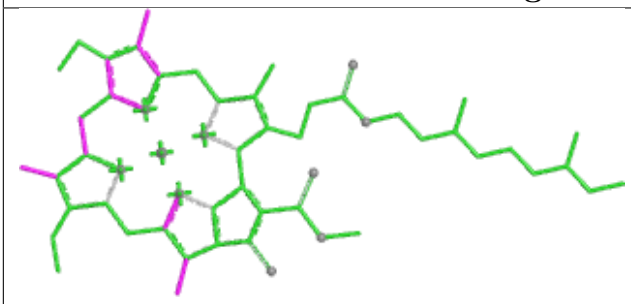


**Torsions**

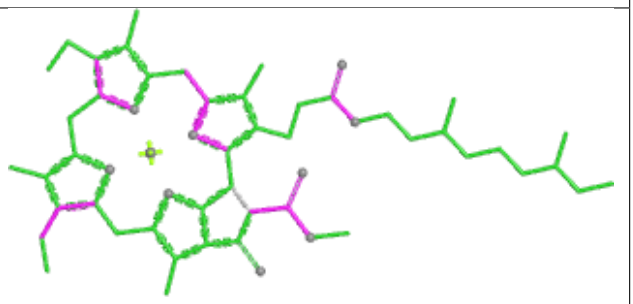


**Rings**

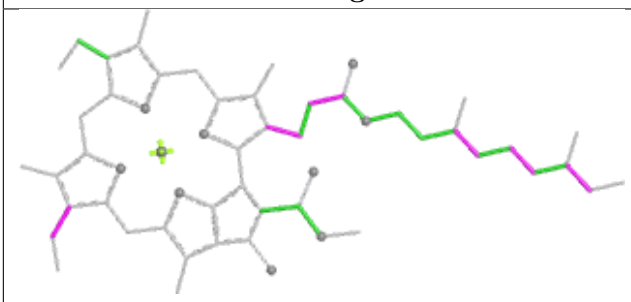
**Ligand CLA B 831**



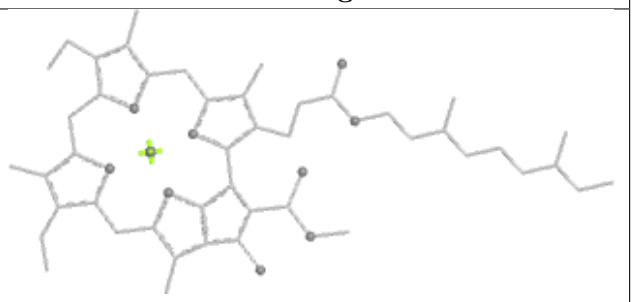
**Bond lengths**



**Bond angles**

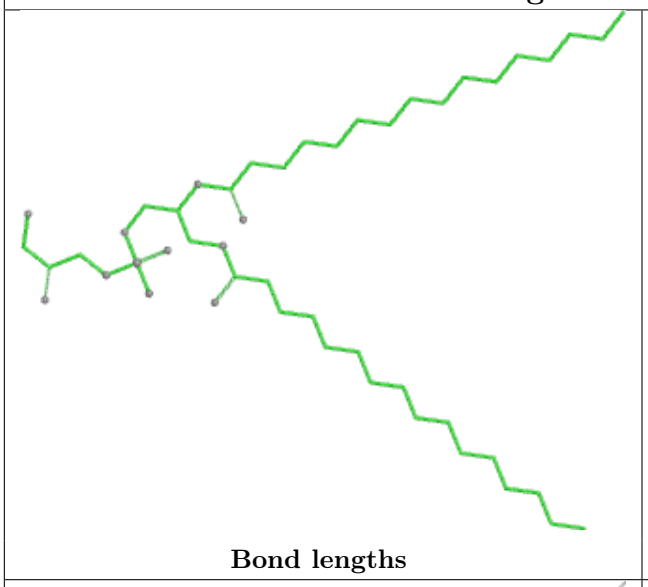


**Torsions**

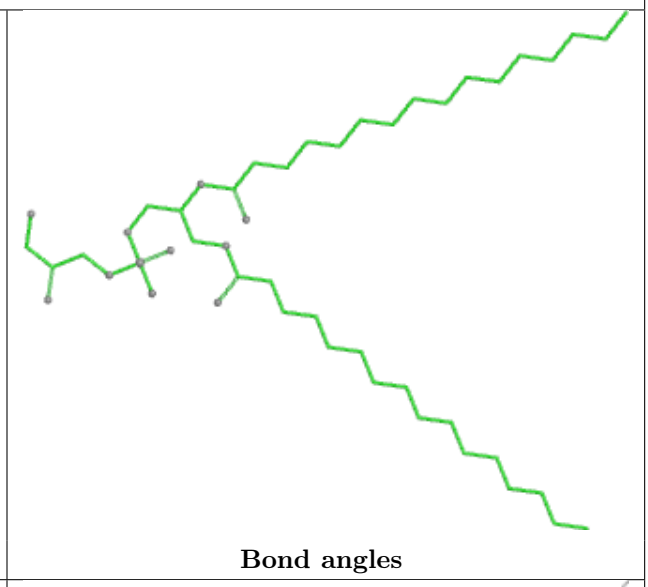


**Rings**

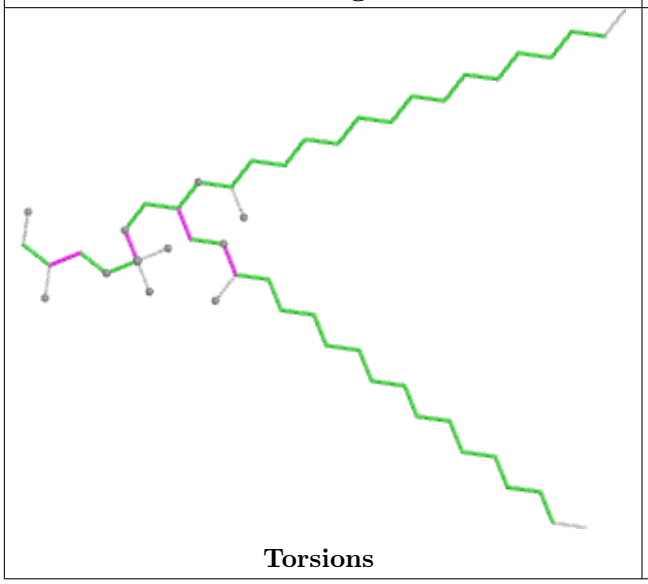
**Ligand LHG b 319**



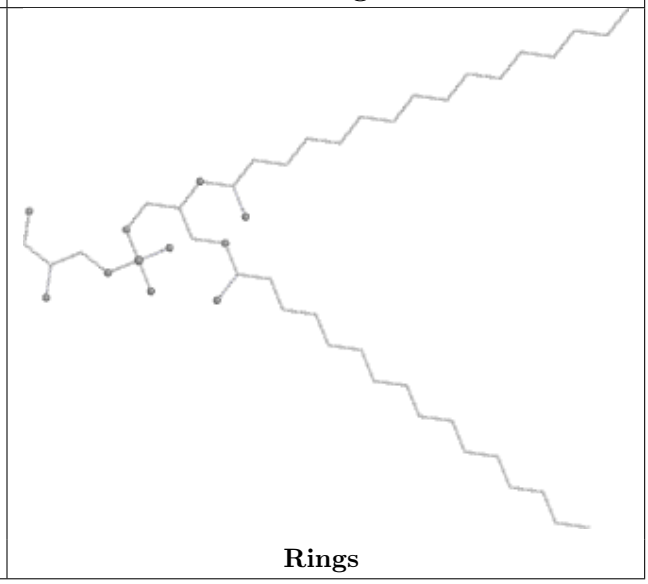
**Bond lengths**



**Bond angles**

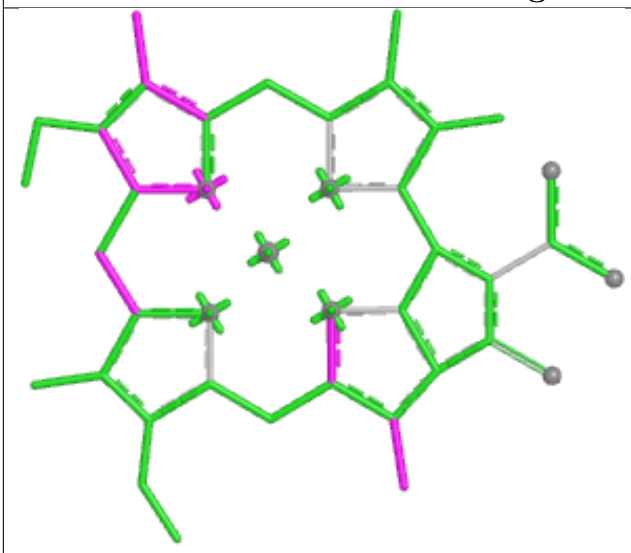


**Torsions**

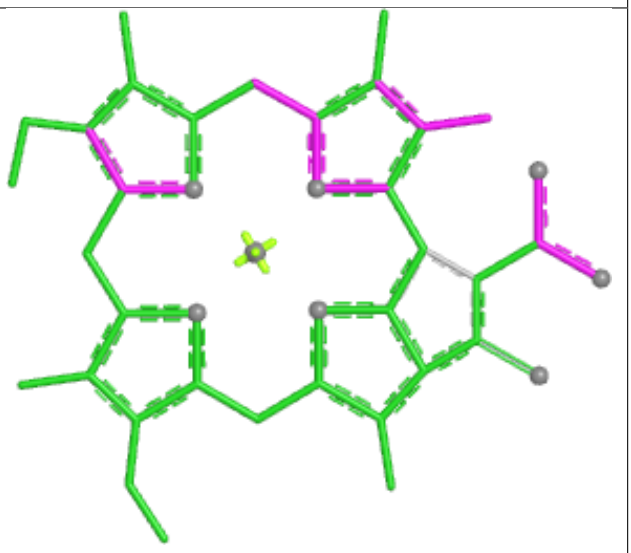


**Rings**

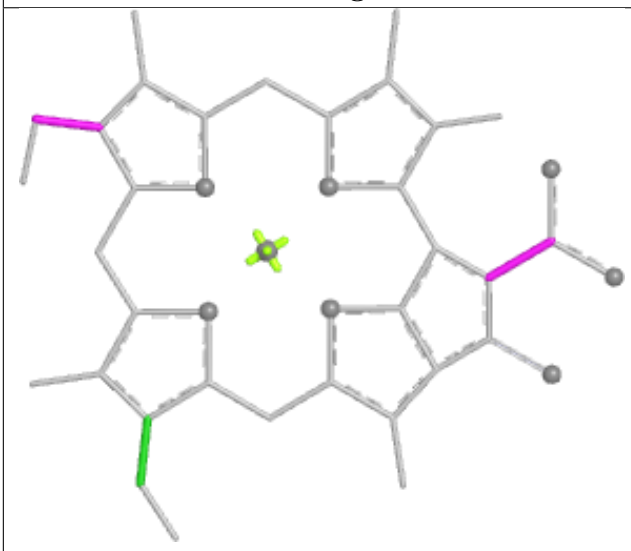
**Ligand CLA 3 410**



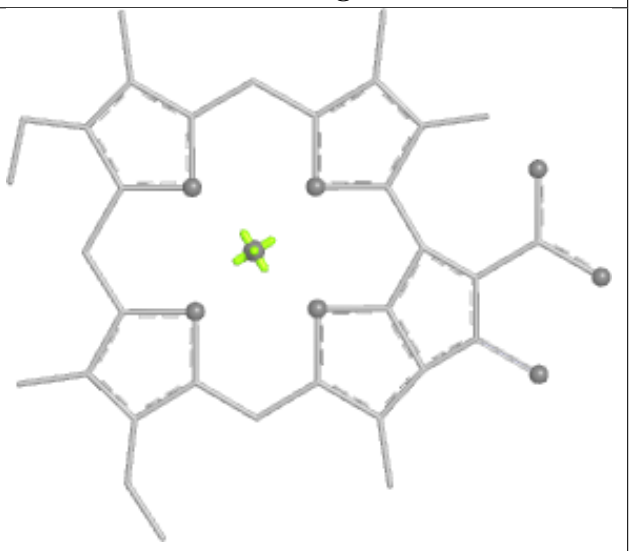
**Bond lengths**



**Bond angles**

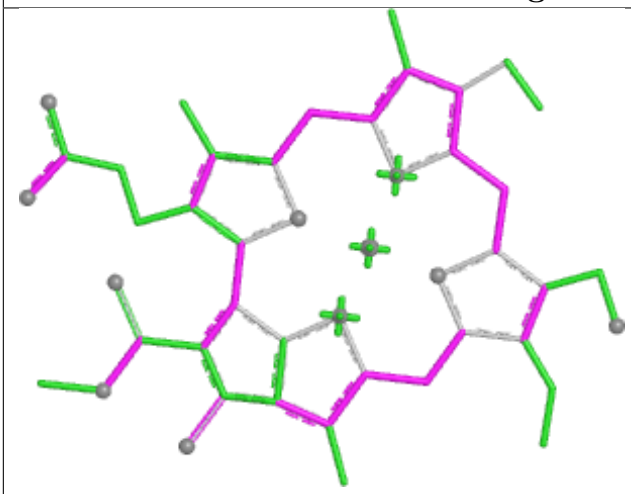


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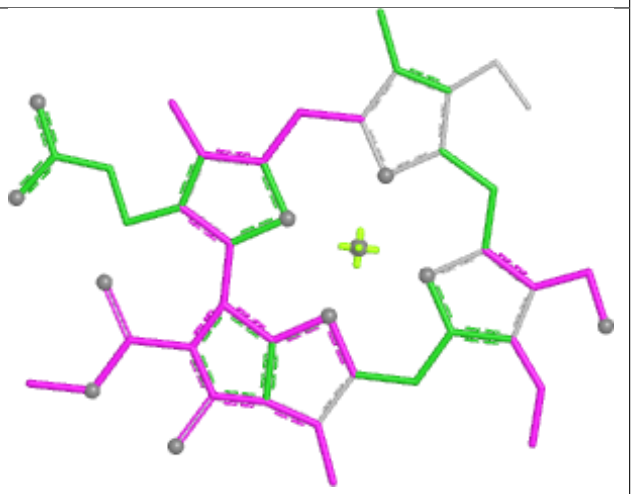


**Rings**

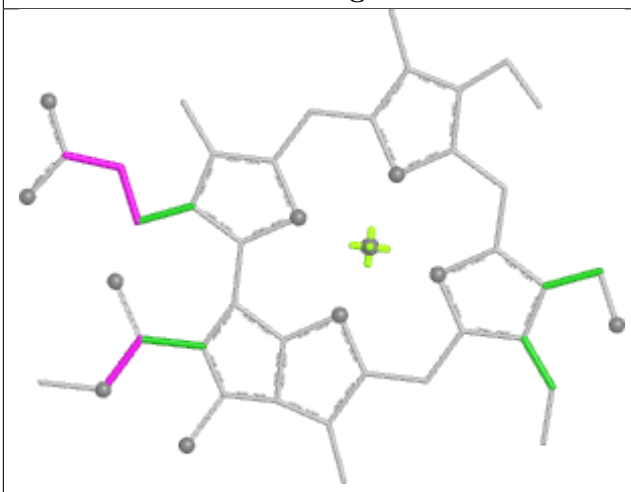
## Ligand CHL 6 614



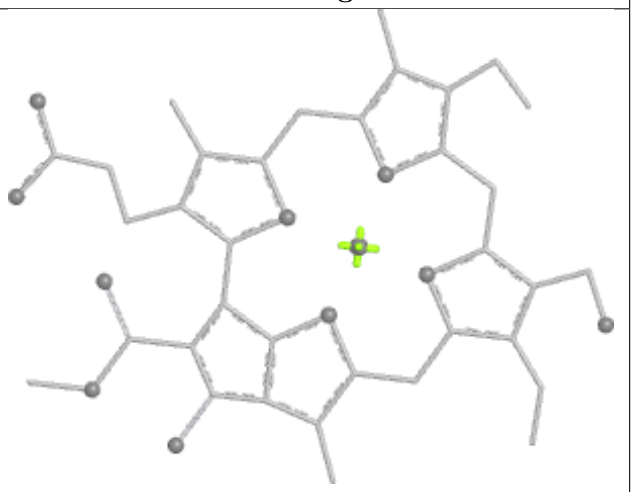
Bond lengths



Bond angles

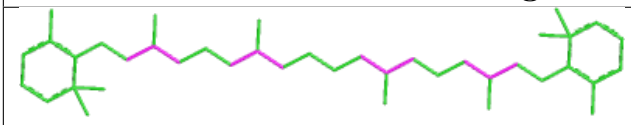


Torsions



Rings

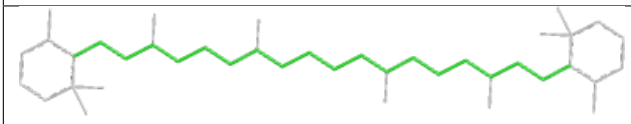
## Ligand BCR G 201



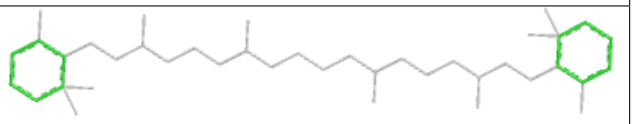
Bond lengths



Bond angles

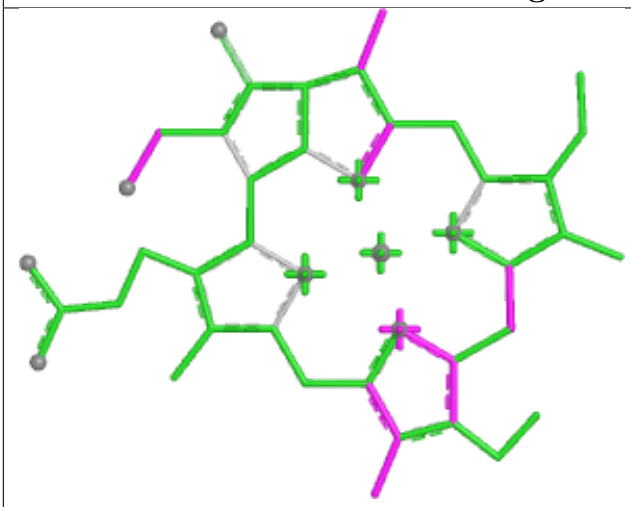


Torsions

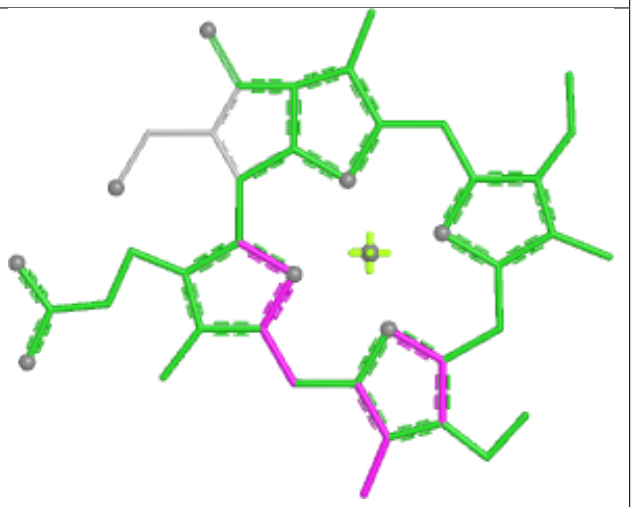


Rings

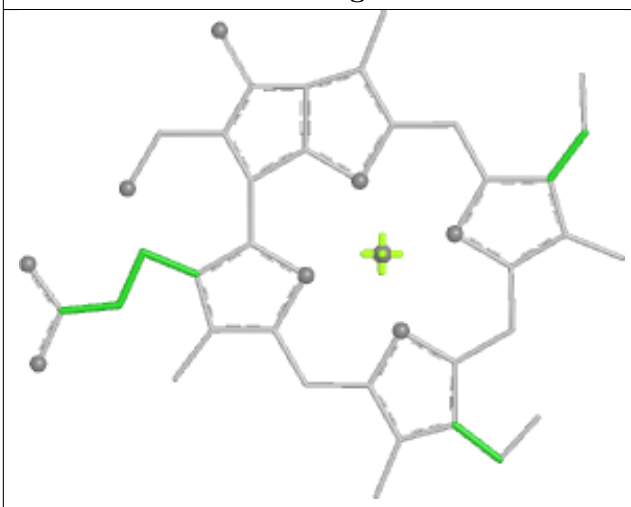
**Ligand CLA 4 608**



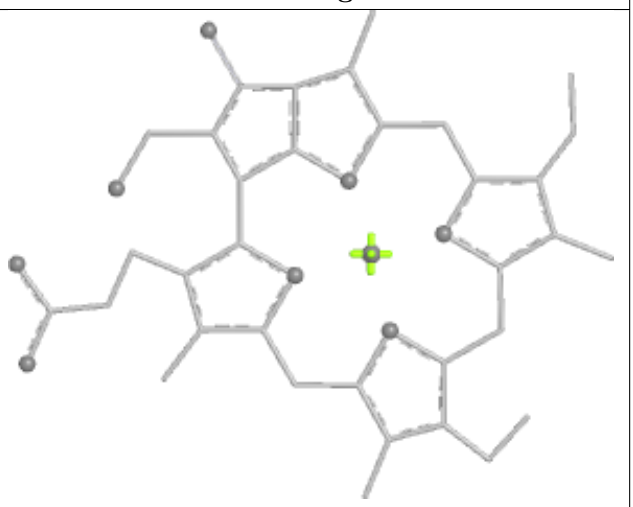
**Bond lengths**



**Bond angles**

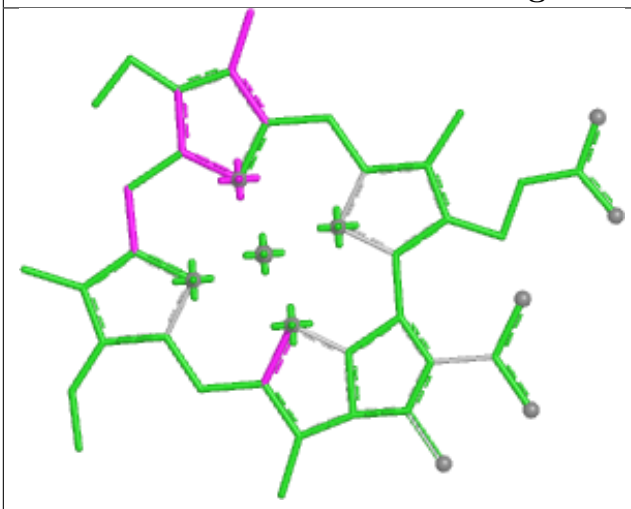


**Torsions**

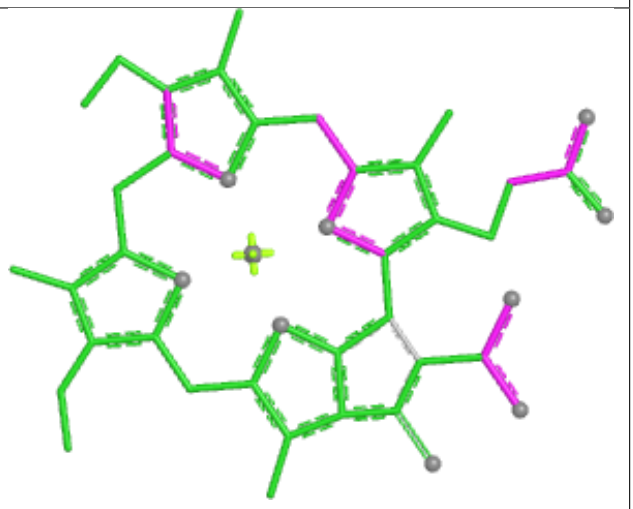


**Rings**

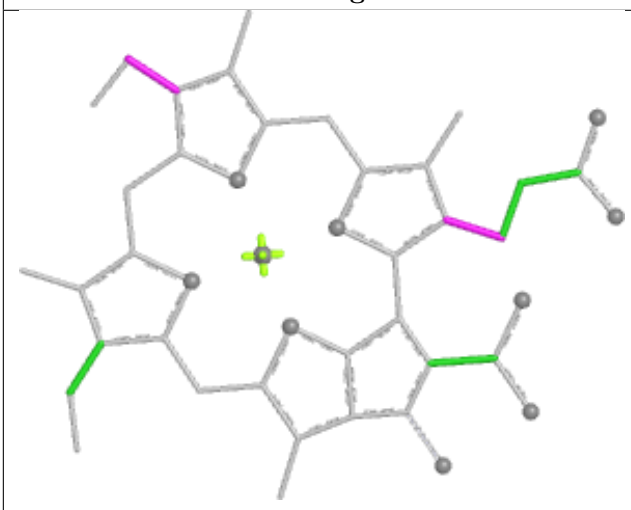
**Ligand CLA 5 607**



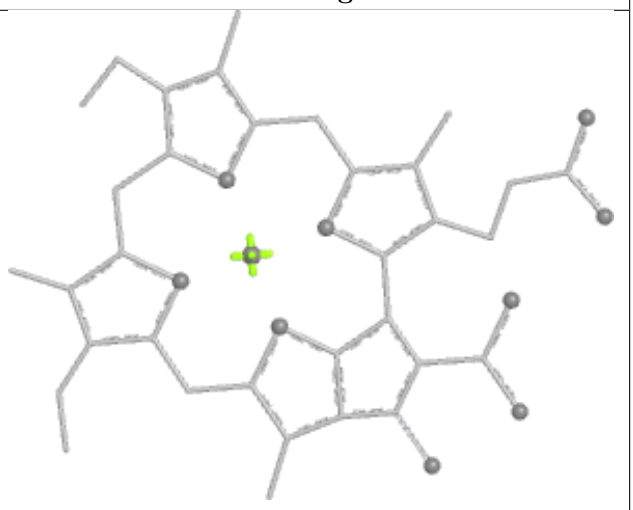
**Bond lengths**



**Bond angles**

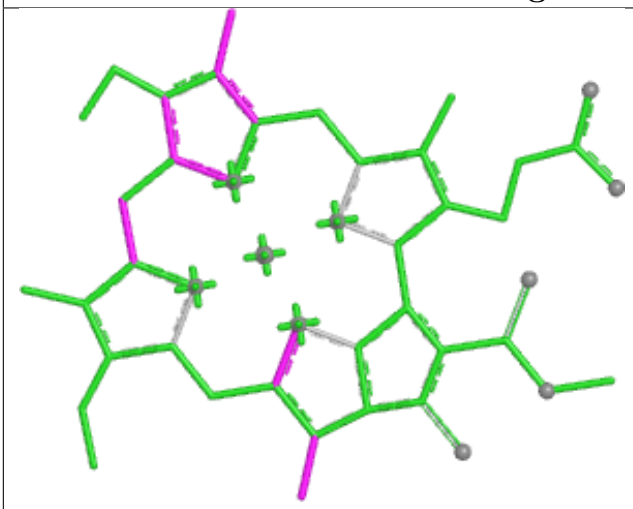


**Torsions**

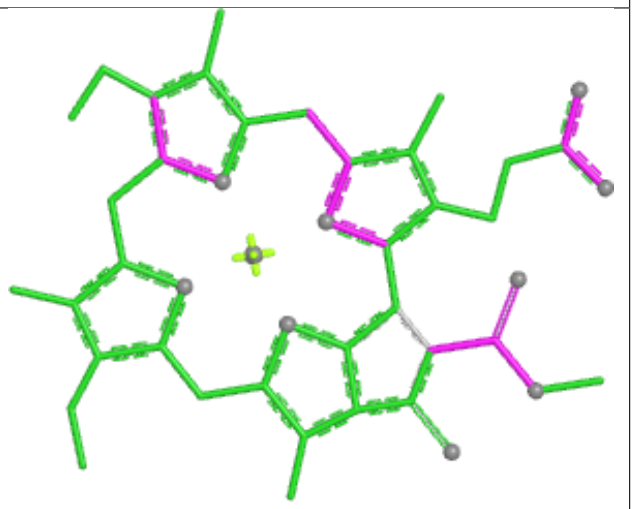


**Rings**

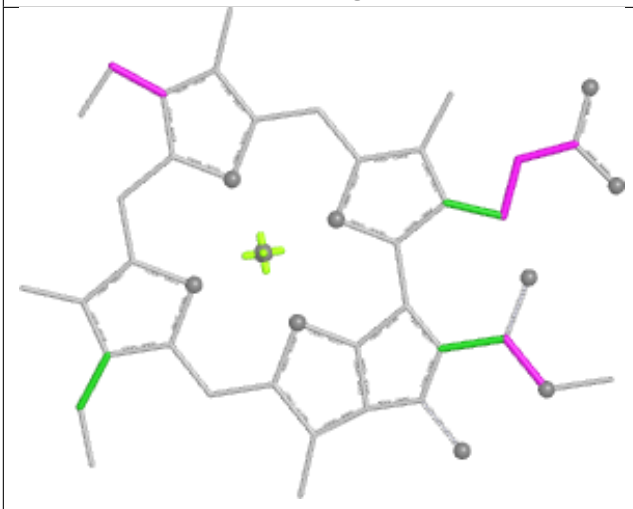
**Ligand CLA 2 612**



**Bond lengths**



**Bond angles**

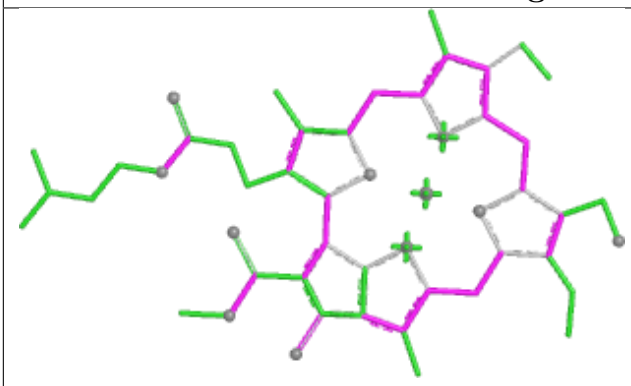


**Torsions**

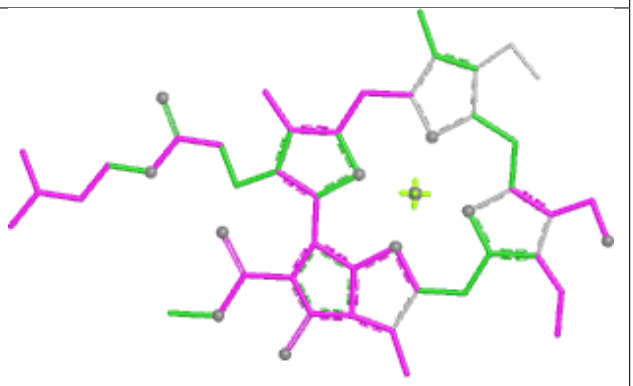


**Rings**

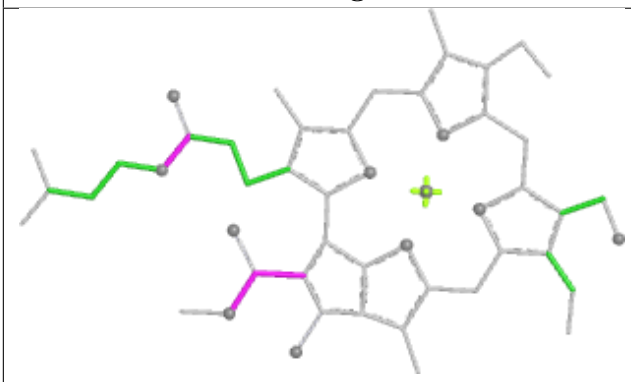
**Ligand CHL 2 607**



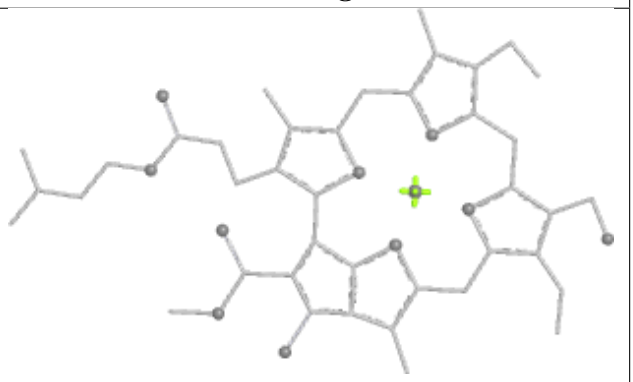
**Bond lengths**



**Bond angles**

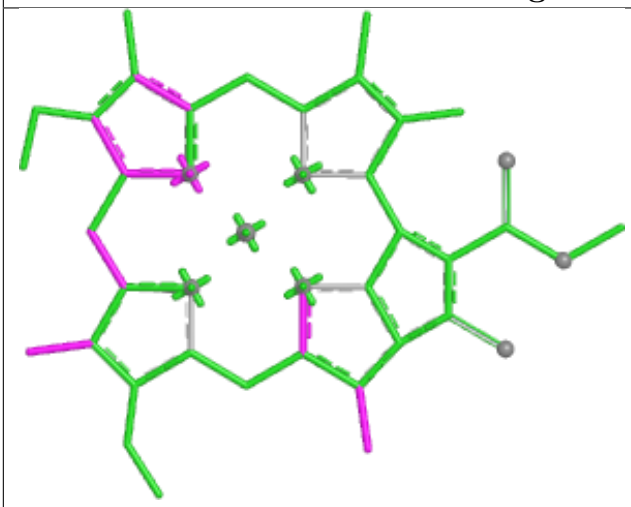


**Torsions**

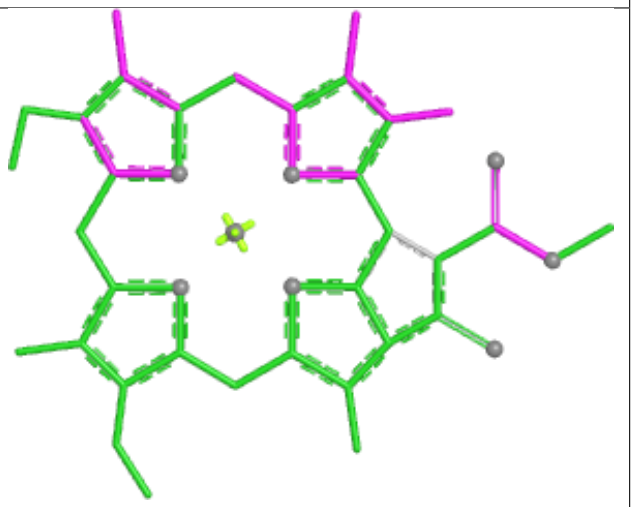


**Rings**

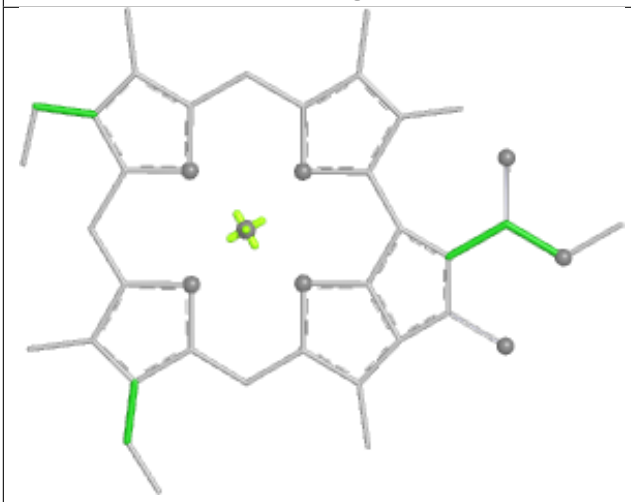
## Ligand CLA 2 611



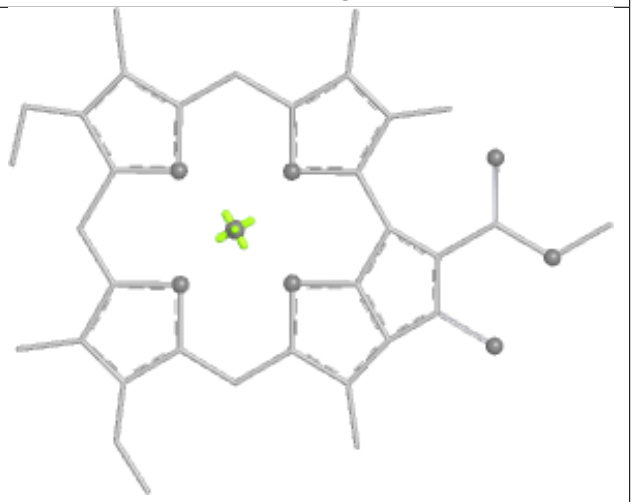
Bond lengths



Bond angles

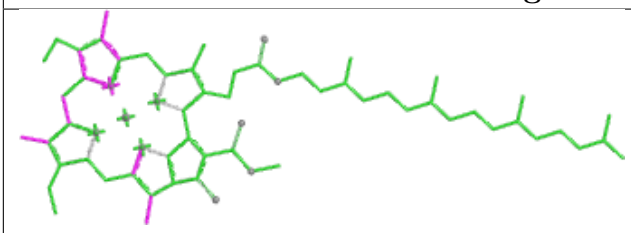


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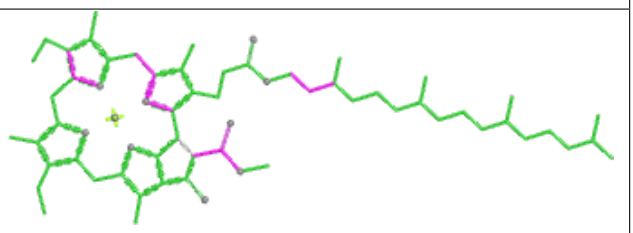


Rings

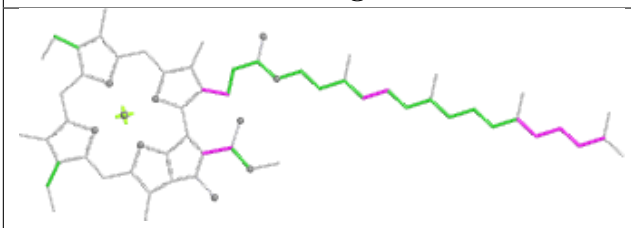
## Ligand CLA A 804



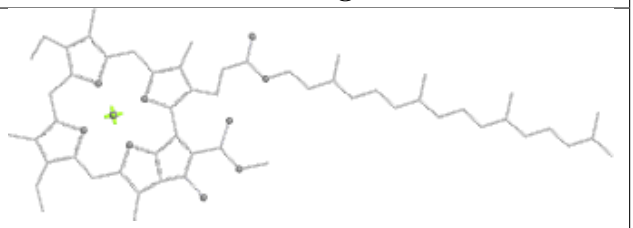
Bond lengths



Bond angles

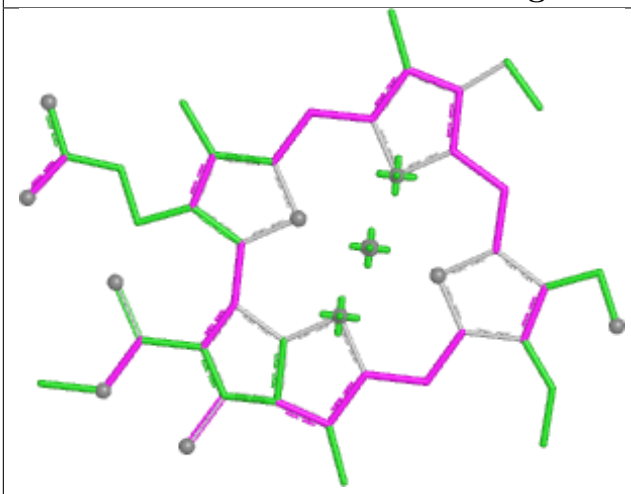


Torsions

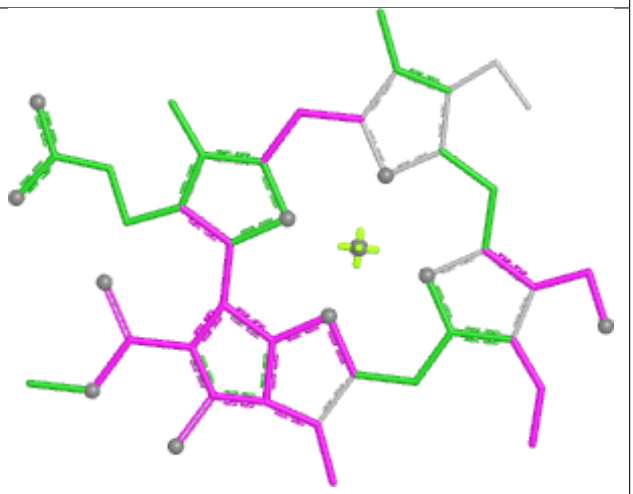


Rings

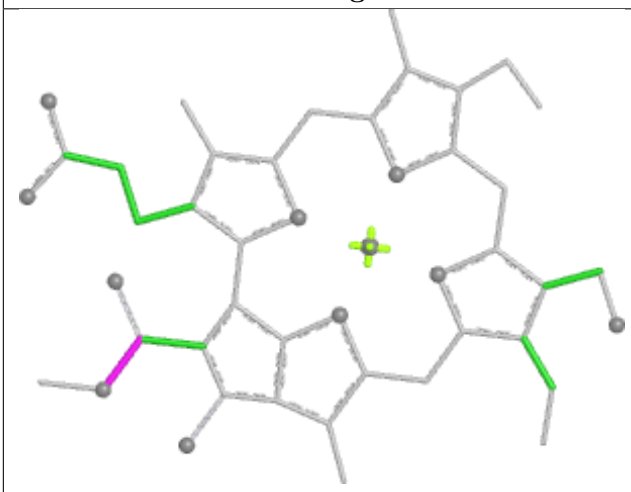
**Ligand CHL a 601**



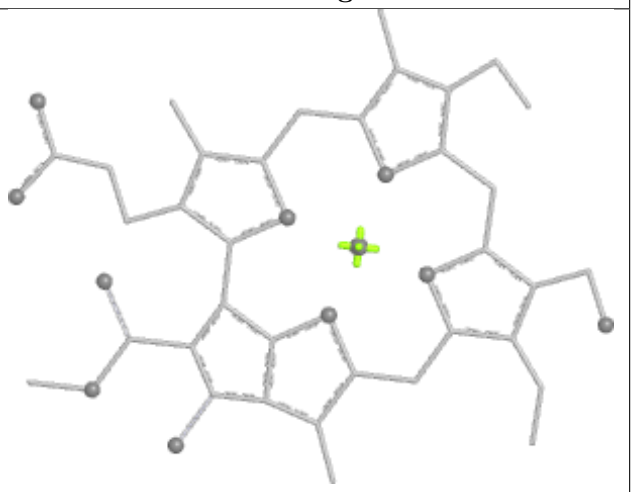
**Bond lengths**



**Bond angles**

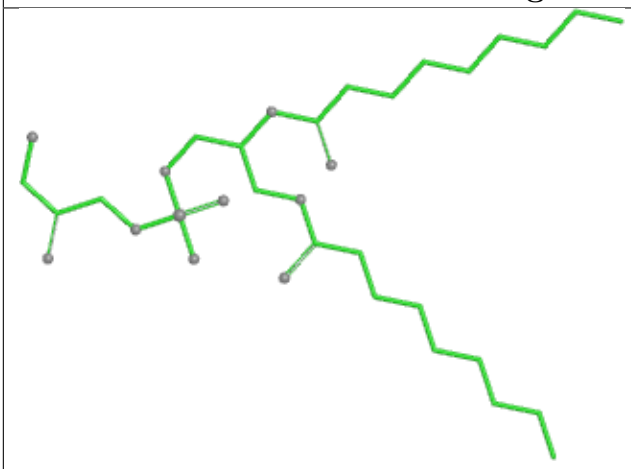


**Torsions**

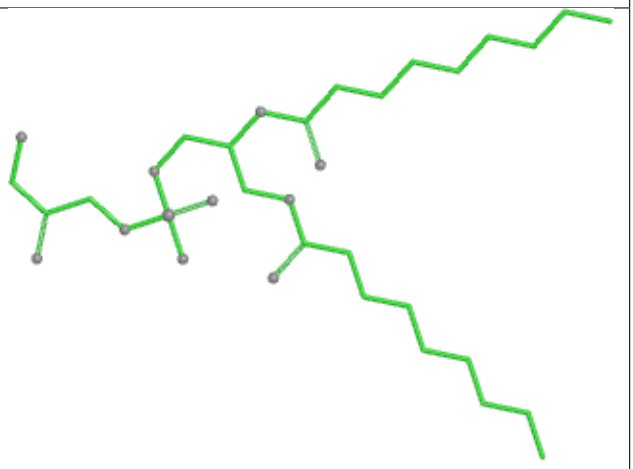


**Rings**

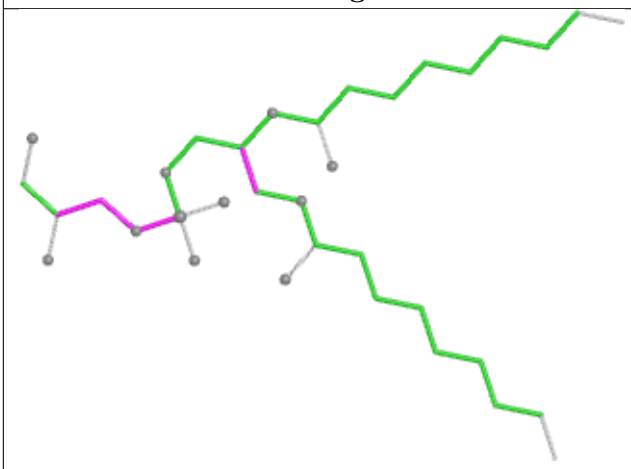
**Ligand LHG 2 619**



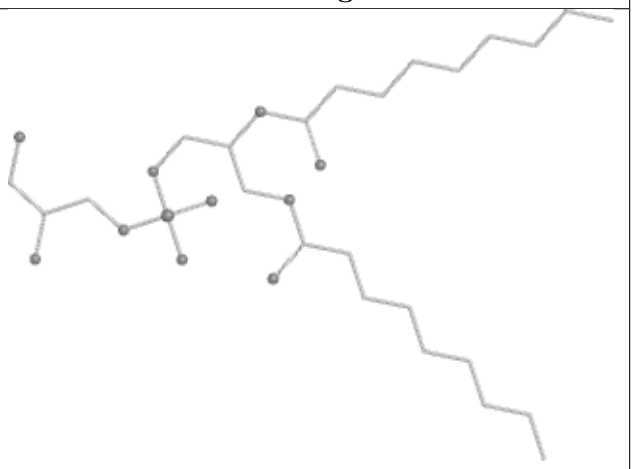
**Bond lengths**



**Bond angles**

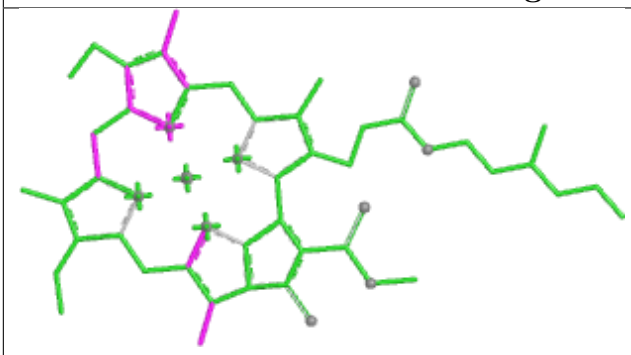


**Torsions**

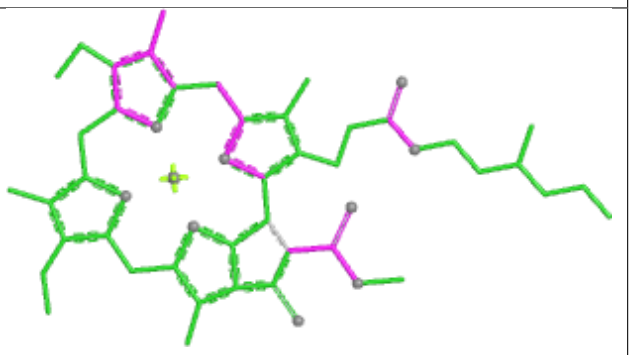


**Rings**

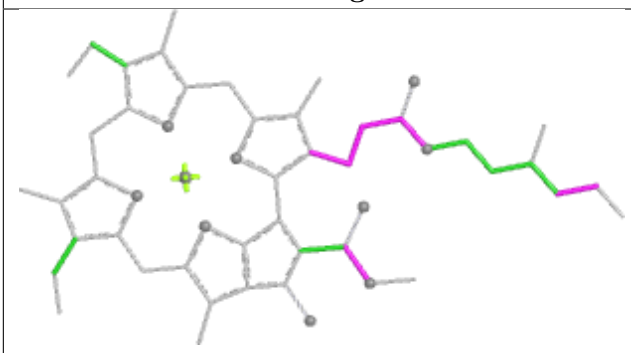
**Ligand CLA B 826**



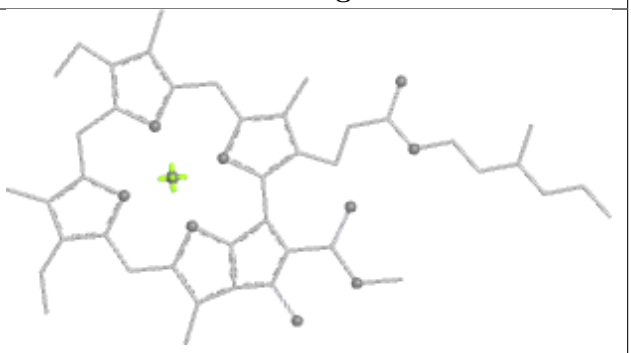
**Bond lengths**



**Bond angles**

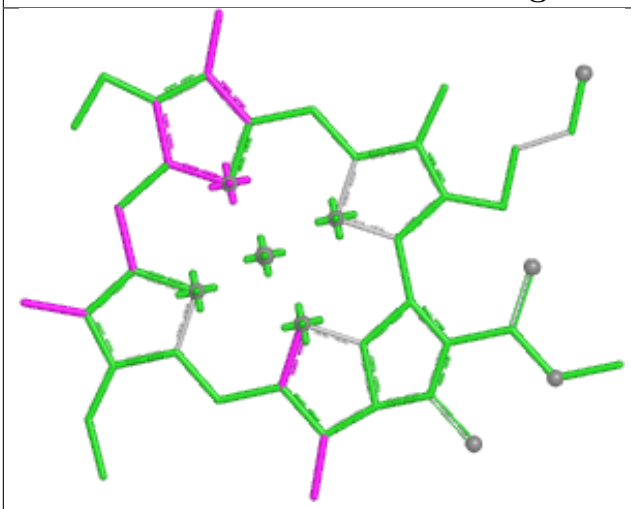


**Torsions**



**Rings**

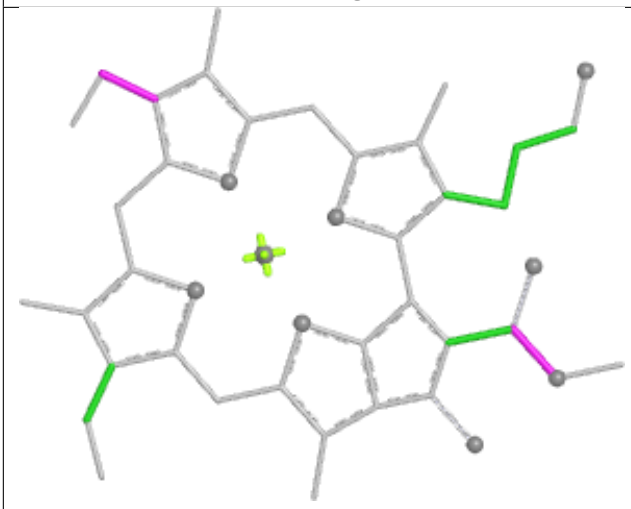
## Ligand CLA c 612



Bond lengths



Bond angles

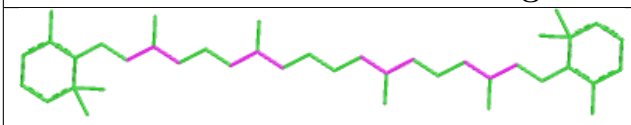


Torsions

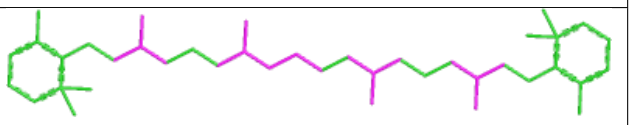


Rings

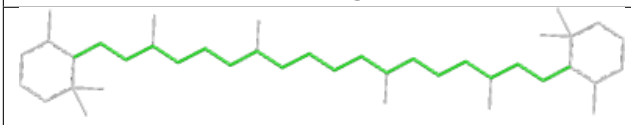
## Ligand BCR A 854



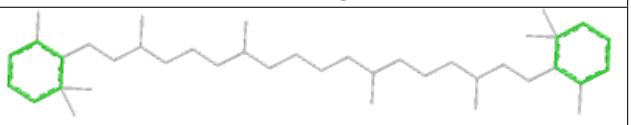
Bond lengths



Bond angles

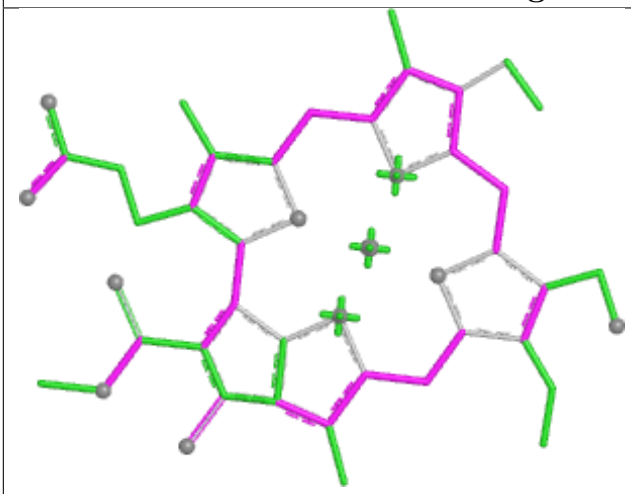


Torsions

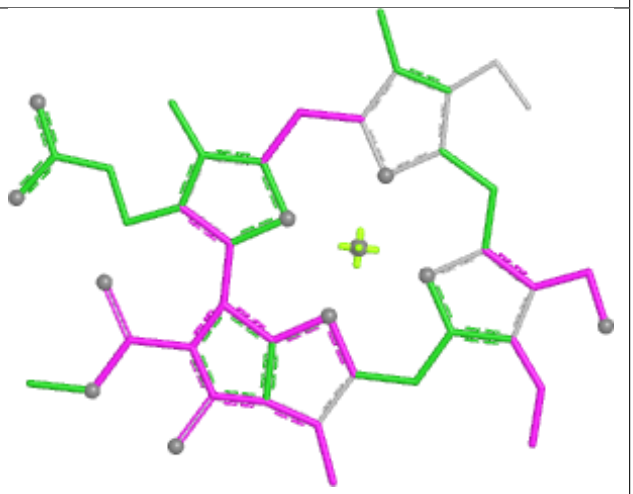


Rings

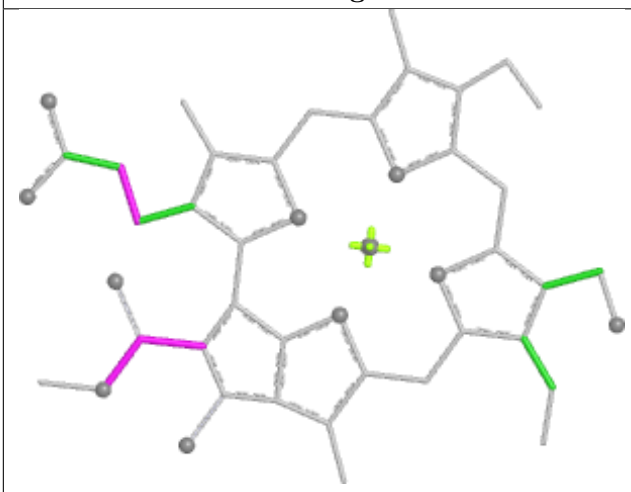
## Ligand CHL 6 605



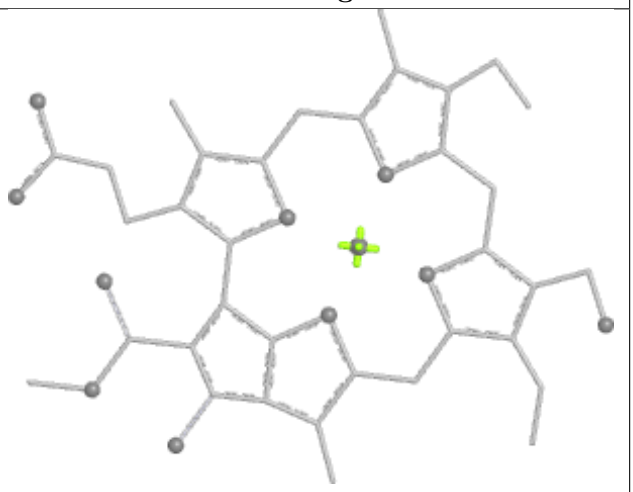
Bond lengths



Bond angles

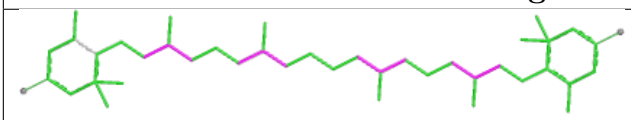


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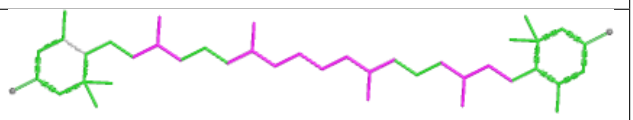


Rings

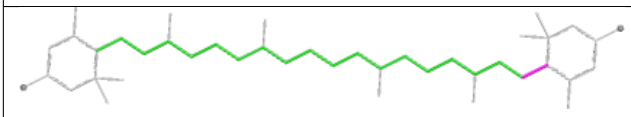
## Ligand LUT 9 615



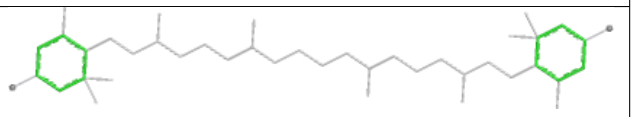
Bond lengths



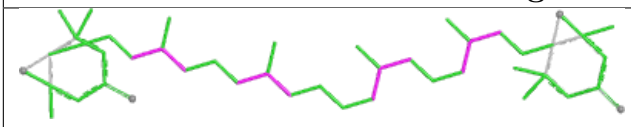
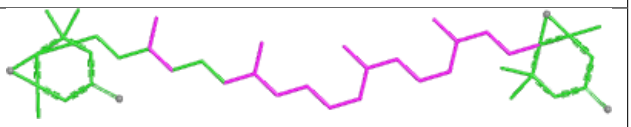
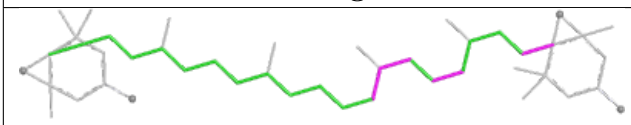
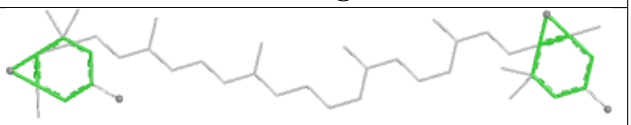
Bond angles

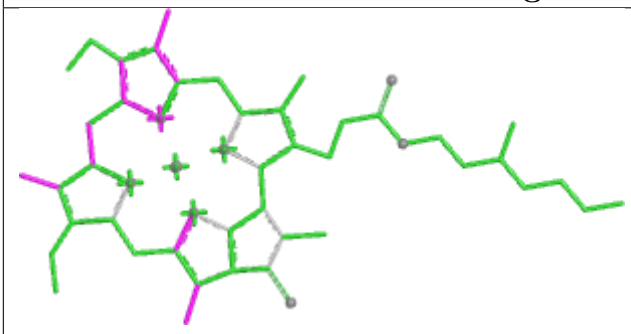
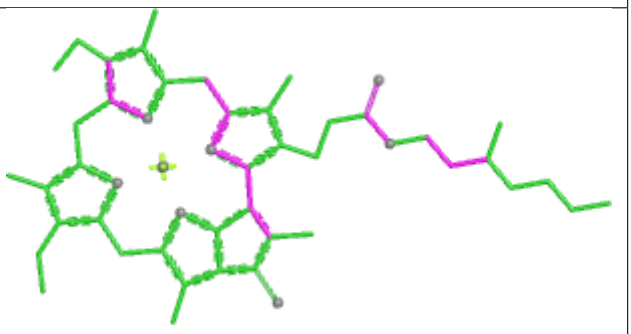
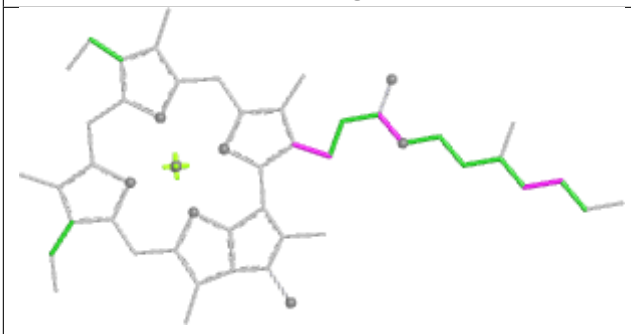
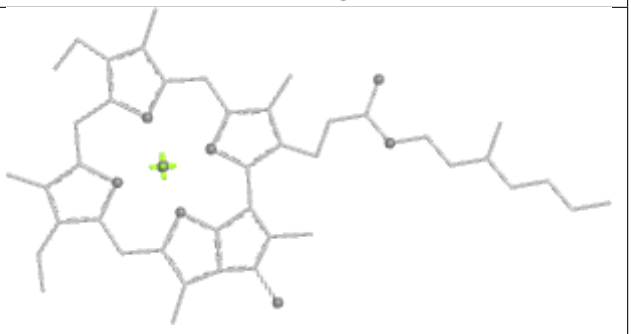


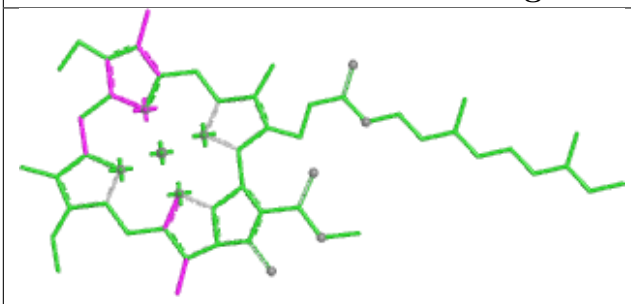
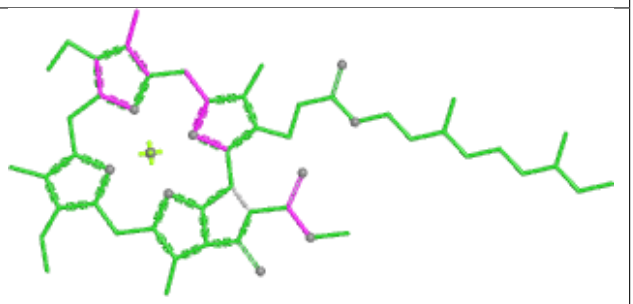
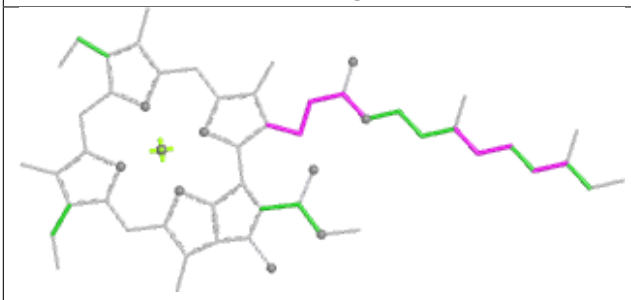
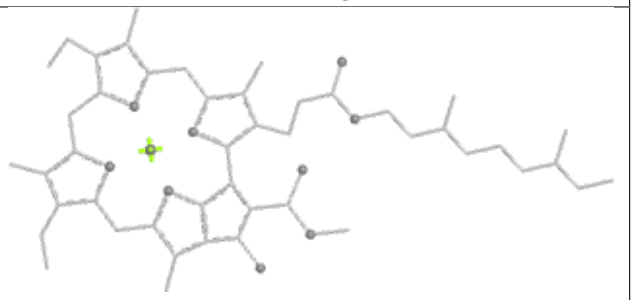
Torsions



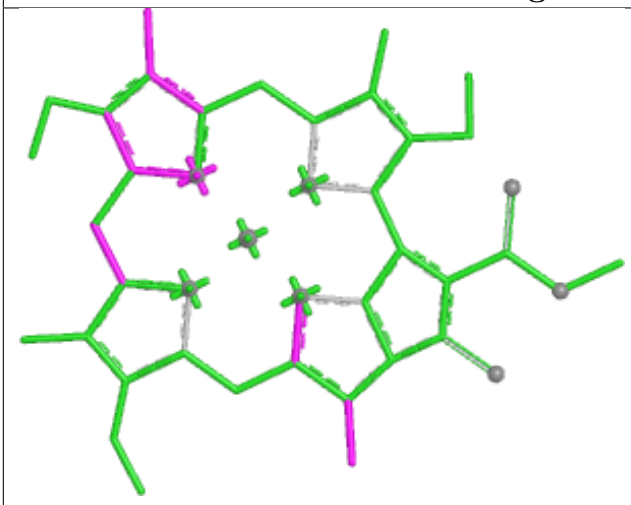
Rings

| Ligand XAT 6 617 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

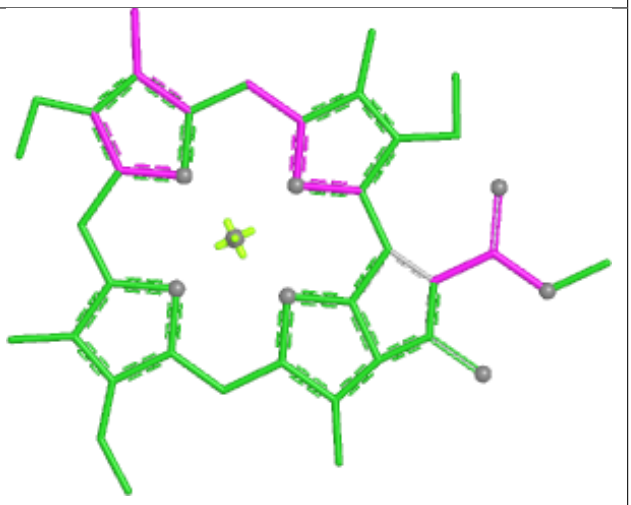
| Ligand CLA O 203 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA B 830 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

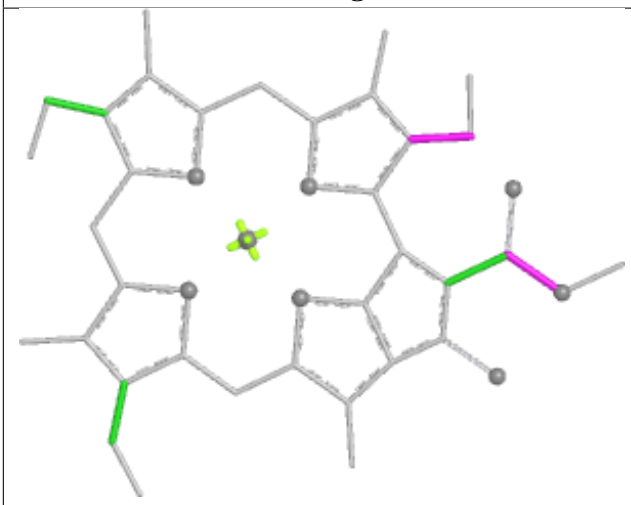
**Ligand CLA 6 609**



**Bond lengths**



**Bond angles**

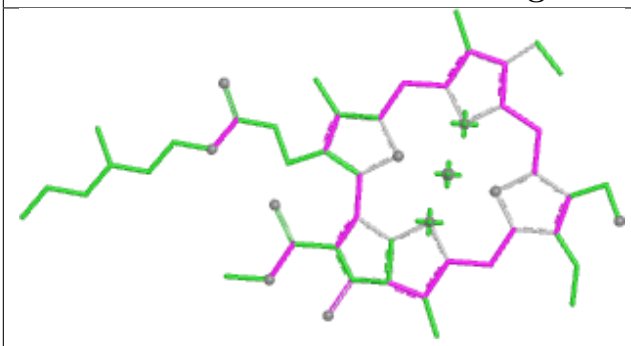


**Torsions**

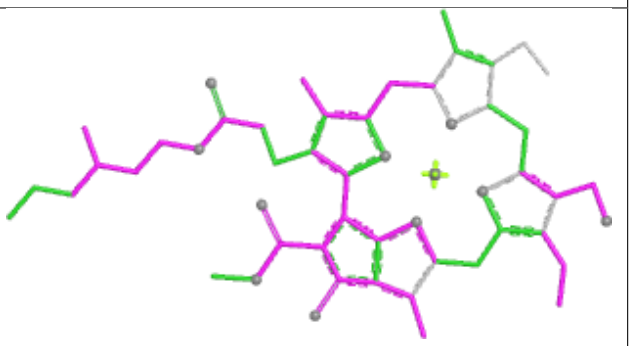


**Rings**

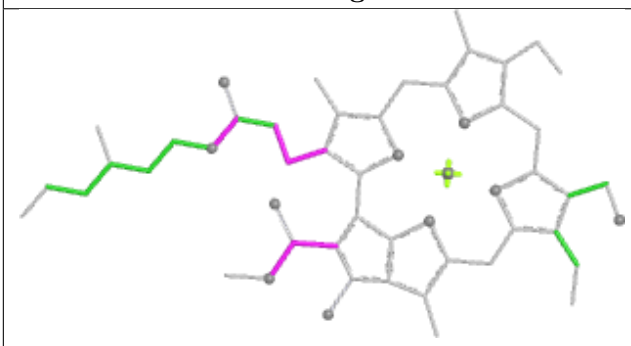
**Ligand CHL 2 602**



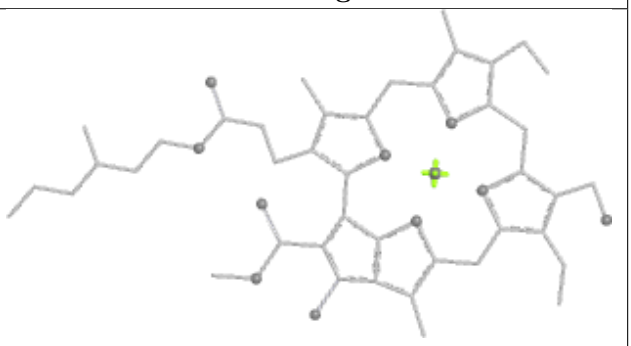
**Bond lengths**



**Bond angles**

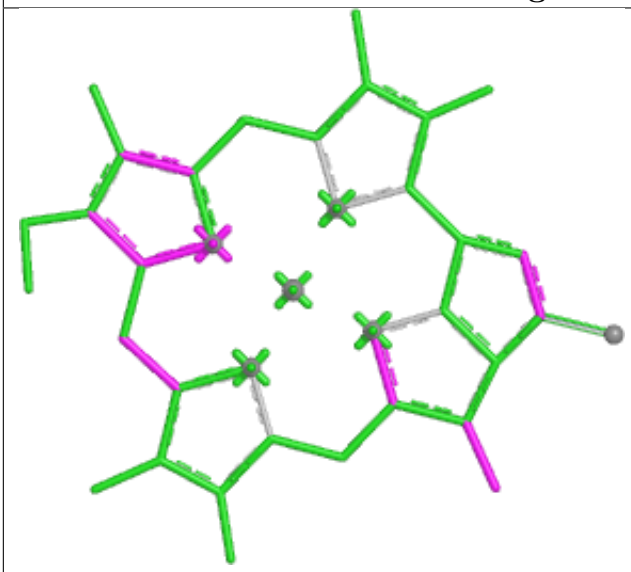


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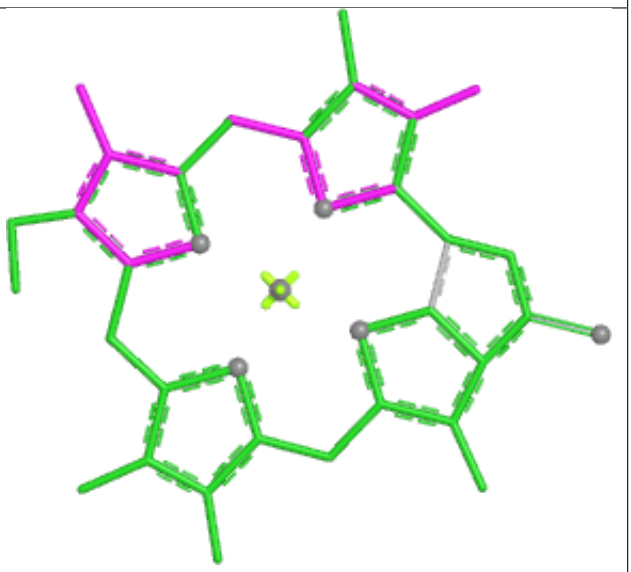


**Rings**

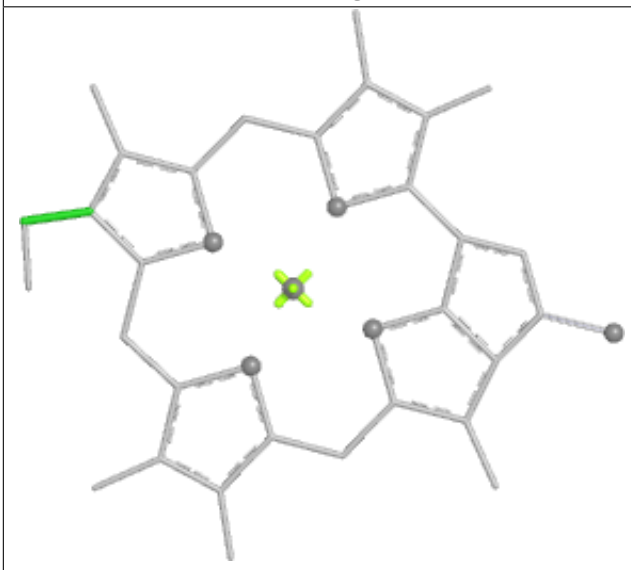
**Ligand CLA 7 413**



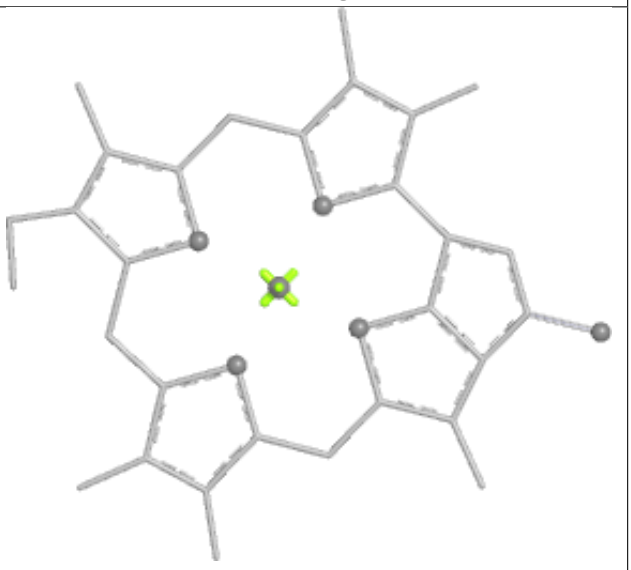
**Bond lengths**



**Bond angles**

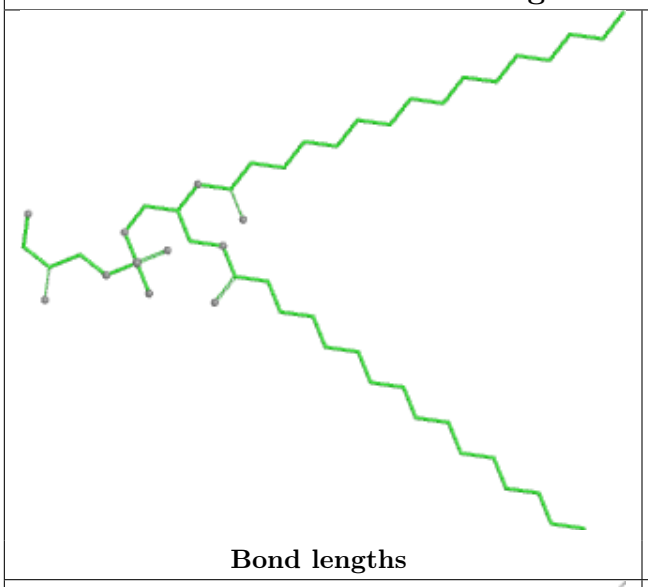


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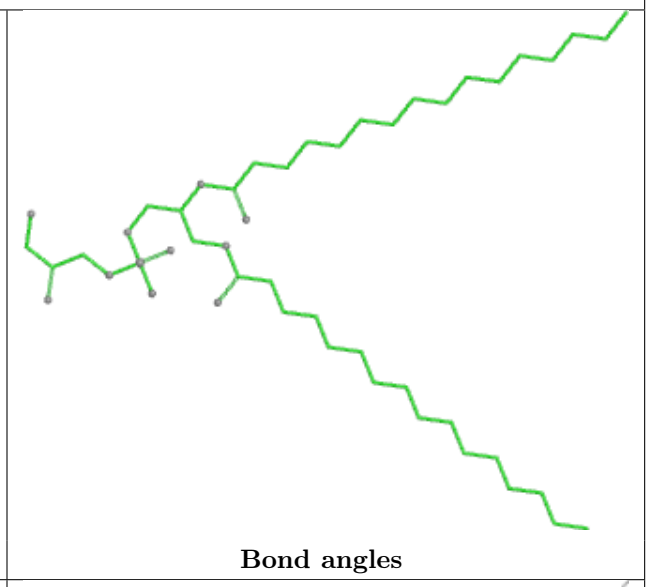


**Rings**

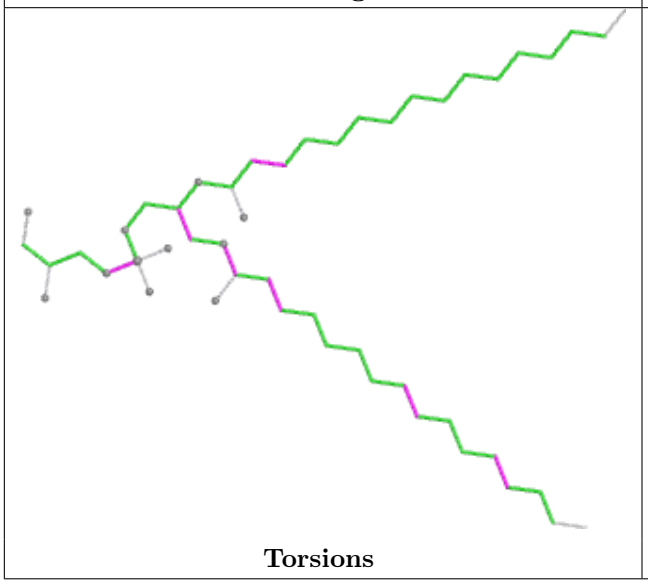
**Ligand LHG 9 618**



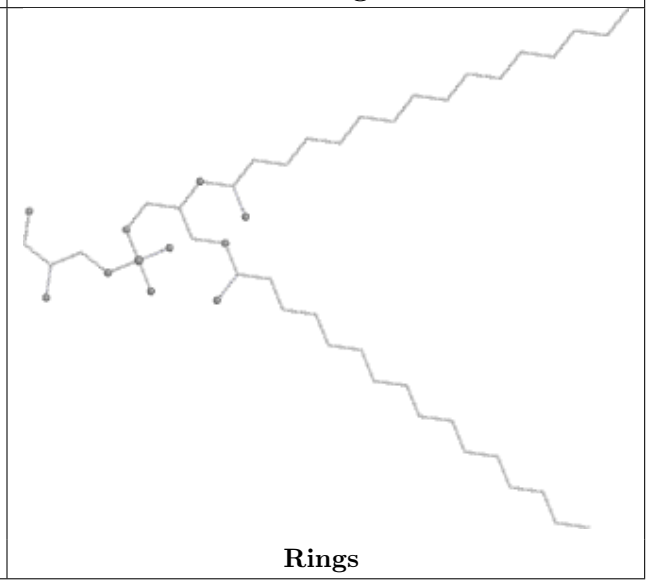
**Bond lengths**



**Bond angles**

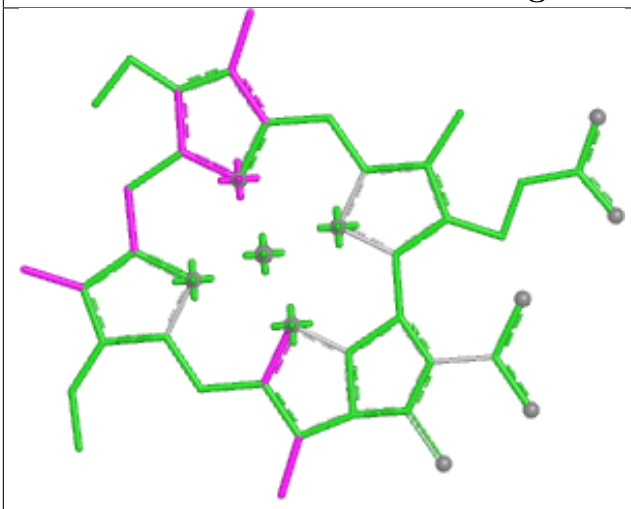


**Torsions**

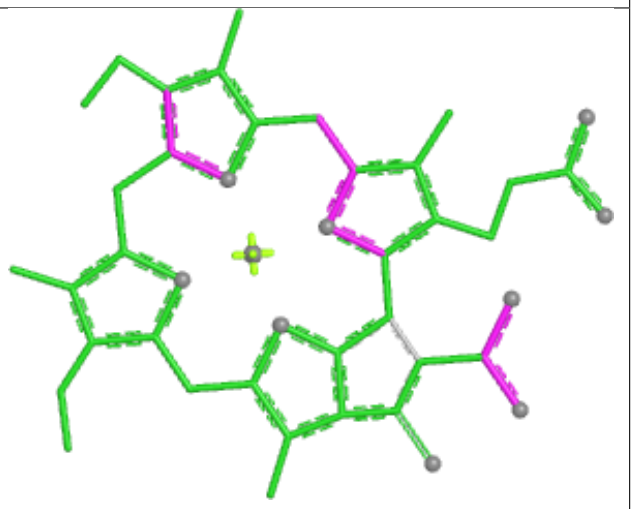


**Rings**

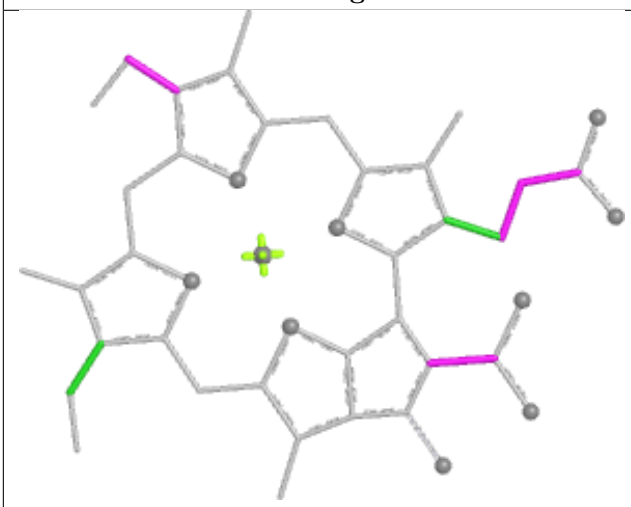
## Ligand CLA 4 603



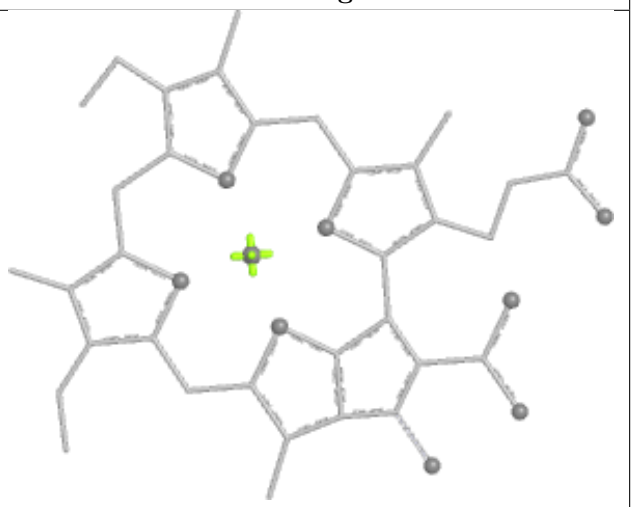
Bond lengths



Bond angles

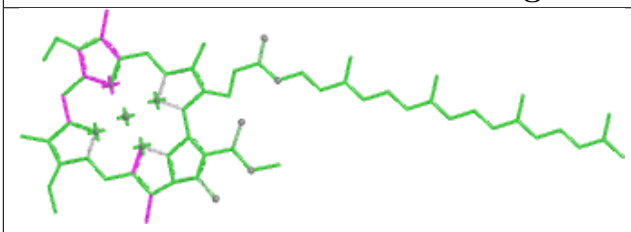


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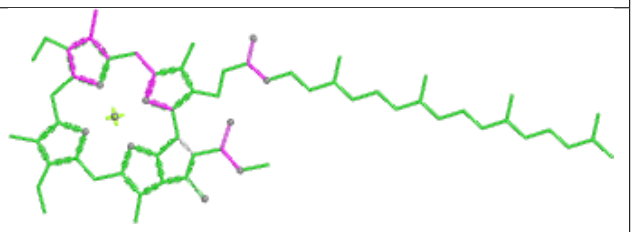


Rings

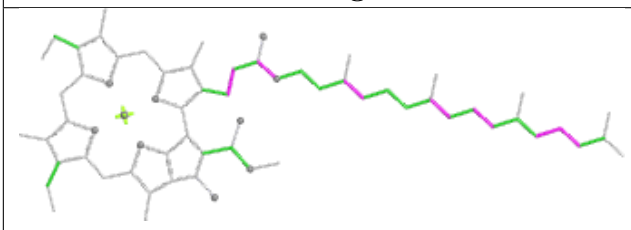
## Ligand CLA A 838



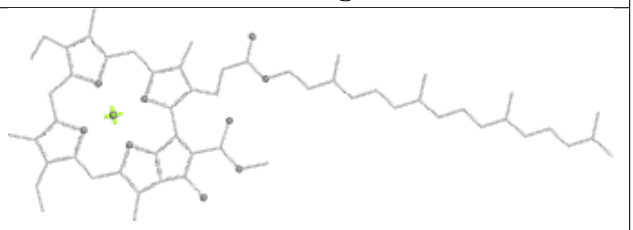
Bond lengths



Bond angles

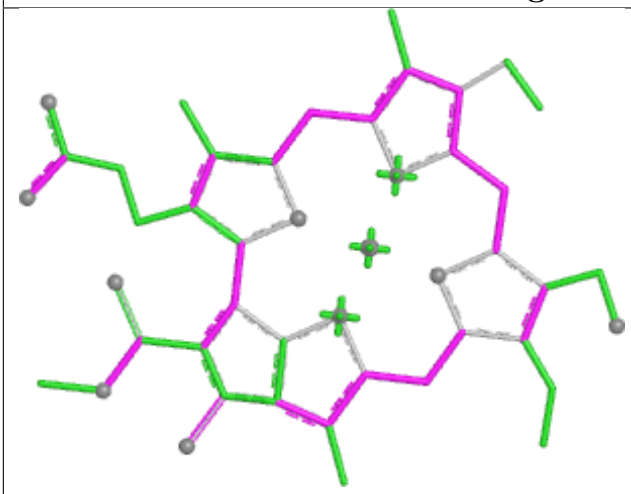


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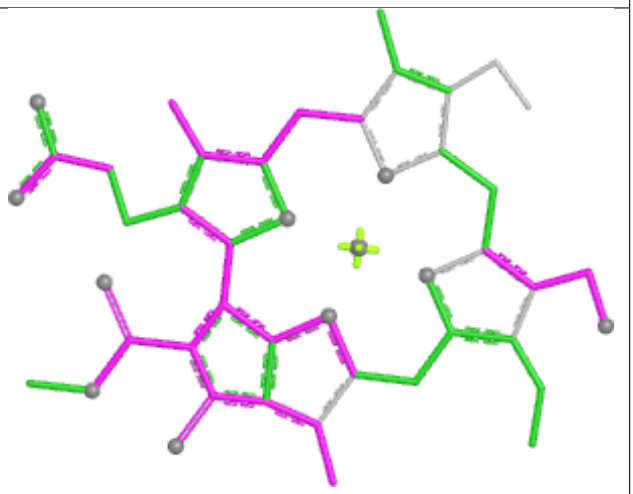


Rings

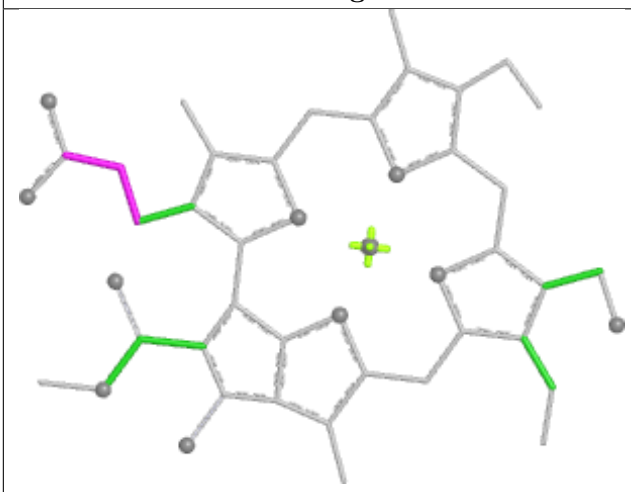
## Ligand CHL 2 614



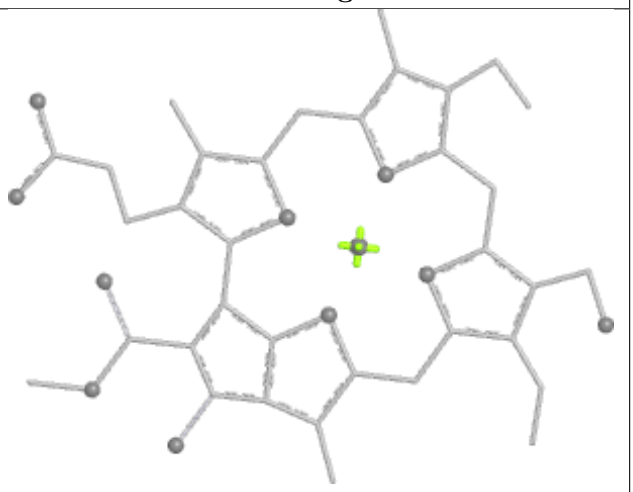
Bond lengths



Bond angles

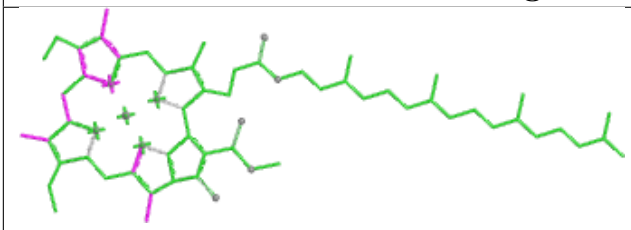


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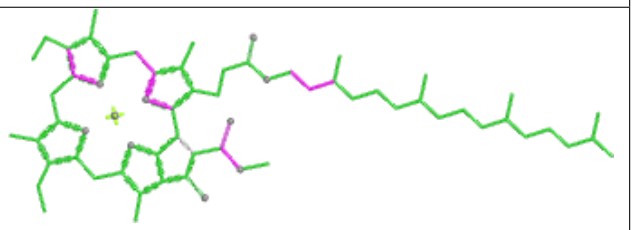


Rings

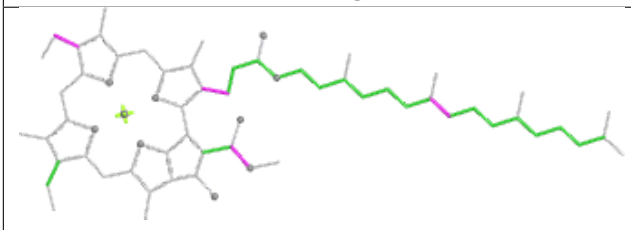
## Ligand CLA A 833



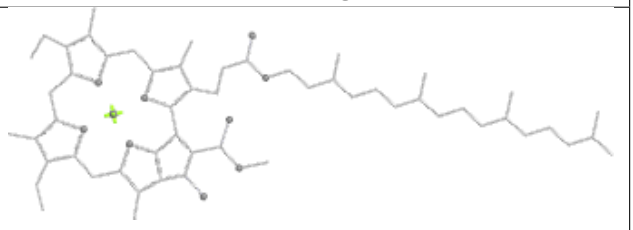
Bond lengths



Bond angles

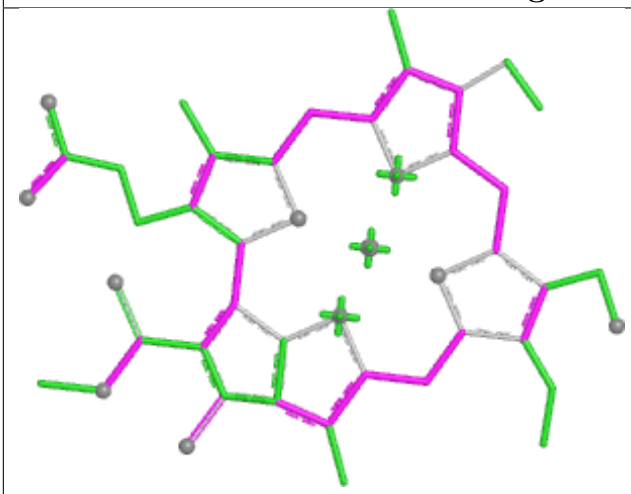


Torsions

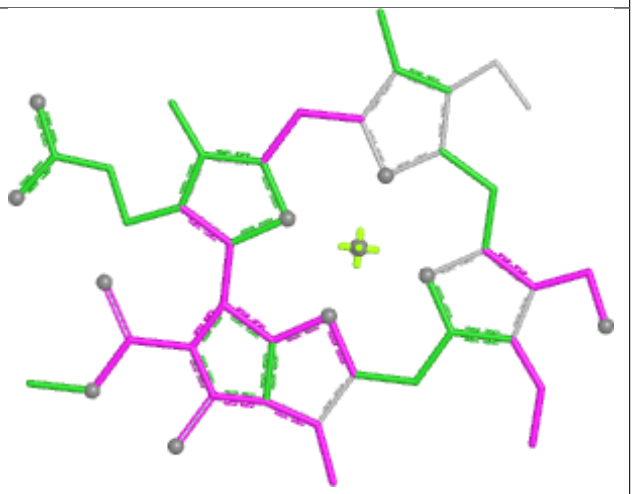


Rings

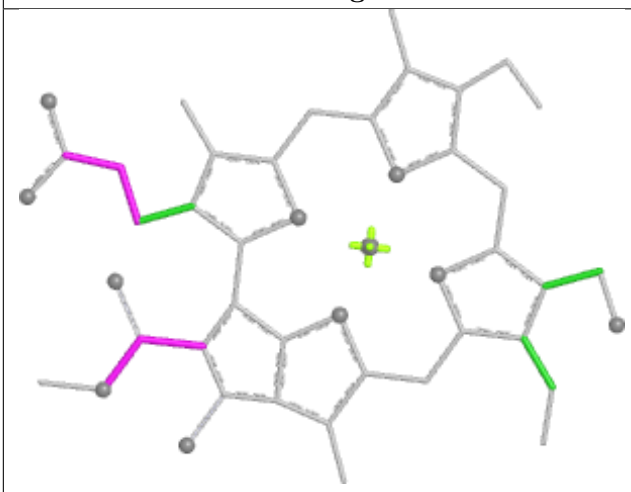
**Ligand CHL a 609**



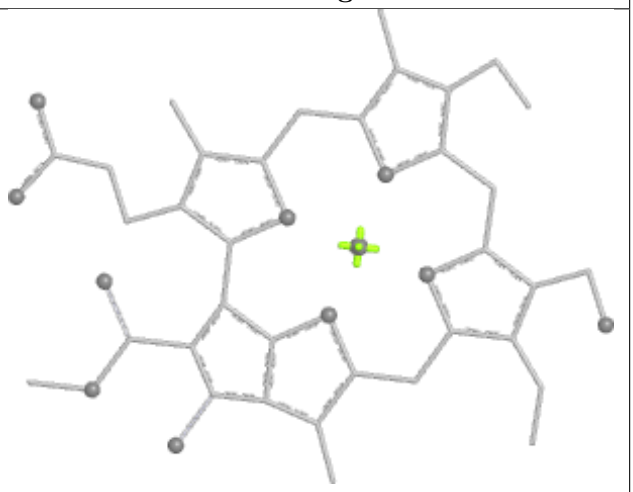
**Bond lengths**



**Bond angles**

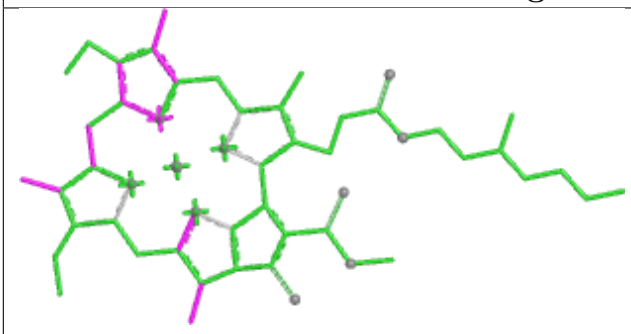


**Torsions**

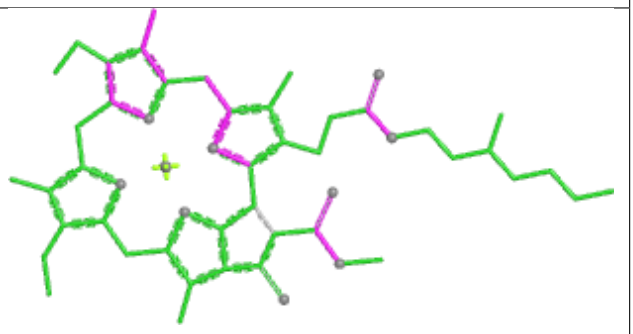


**Rings**

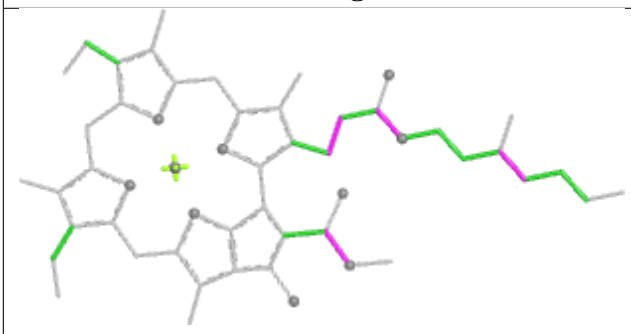
**Ligand CLA b 314**



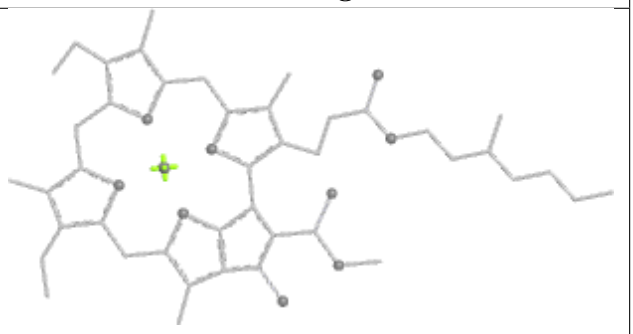
Bond lengths



Bond angles

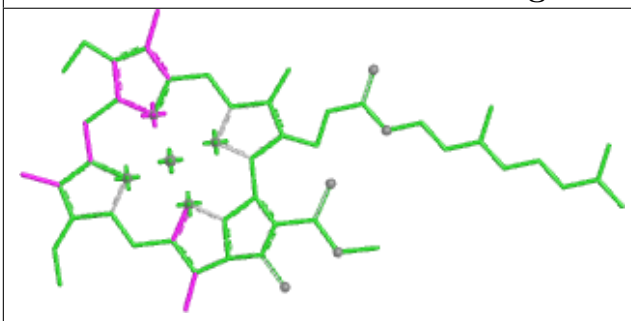


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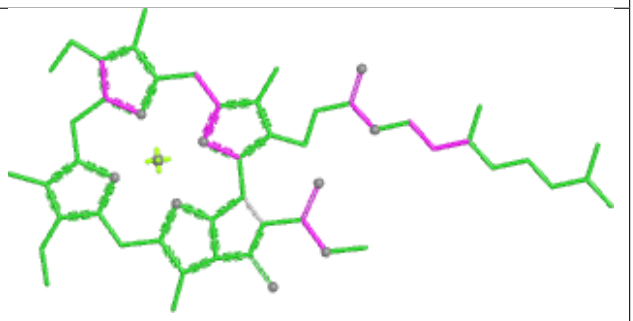


Rings

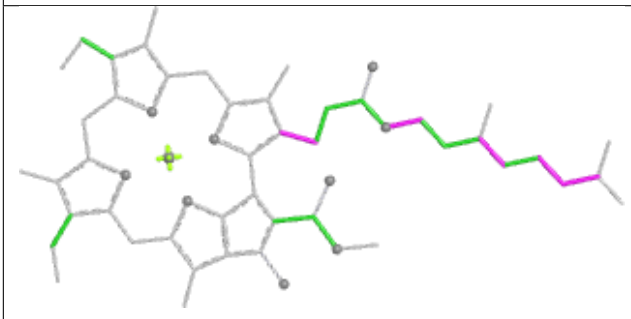
**Ligand CLA 2 608**



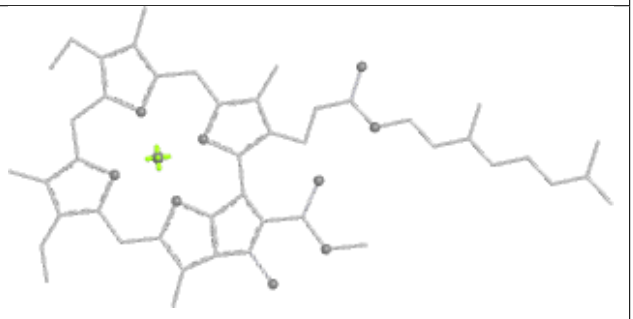
Bond lengths



Bond angles

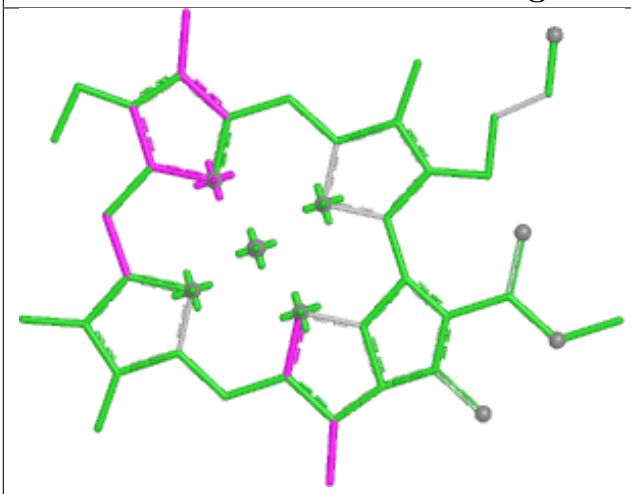


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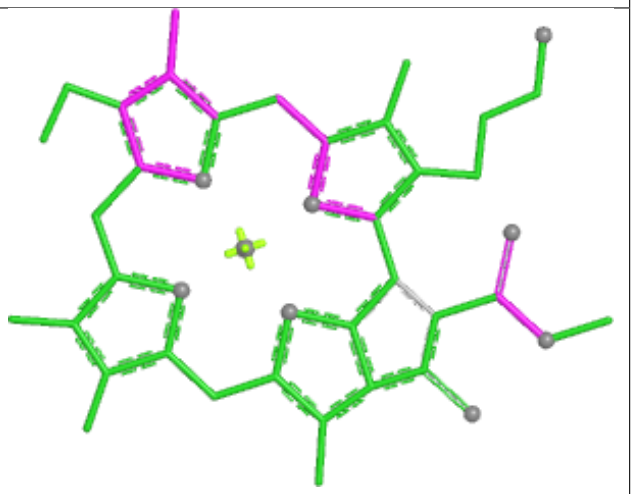


Rings

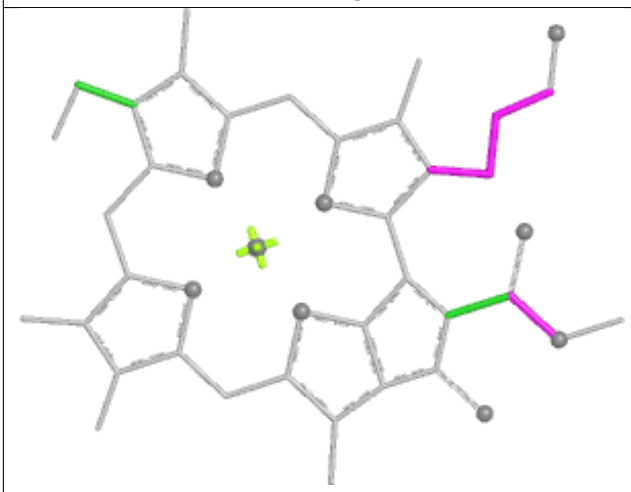
## Ligand CLA 8 604



Bond lengths



Bond angles

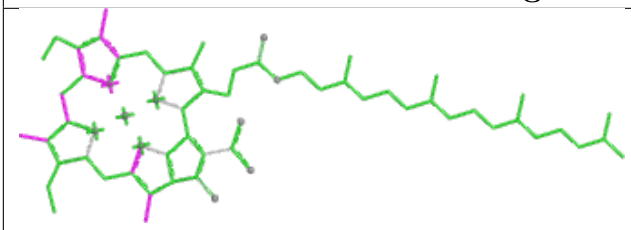


Torsions

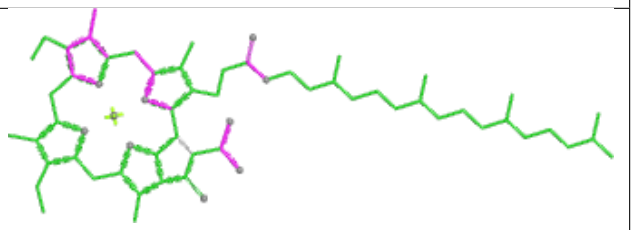


Rings

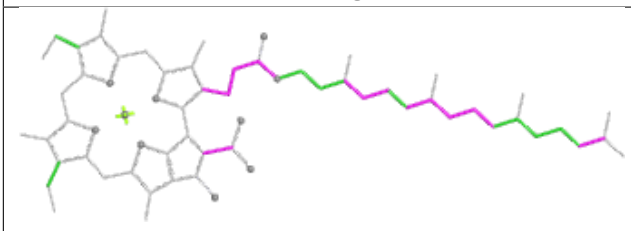
## Ligand CLA A 827



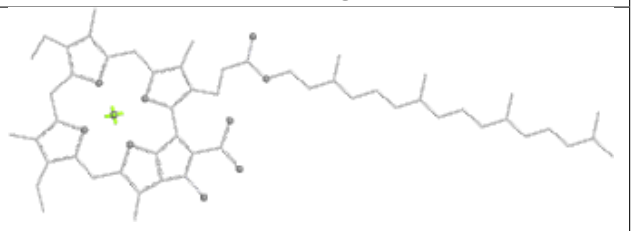
Bond lengths



Bond angles



Torsions

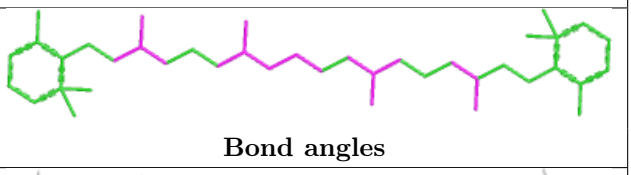


Rings

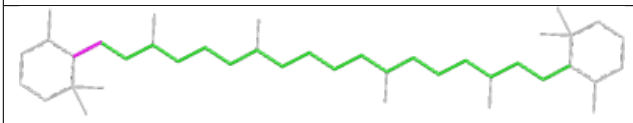
## Ligand BCR 7 417



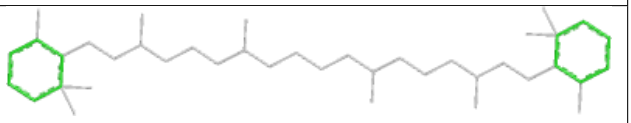
Bond lengths



Bond angles

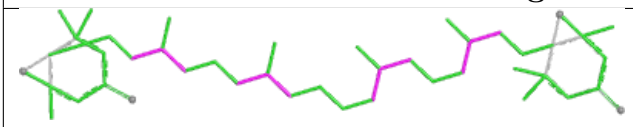


Torsions



Rings

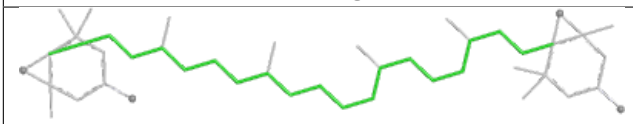
## Ligand XAT 4 616



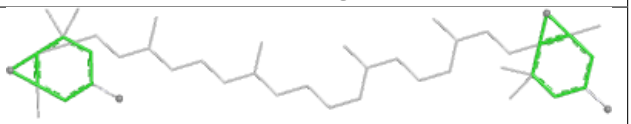
Bond lengths



Bond angles

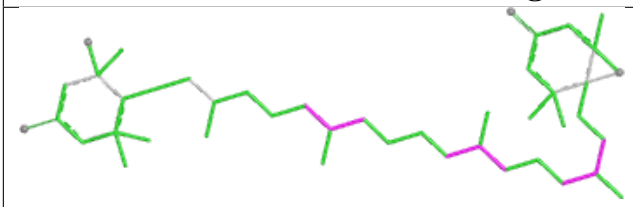


Torsions

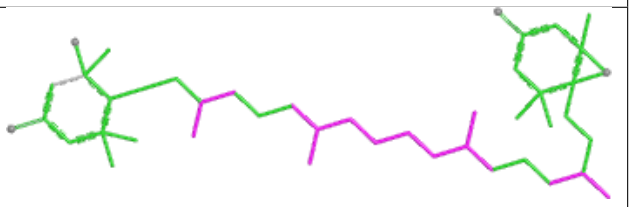


Rings

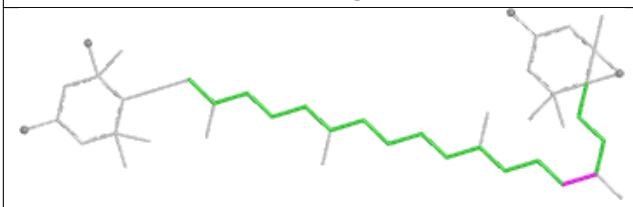
## Ligand NEX 9 617



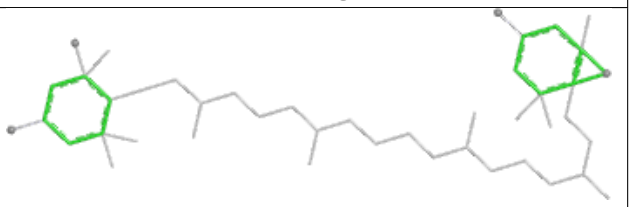
Bond lengths



Bond angles

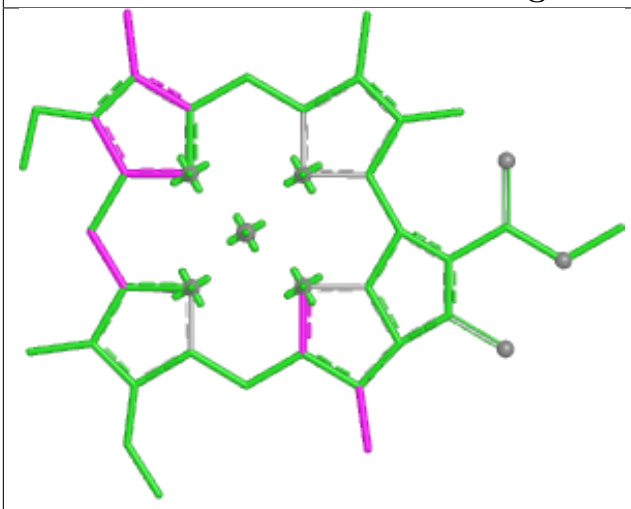


Torsions

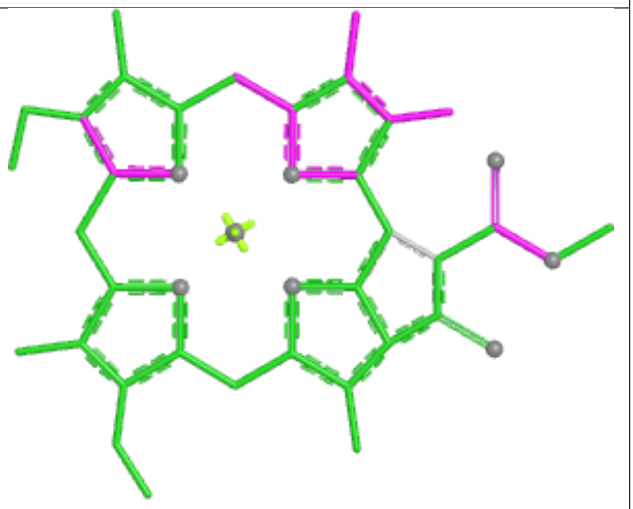


Rings

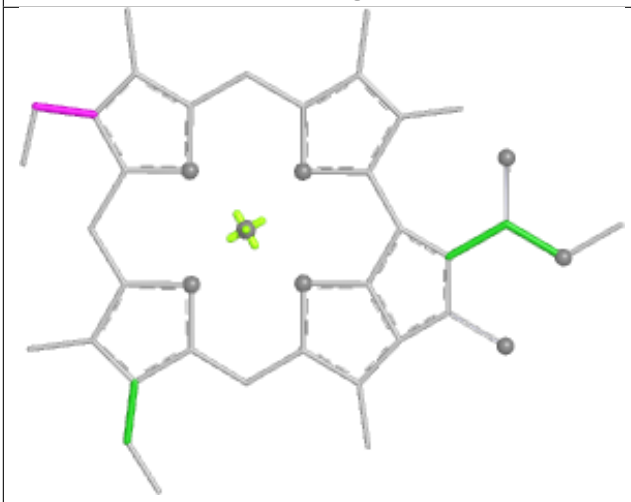
## Ligand CLA a 603



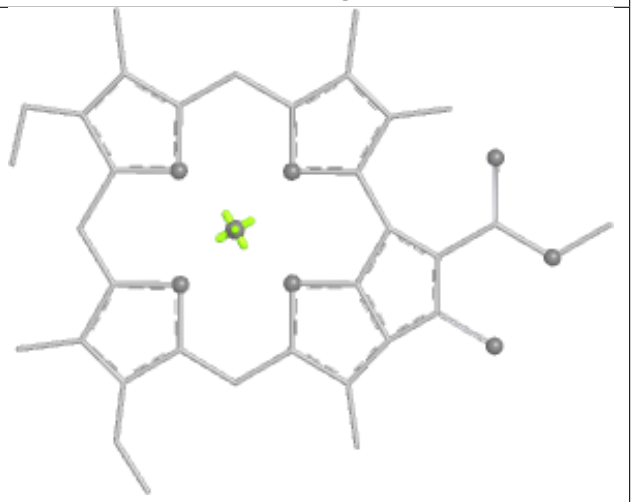
Bond lengths



Bond angles

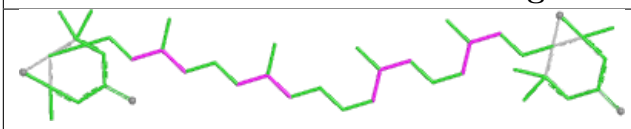


Torsions

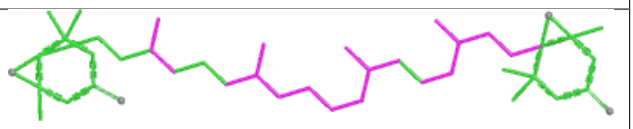


Rings

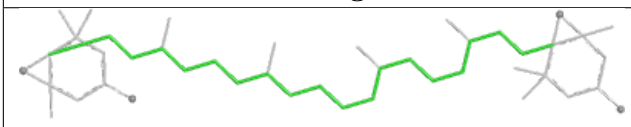
## Ligand XAT 1 318



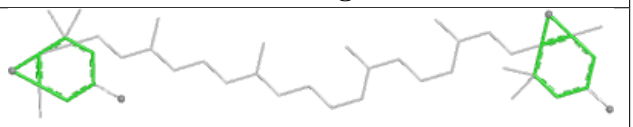
Bond lengths



Bond angles

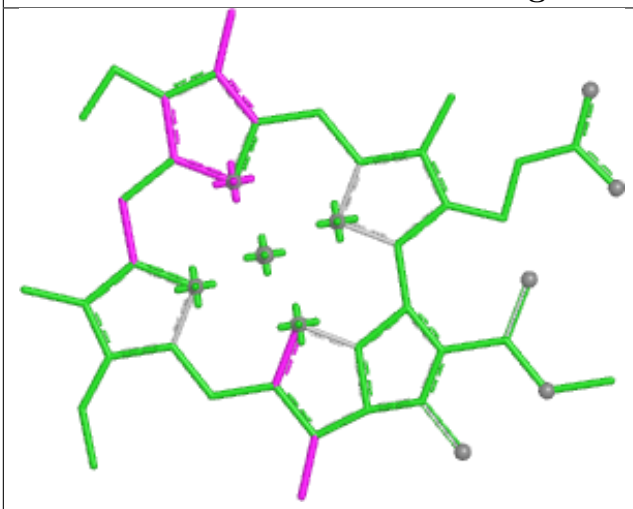


Torsions

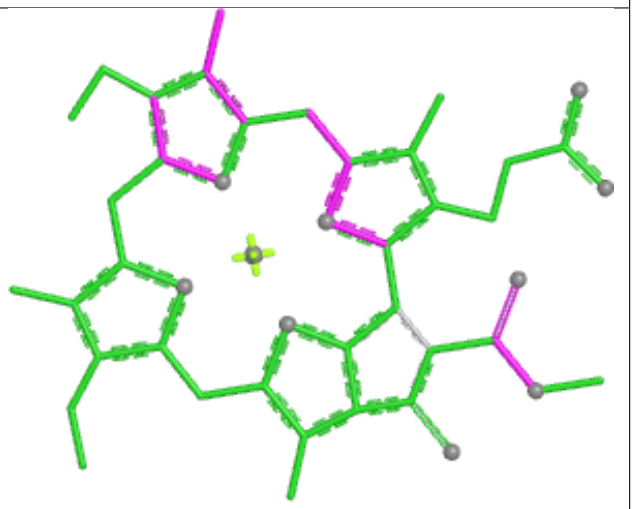


Rings

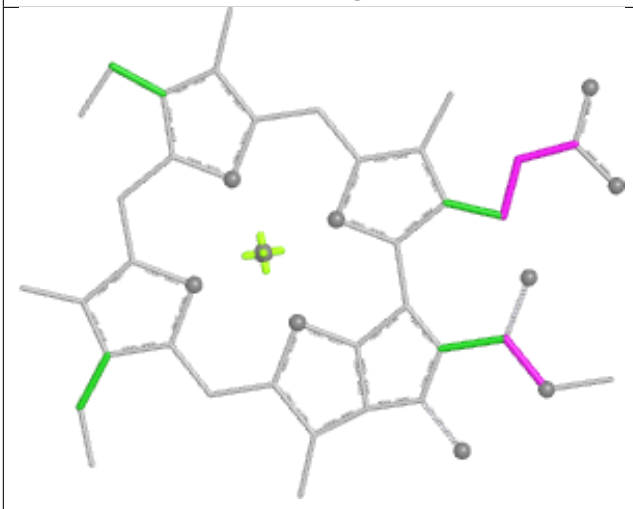
## Ligand CLA 5 611



Bond lengths



Bond angles

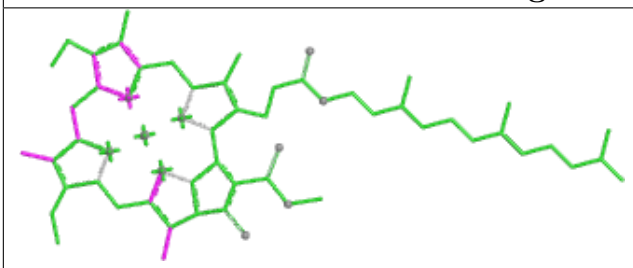


Torsions

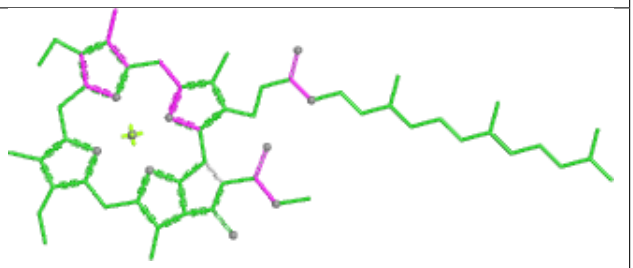


Rings

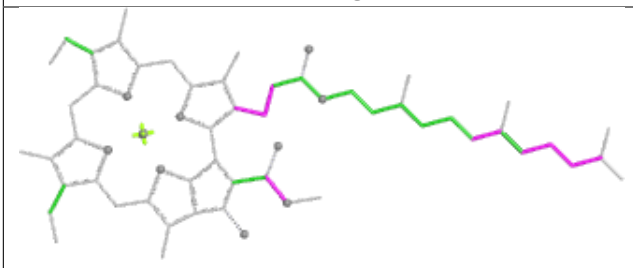
## Ligand CLA a 602



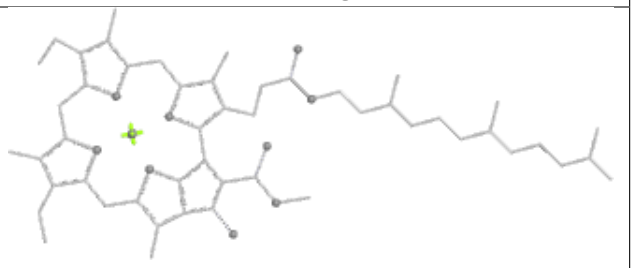
Bond lengths



Bond angles

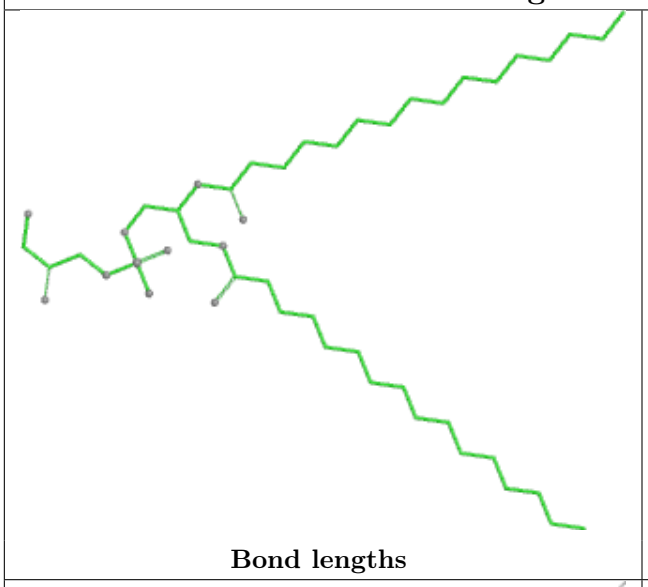


Torsions

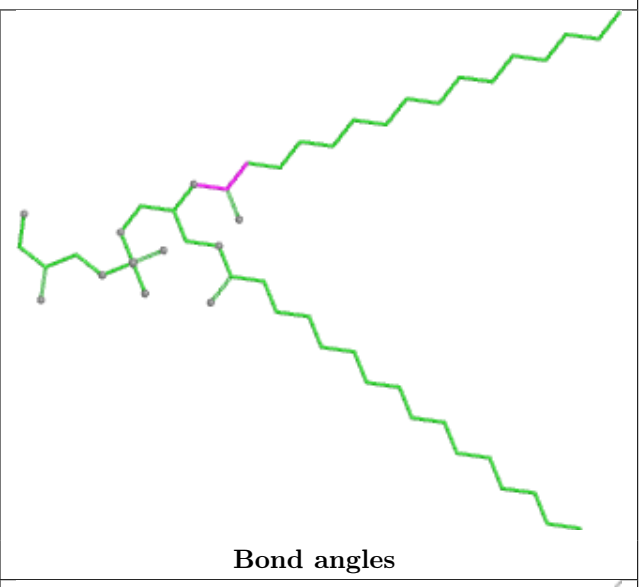


Rings

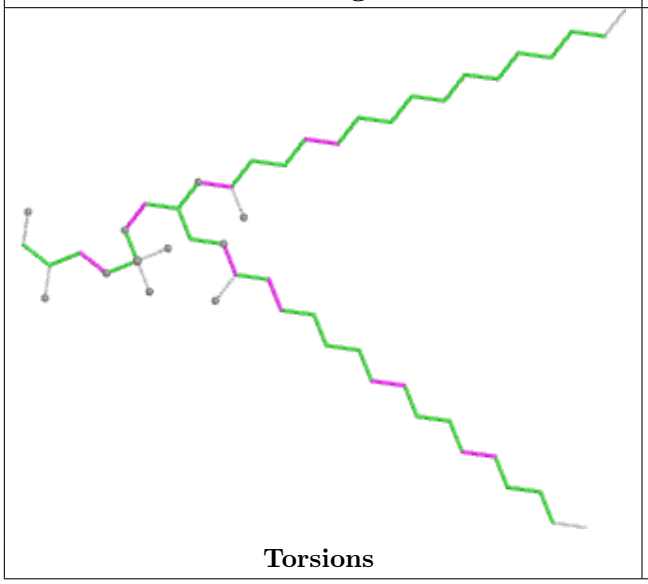
**Ligand LHG 4 619**



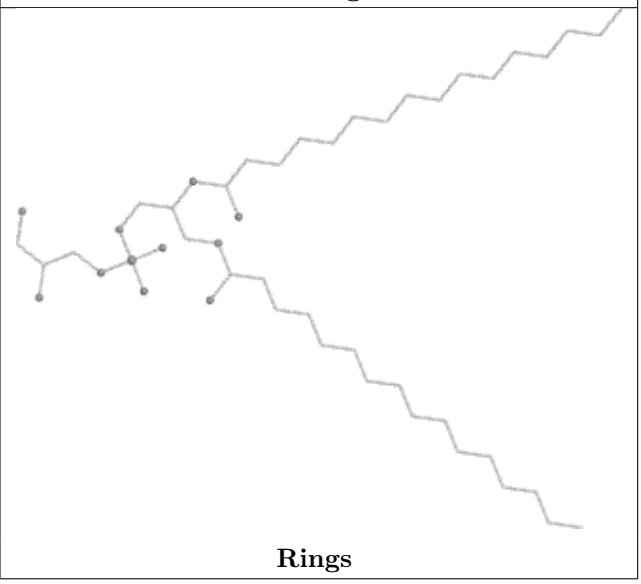
**Bond lengths**



**Bond angles**

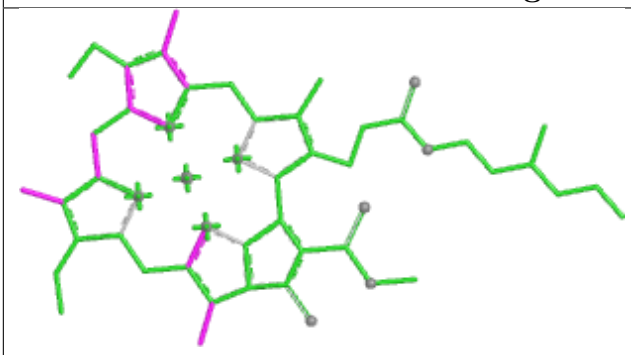


**Torsions**

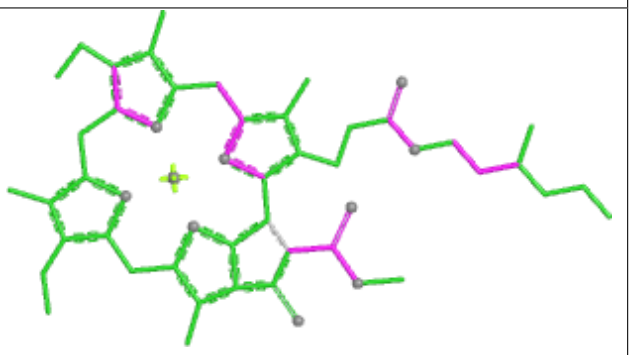


**Rings**

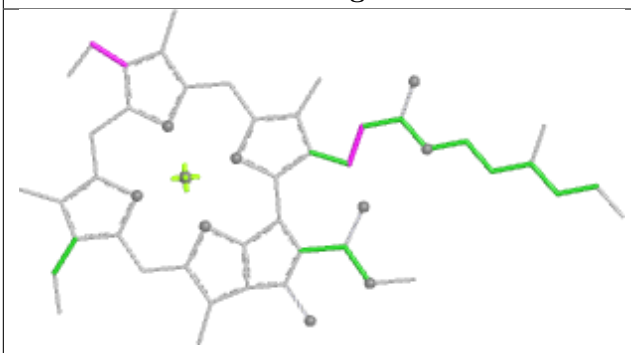
**Ligand CLA A 802**



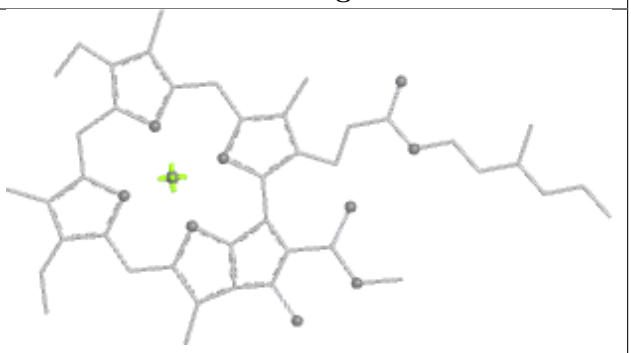
**Bond lengths**



**Bond angles**

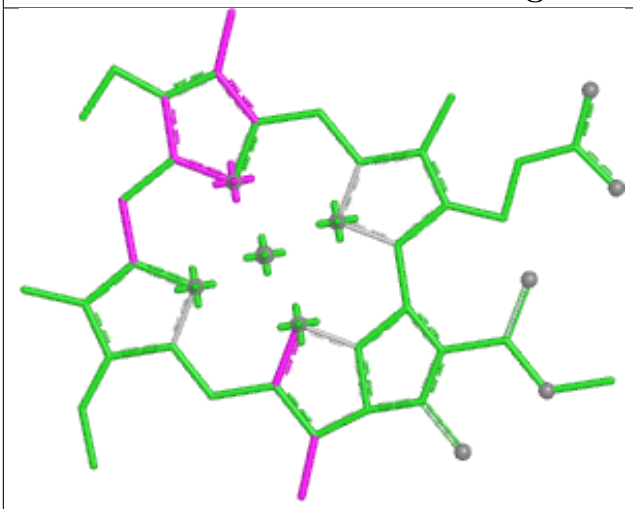


**Torsions**

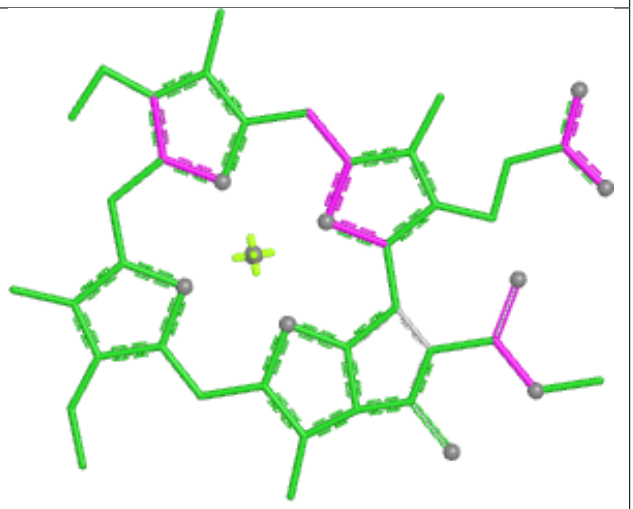


**Rings**

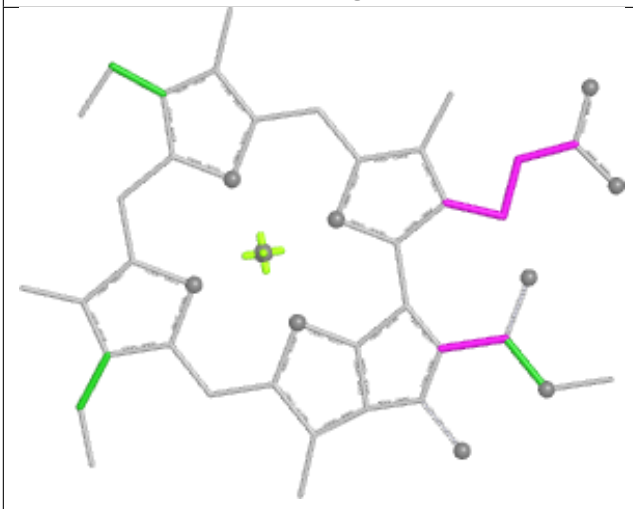
**Ligand CLA L 302**



**Bond lengths**



**Bond angles**

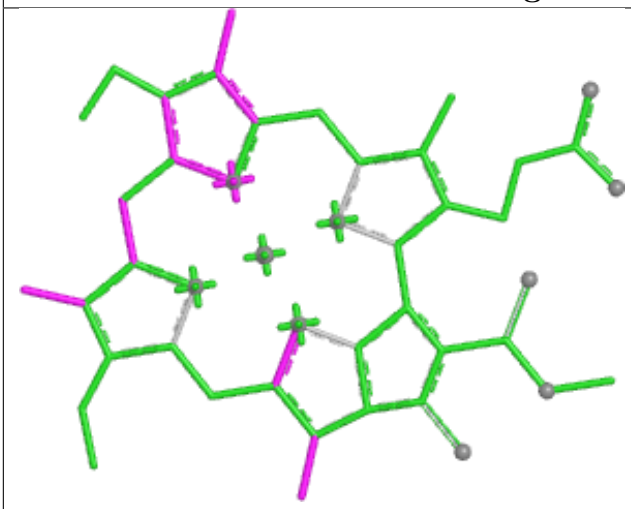


**Torsions**

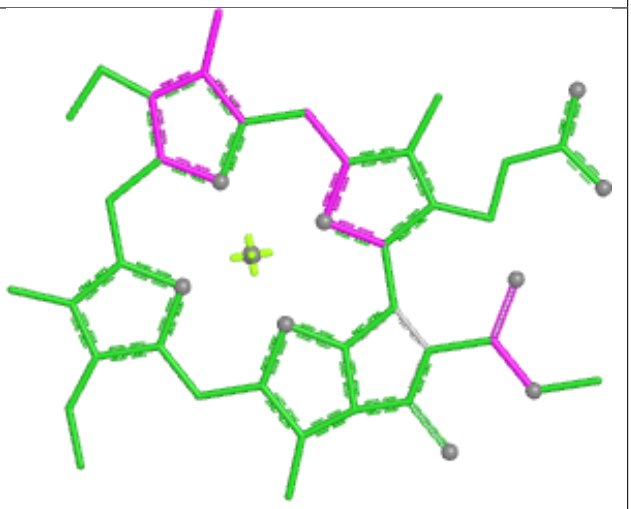


**Rings**

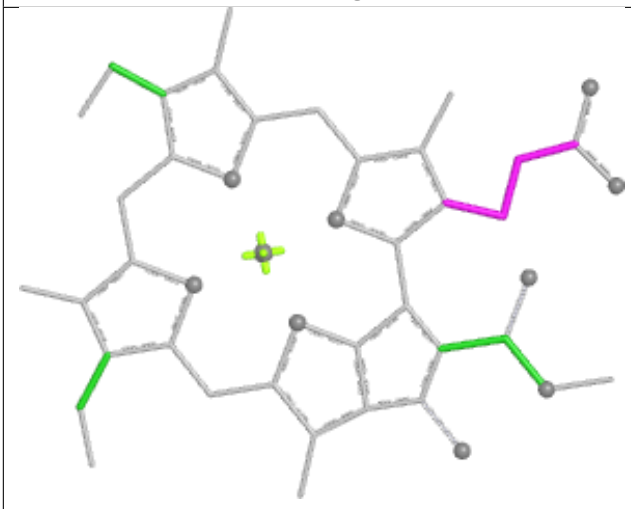
## Ligand CLA A 832



Bond lengths



Bond angles

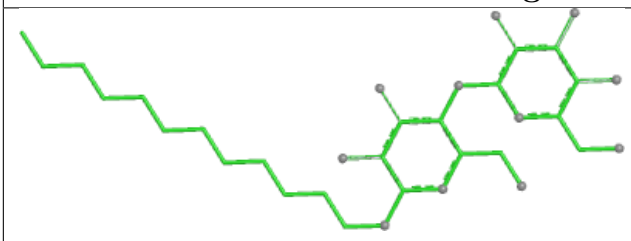


Torsions

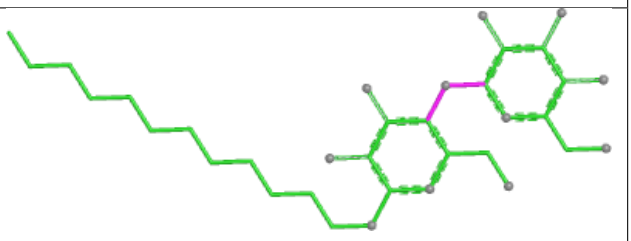


Rings

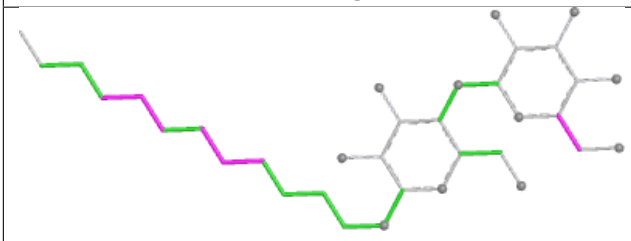
## Ligand LMU b 301



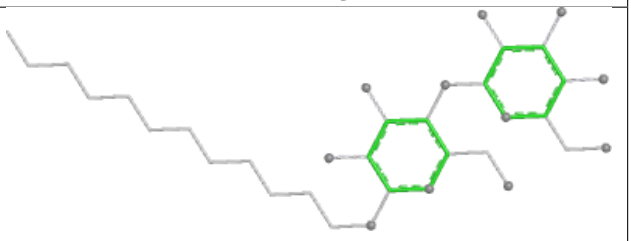
Bond lengths



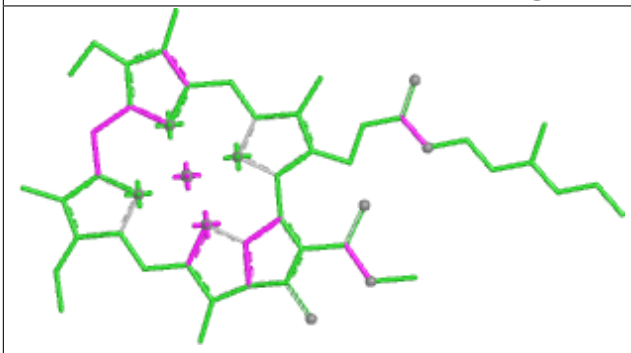
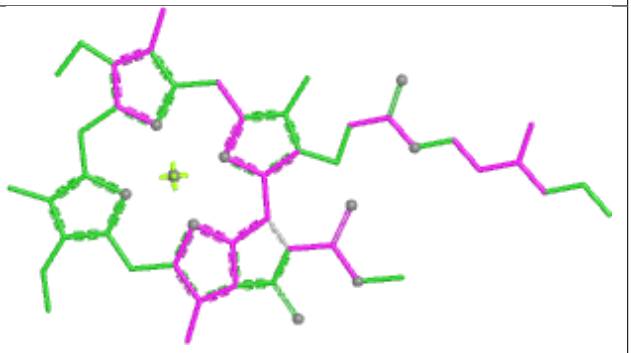
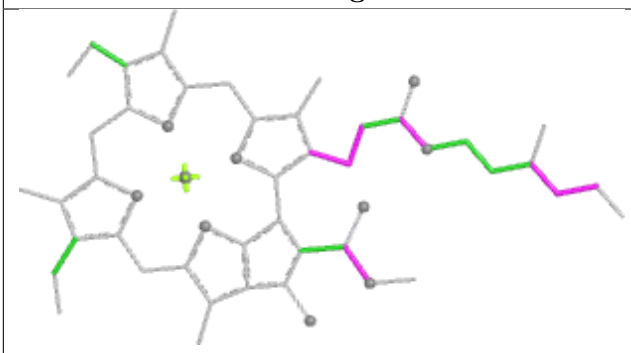
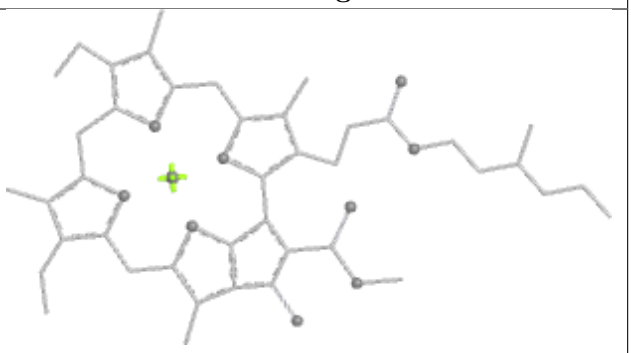
Bond angles

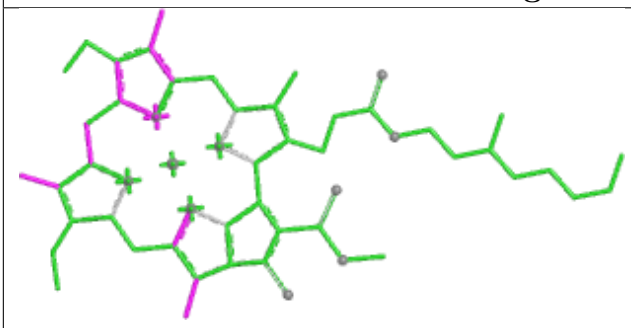
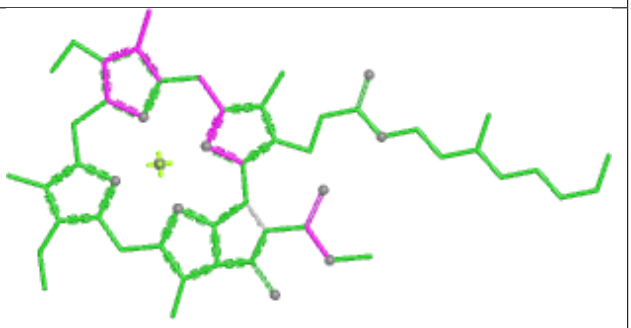
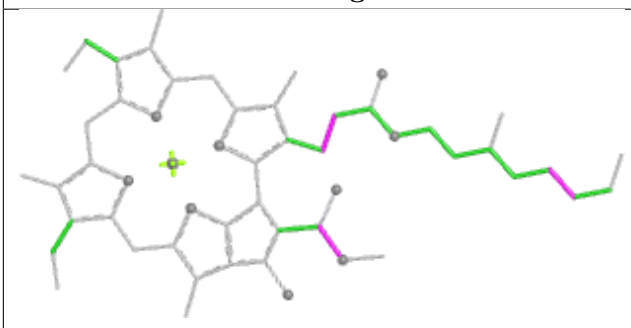
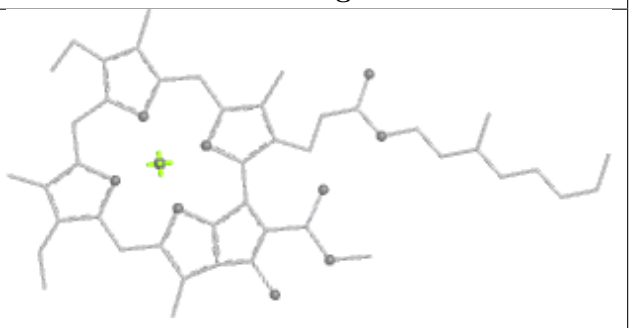


Torsions

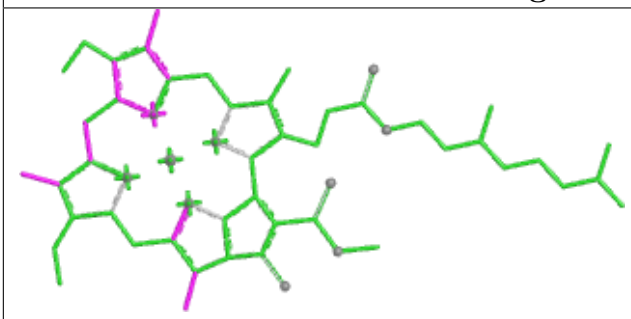


Rings

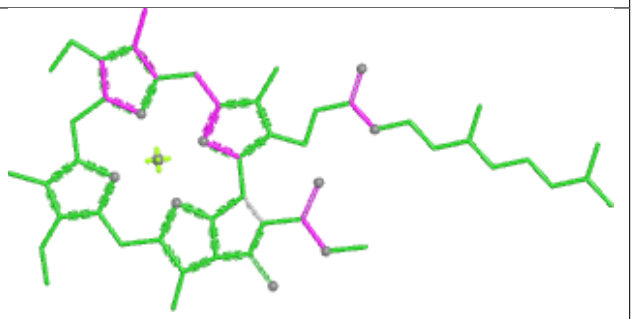
| Ligand CLA 3 409 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA A 813 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

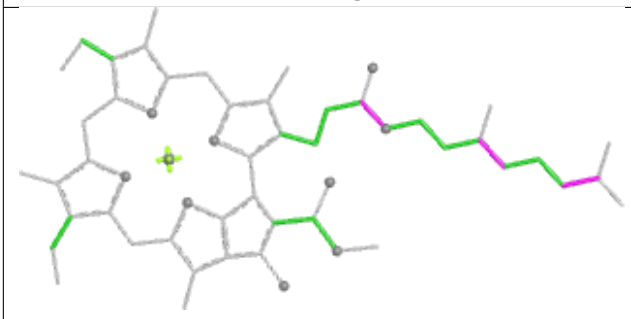
**Ligand CLA c 603**



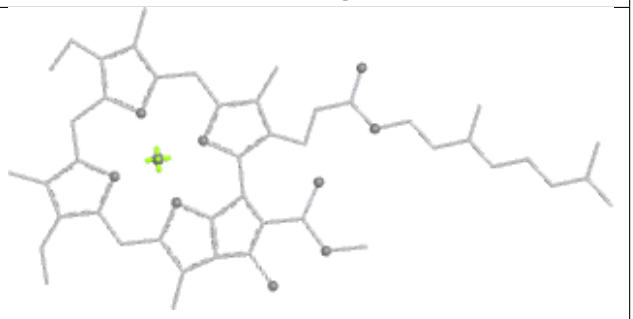
**Bond lengths**



**Bond angles**

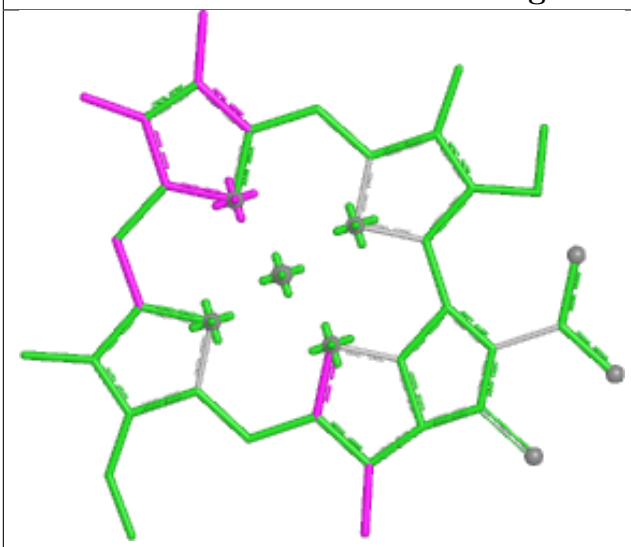


**Torsions**

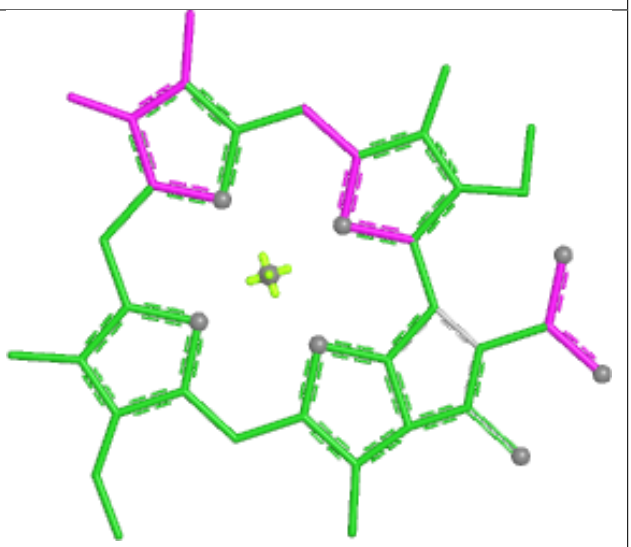


**Rings**

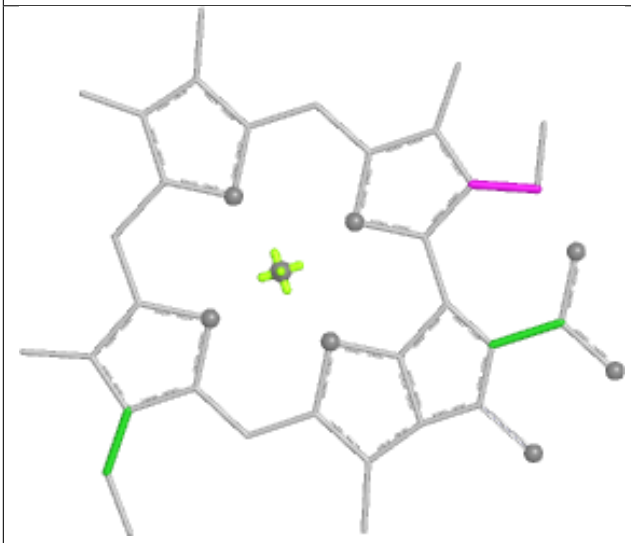
**Ligand CLA 7 405**



**Bond lengths**



**Bond angles**

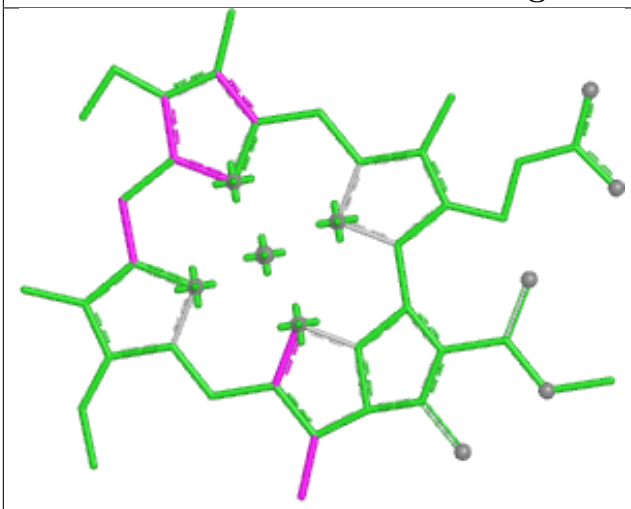


**Torsions**

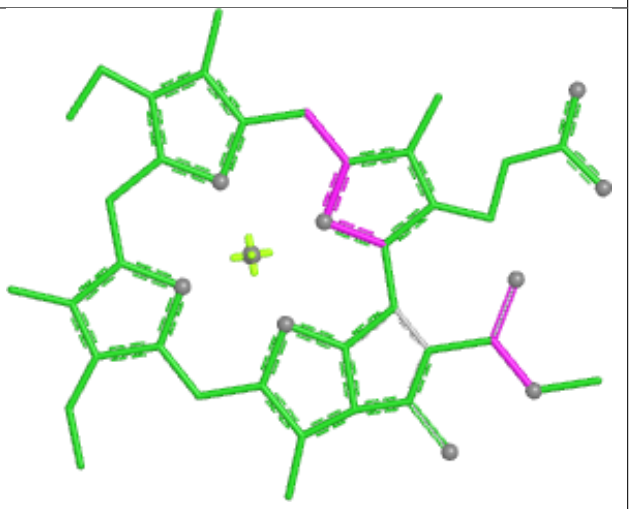


**Rings**

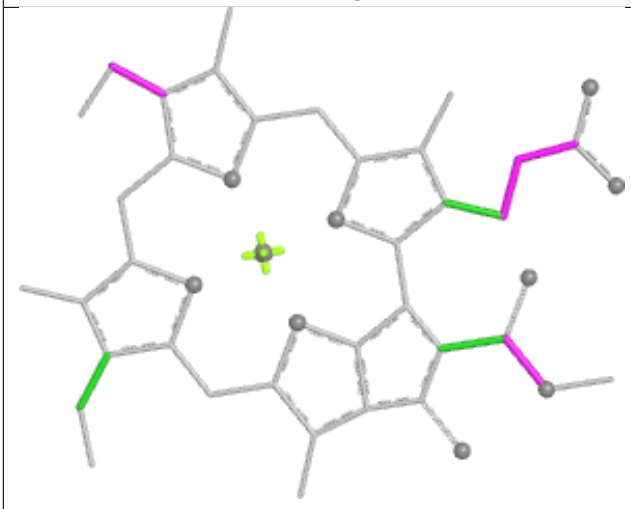
**Ligand CLA 6 603**



**Bond lengths**



**Bond angles**

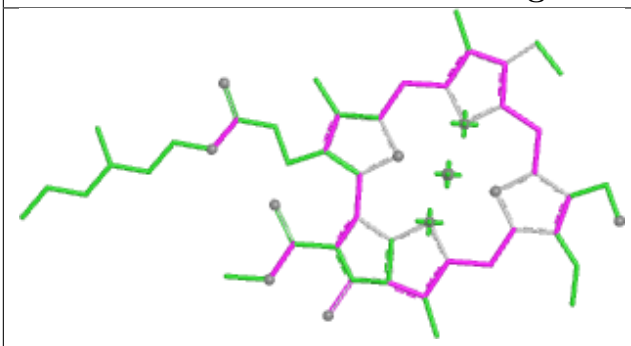


**Torsions**

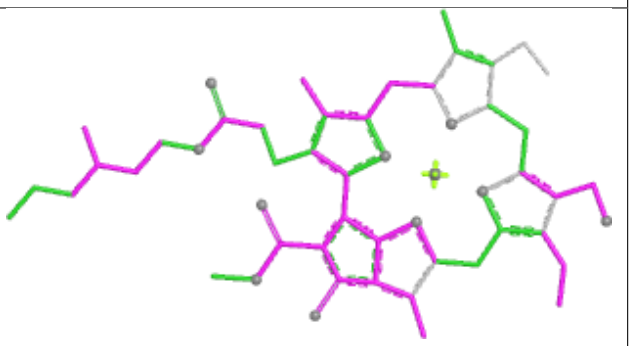


**Rings**

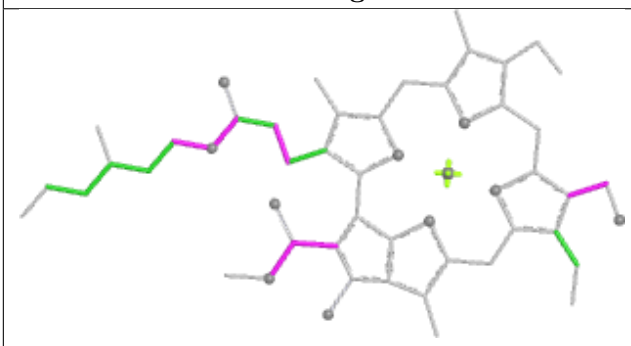
**Ligand CHL 6 602**



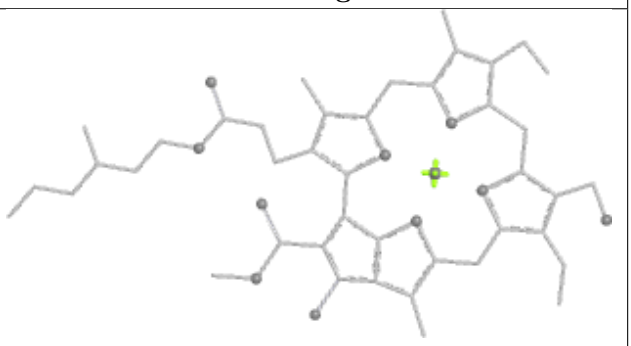
**Bond lengths**



**Bond angles**

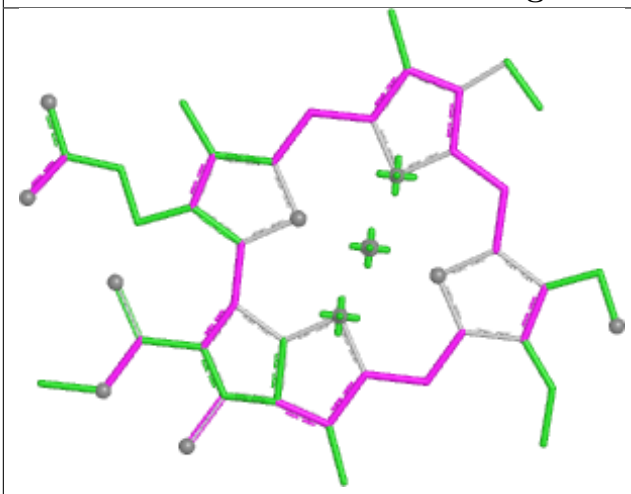


**Torsions**

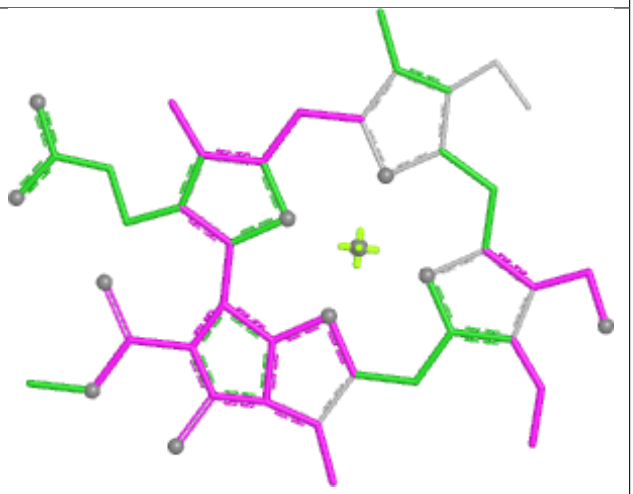


**Rings**

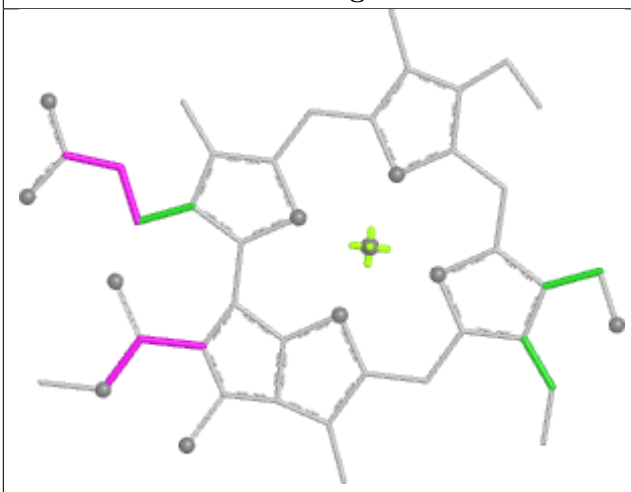
## Ligand CHL b 306



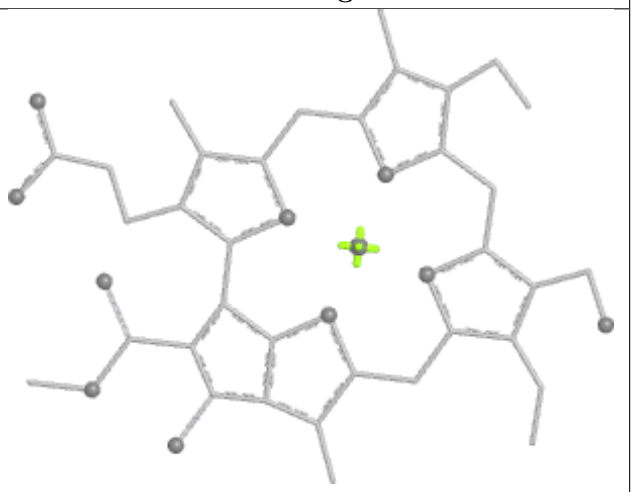
Bond lengths



Bond angles

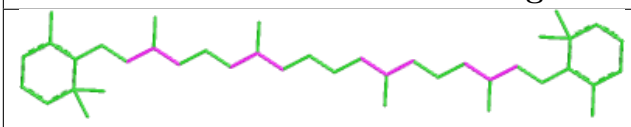


Torsions

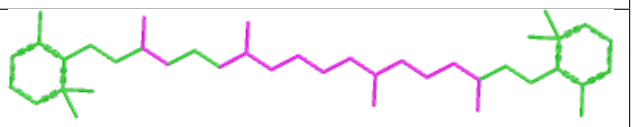


Rings

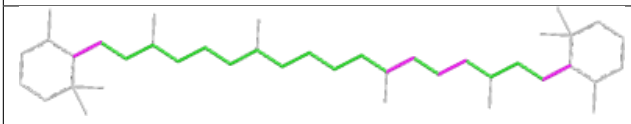
## Ligand BCR J 101



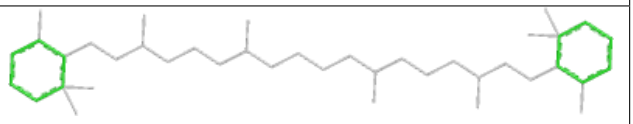
Bond lengths



Bond angles

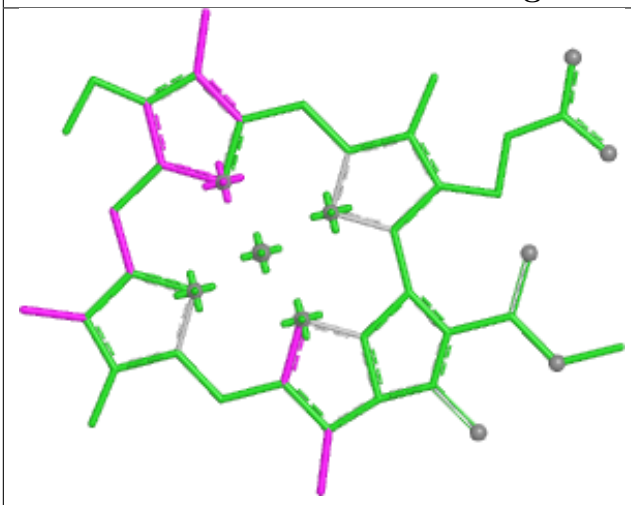


Torsions

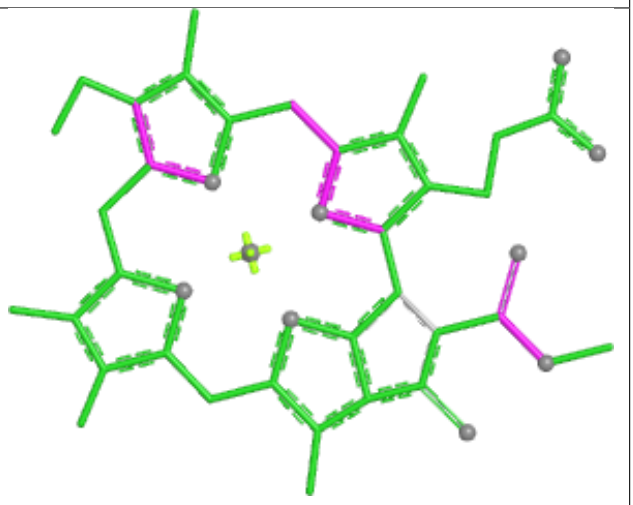


Rings

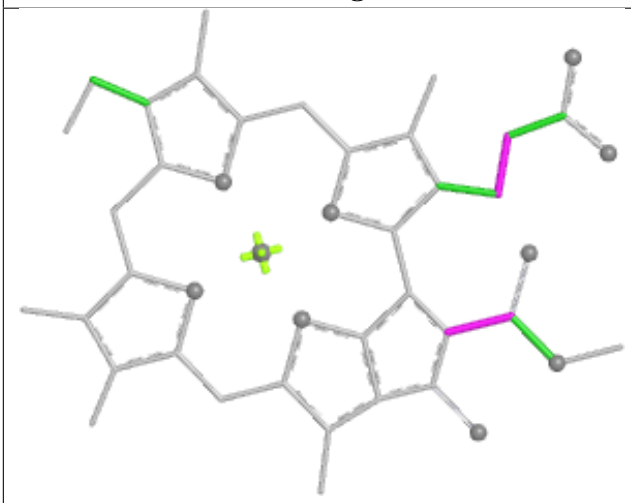
**Ligand CLA A 822**



**Bond lengths**



**Bond angles**

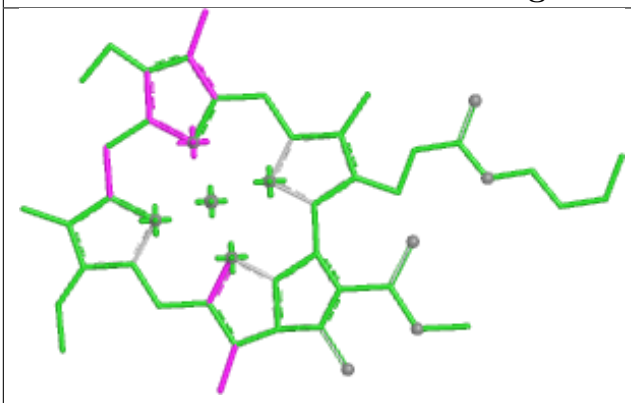


**Torsions**

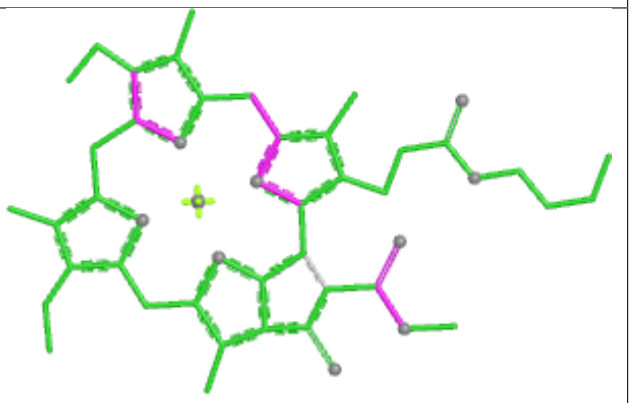


**Rings**

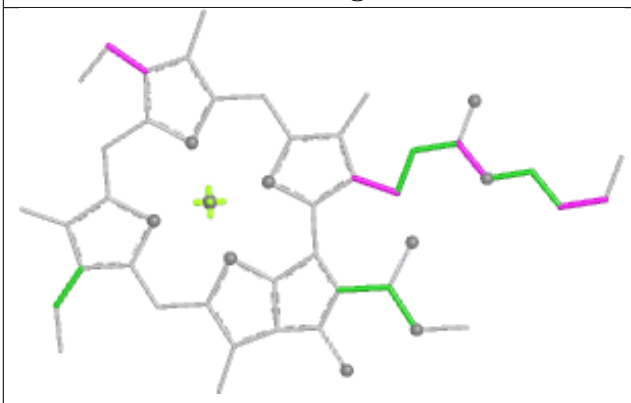
## Ligand CLA 5 604



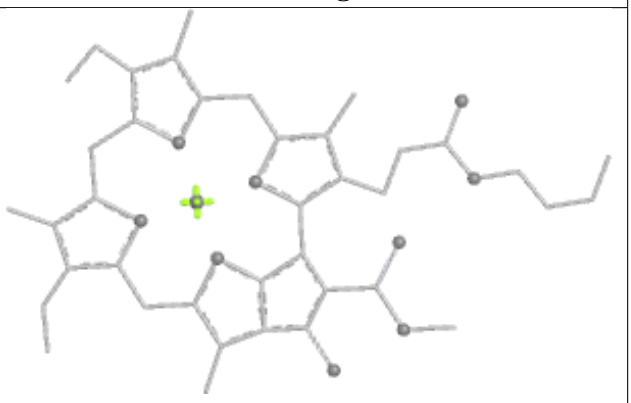
Bond lengths



Bond angles

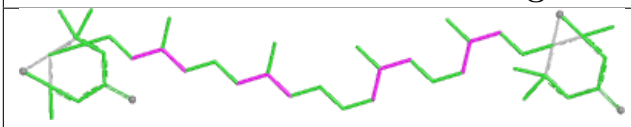


Torsions

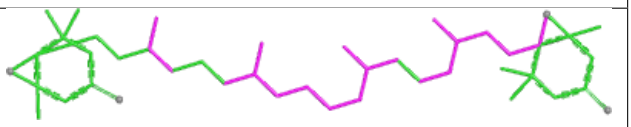


Rings

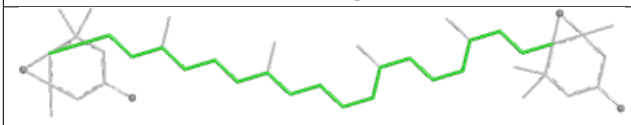
## Ligand XAT 7 416



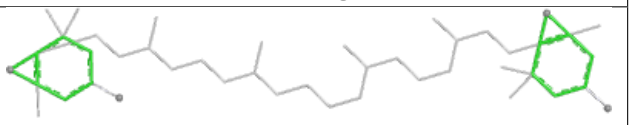
Bond lengths



Bond angles

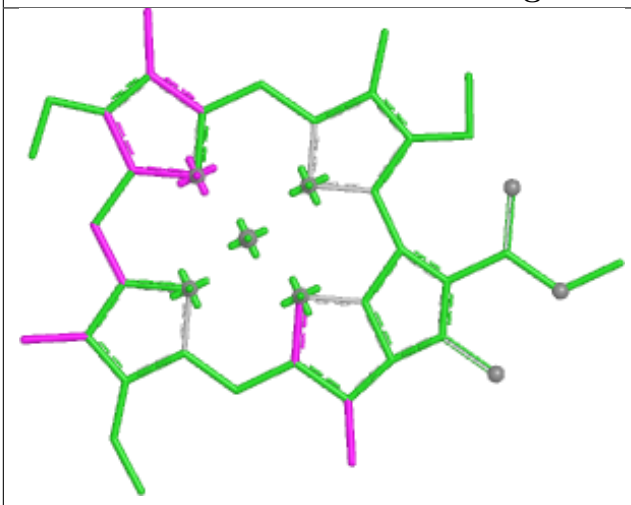


Torsions

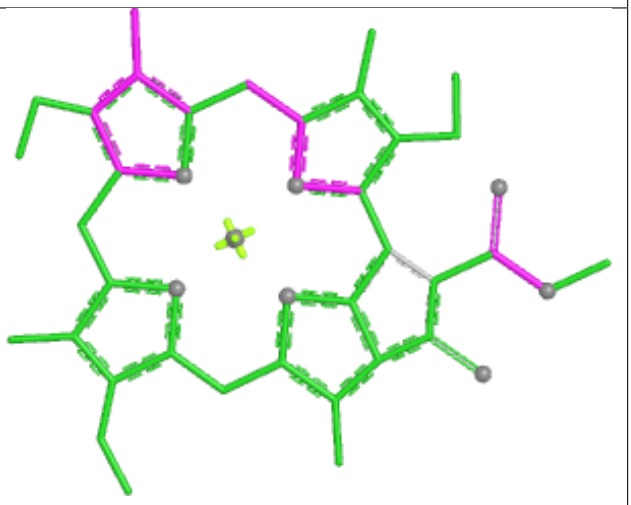


Rings

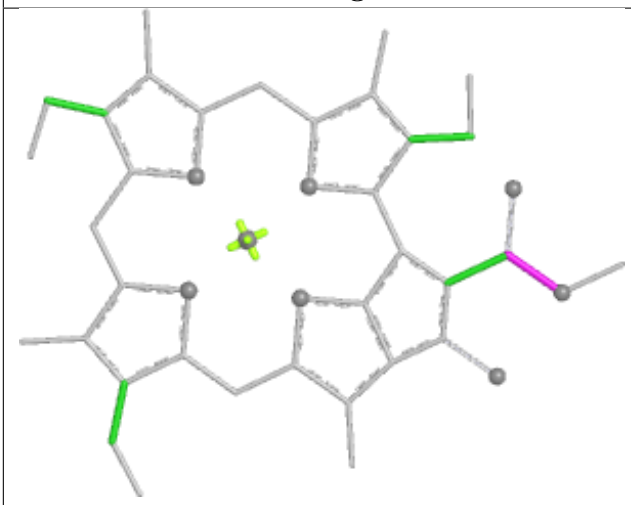
**Ligand CLA A 816**



**Bond lengths**



**Bond angles**

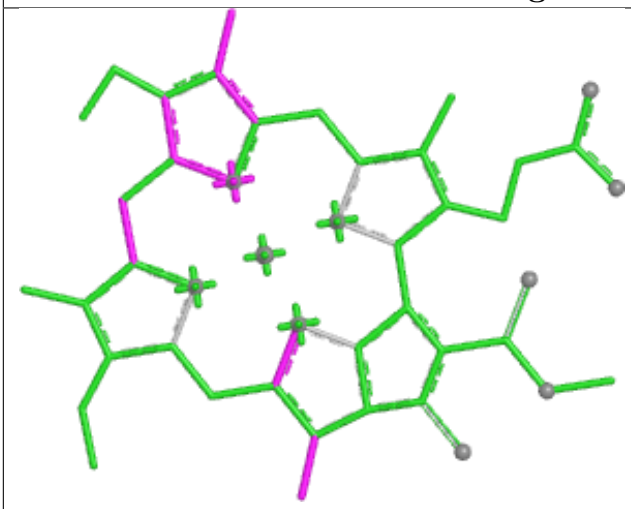


**Torsions**

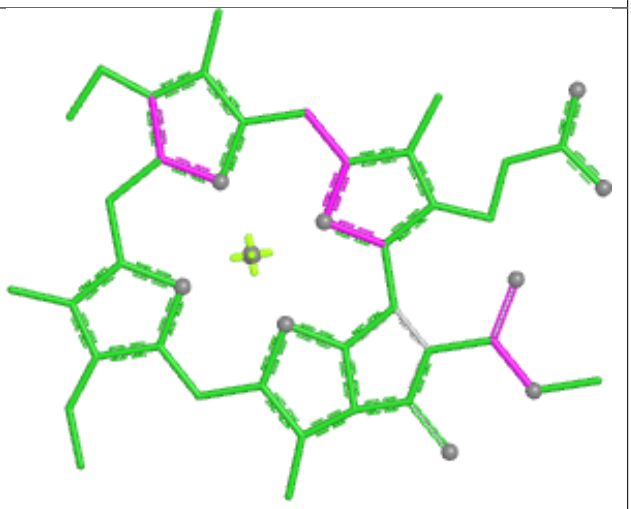


**Rings**

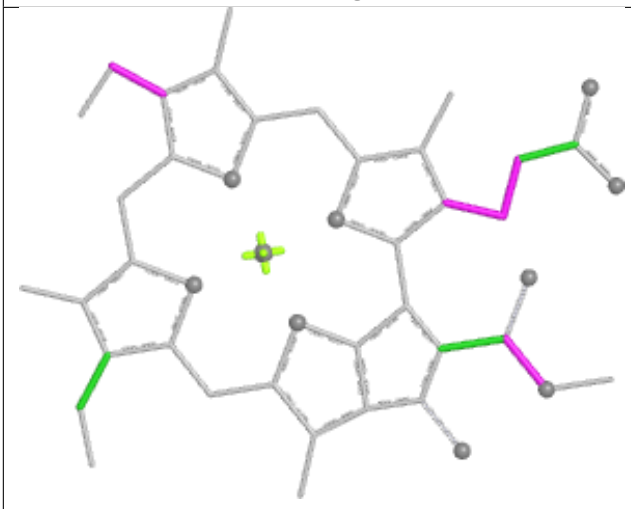
## Ligand CLA 6 608



Bond lengths



Bond angles

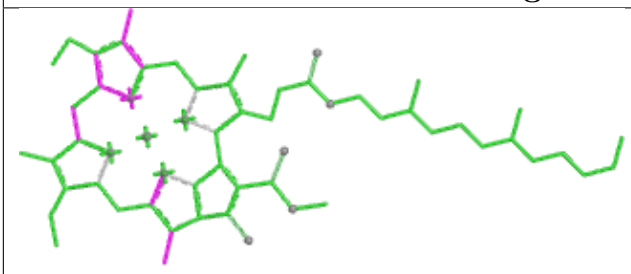


Torsions

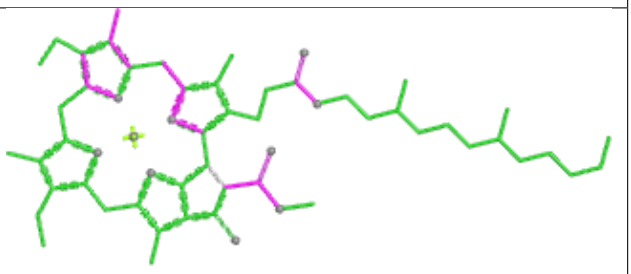


Rings

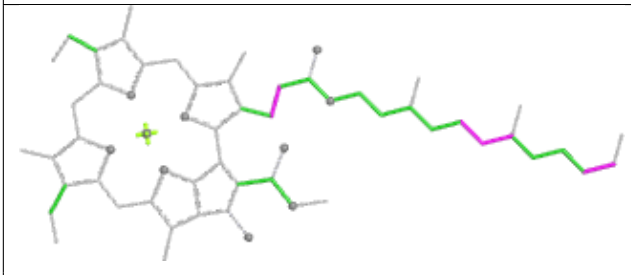
## Ligand CLA A 809



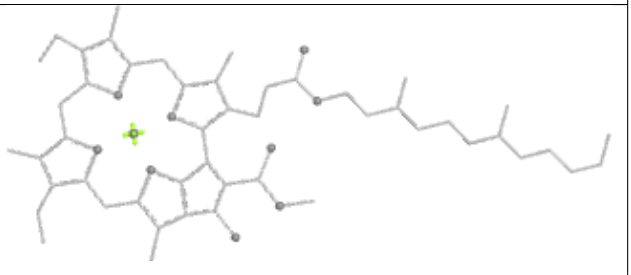
Bond lengths



Bond angles

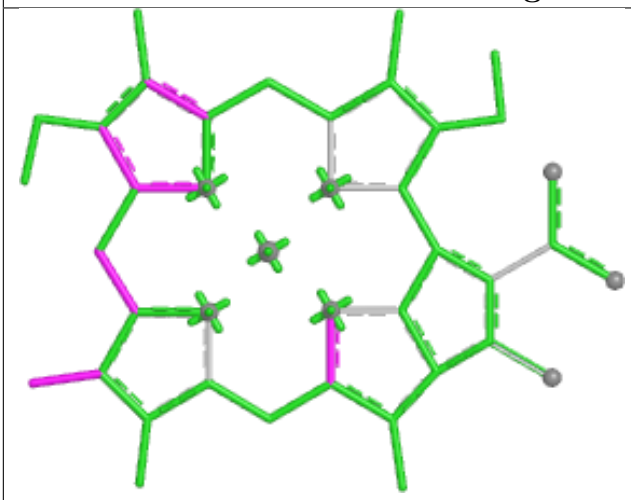


Torsions

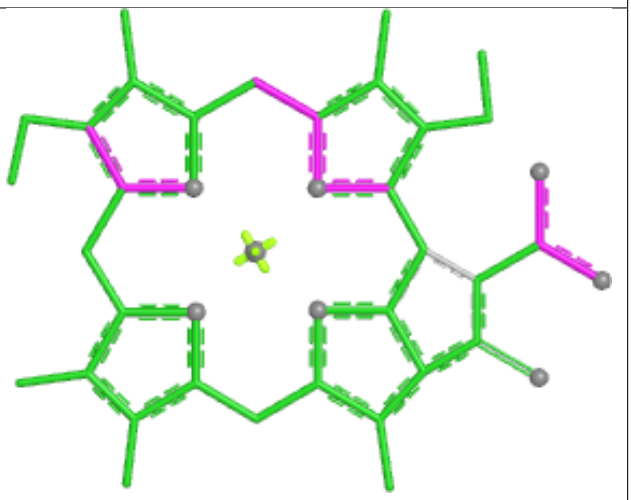


Rings

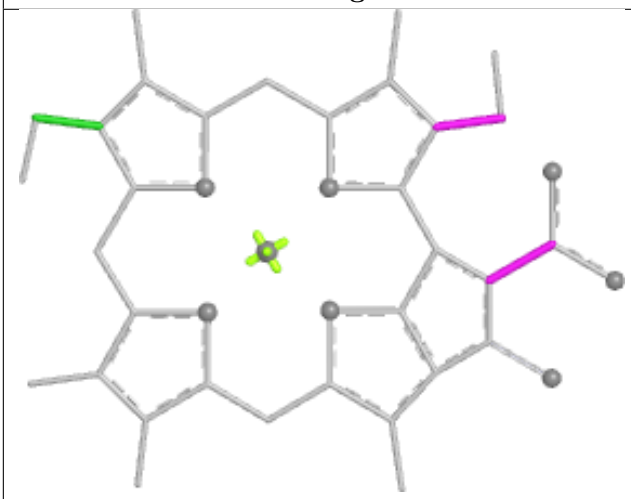
## Ligand CLA O 204



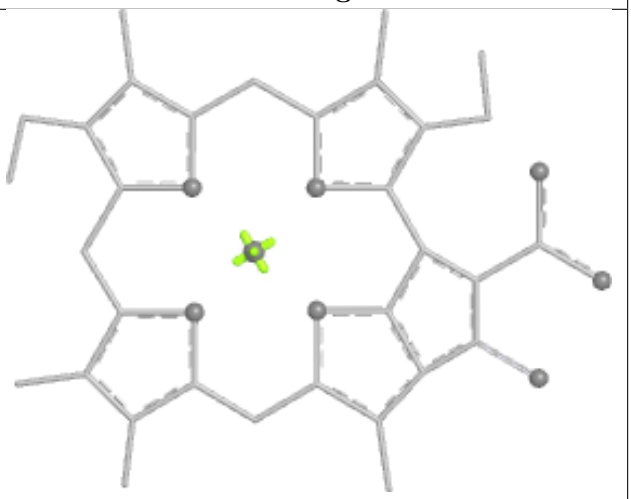
Bond lengths



Bond angles

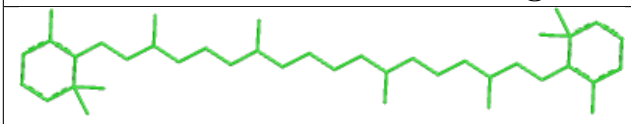


Torsions

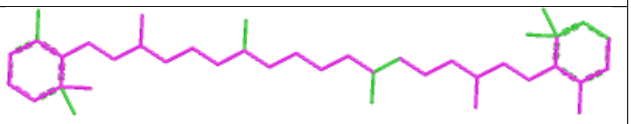


Rings

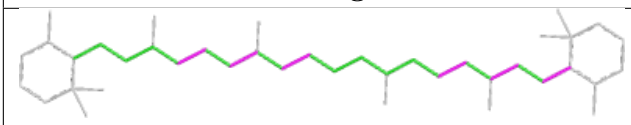
## Ligand BCR J 104



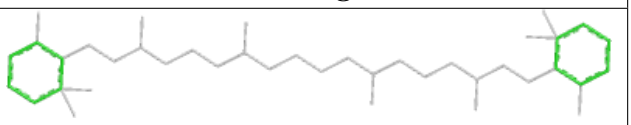
Bond lengths



Bond angles

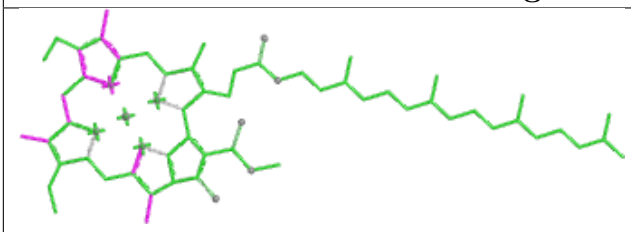


Torsions

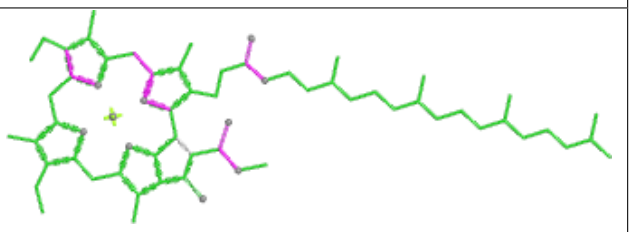


Rings

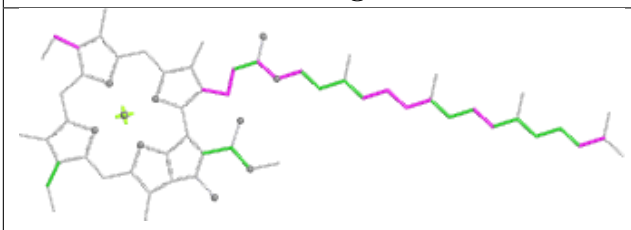
## Ligand CLA A 842



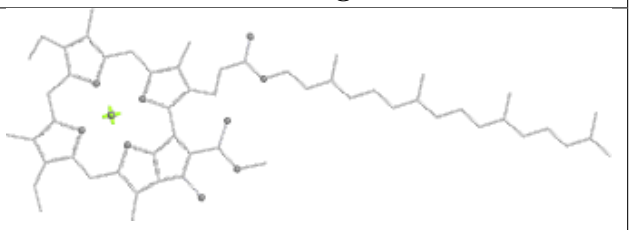
Bond lengths



Bond angles

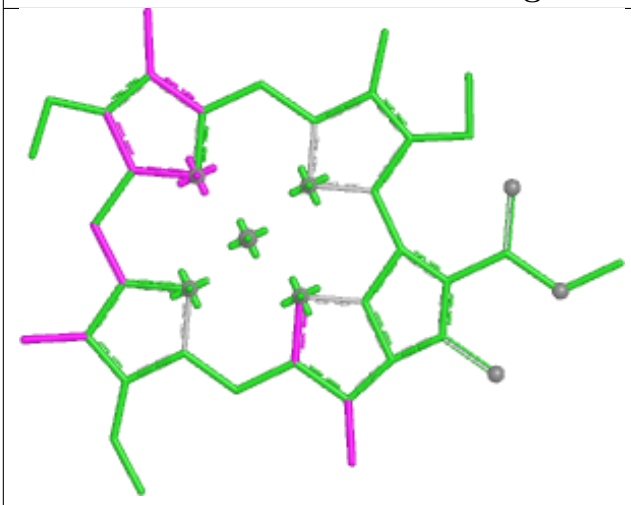


Torsions

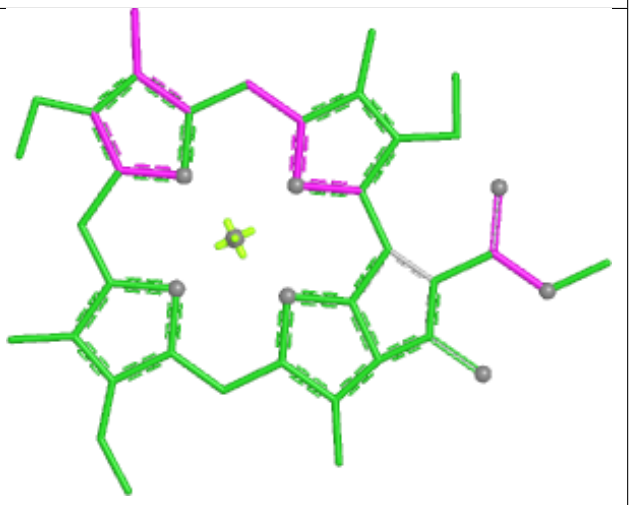


Rings

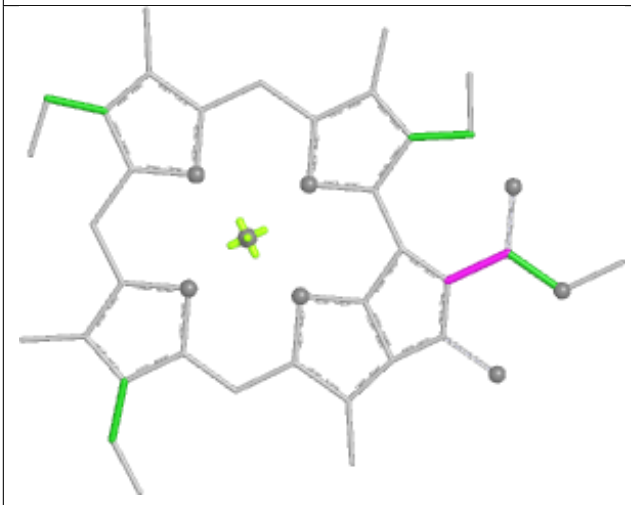
## Ligand CLA O 201



Bond lengths



Bond angles

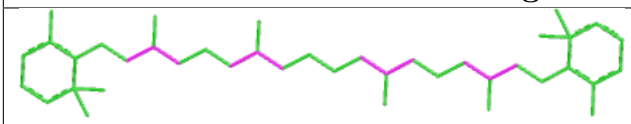


Torsions

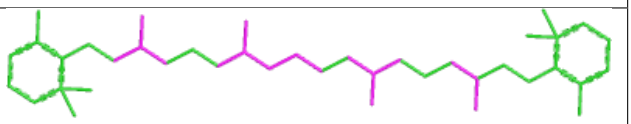


Rings

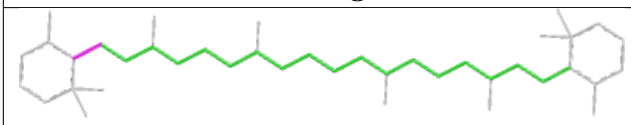
**Ligand BCR A 848**



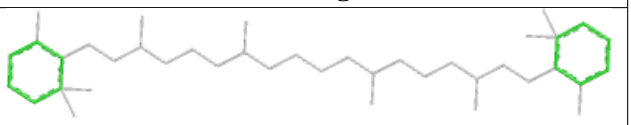
Bond lengths



Bond angles

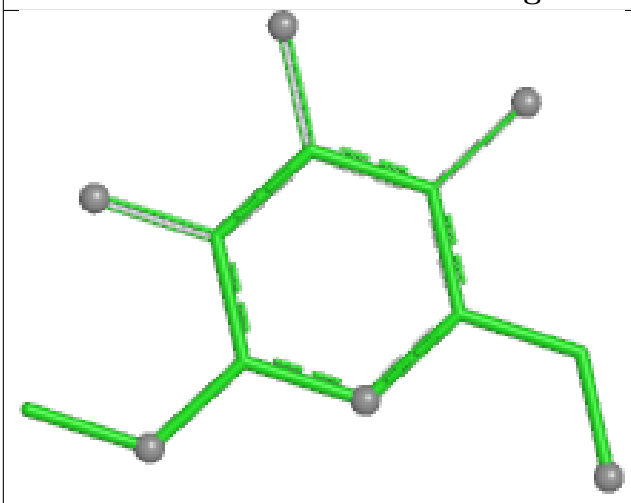


Torsions

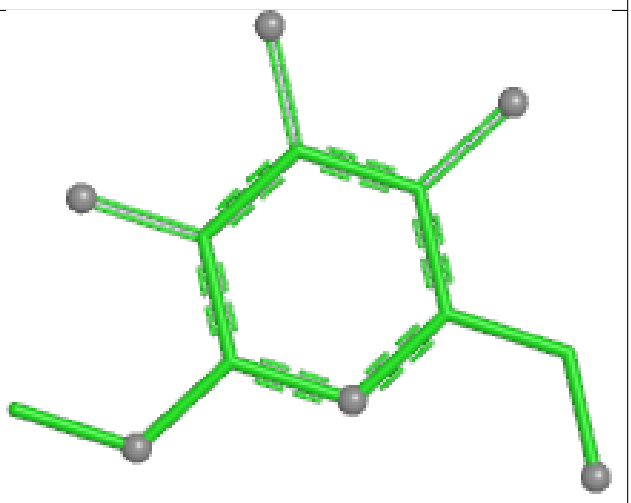


Rings

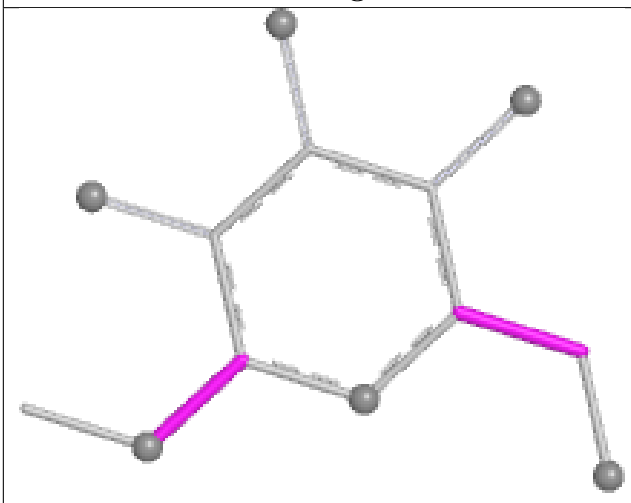
**Ligand LMG 6 615**



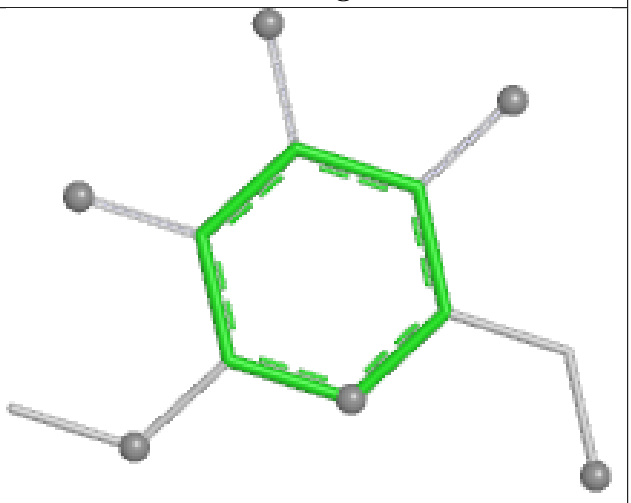
Bond lengths



Bond angles

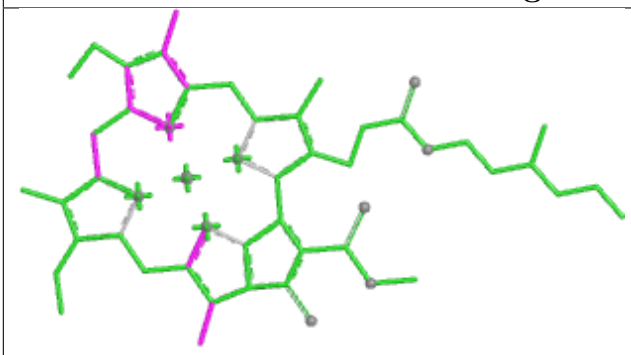


Torsions

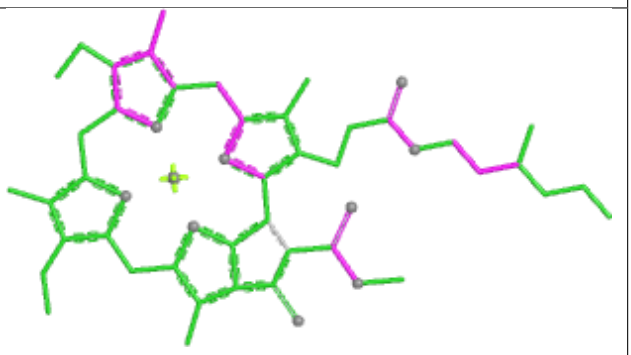


Rings

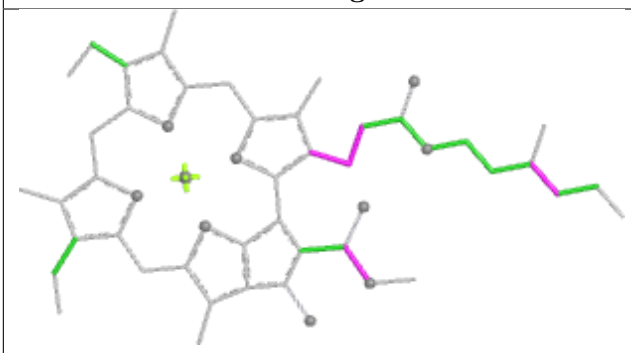
## Ligand CLA A 803



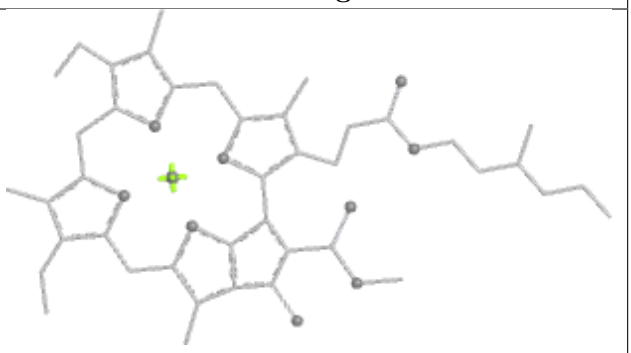
Bond lengths



Bond angles

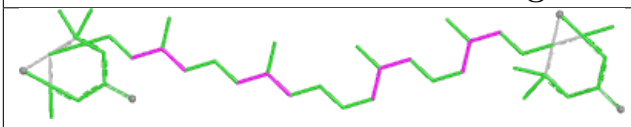


Torsions

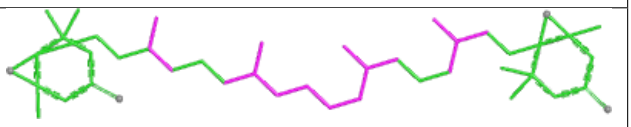


Rings

## Ligand XAT 5 616



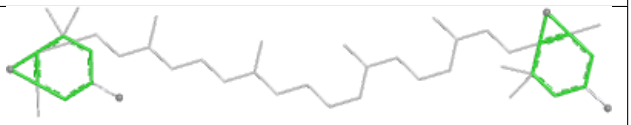
Bond lengths



Bond angles

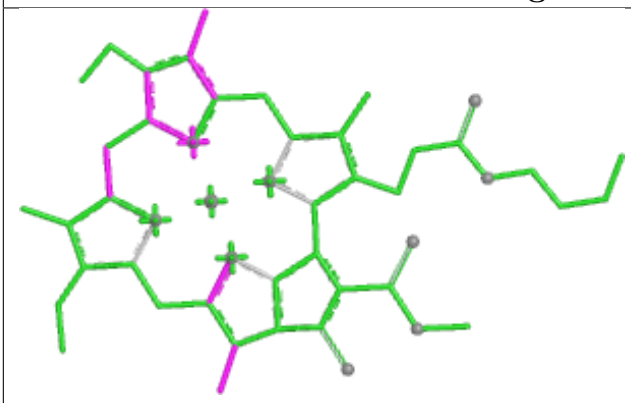


Torsions

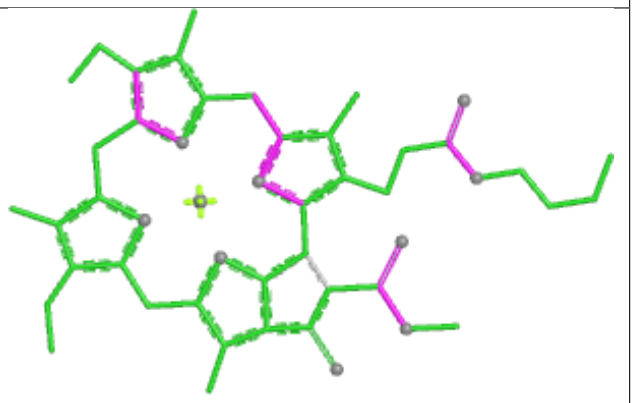


Rings

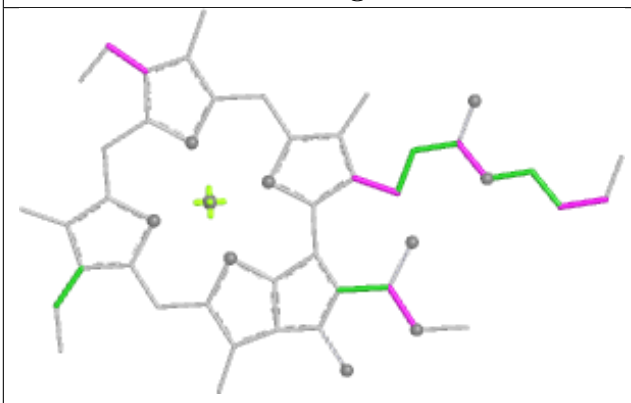
**Ligand CLA 1 305**



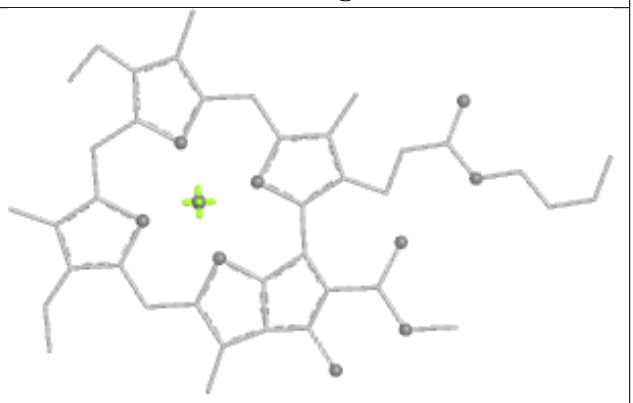
Bond lengths



Bond angles

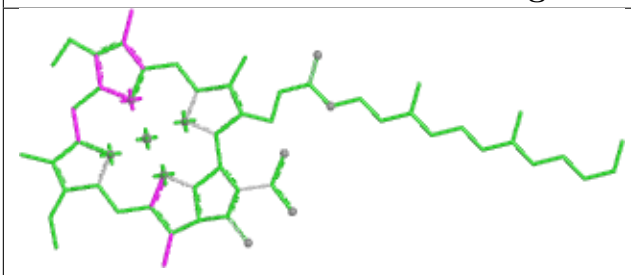


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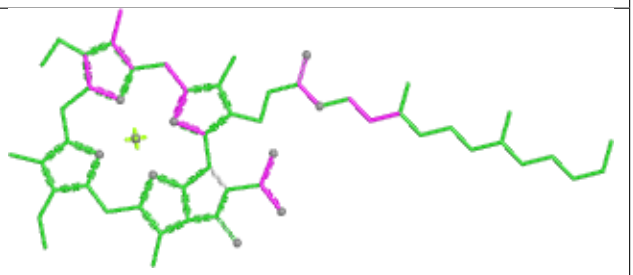


Rings

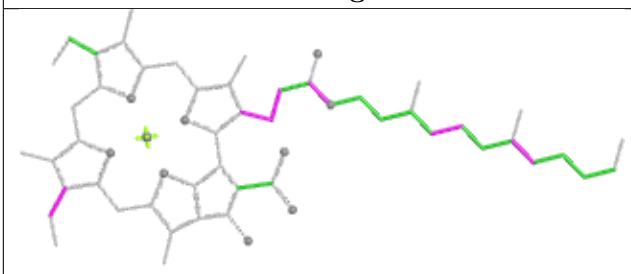
**Ligand CLA 4 602**



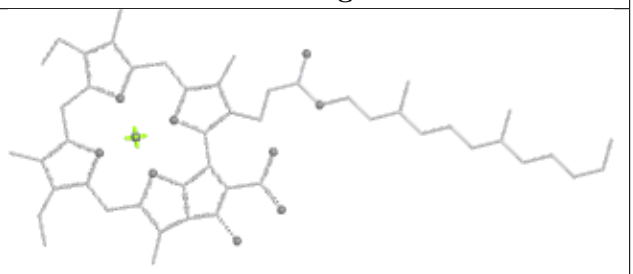
Bond lengths



Bond angles

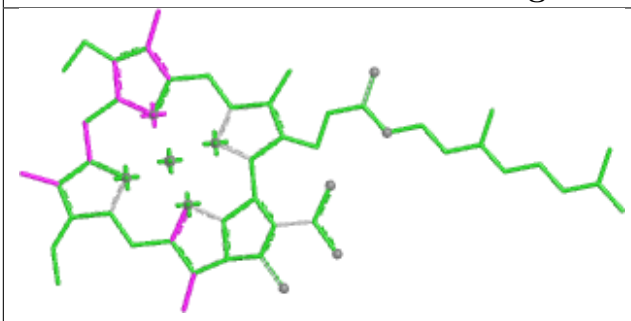


Torsions

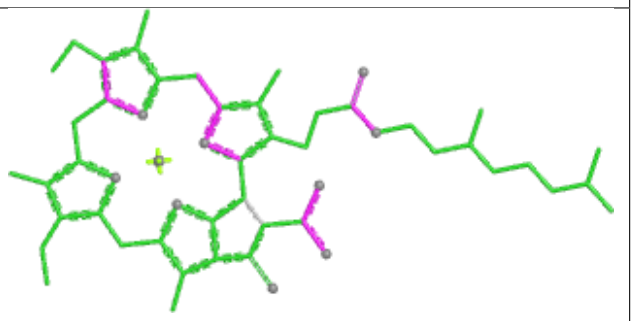


Rings

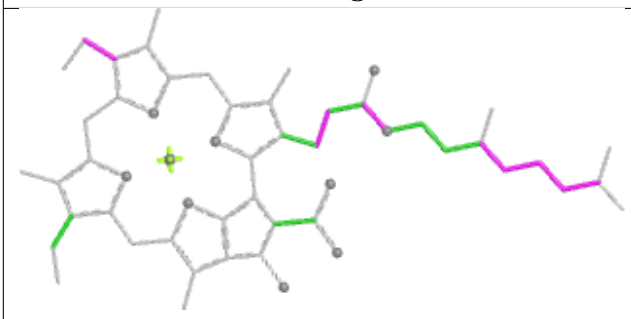
## Ligand CLA 3 412



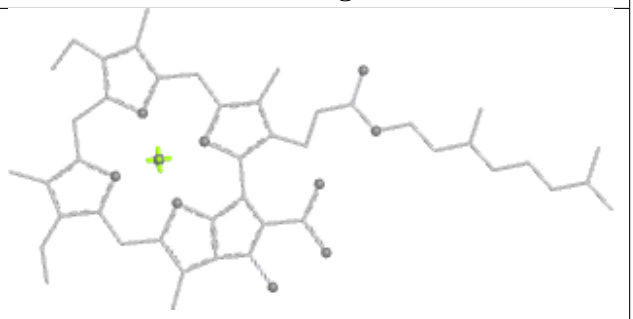
Bond lengths



Bond angles

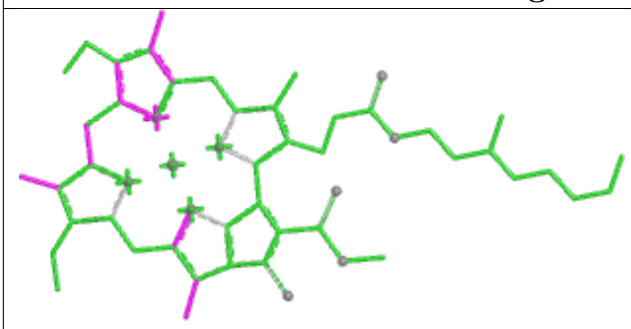


Torsions

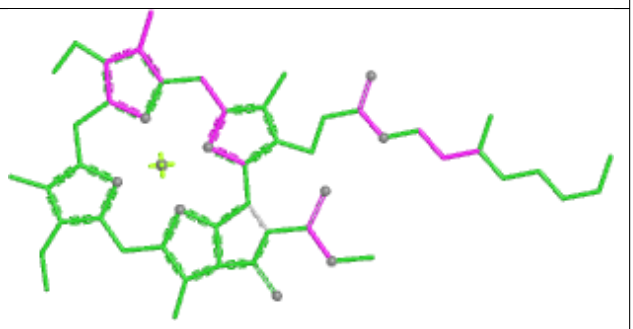


Rings

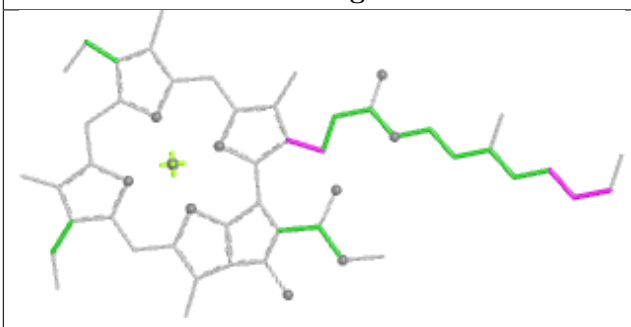
## Ligand CLA 9 610



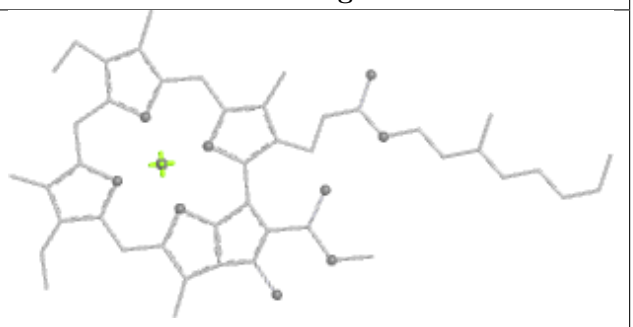
Bond lengths



Bond angles

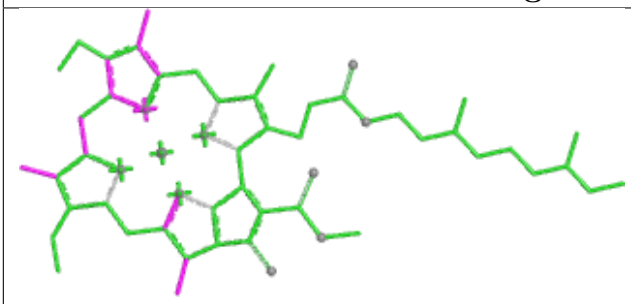


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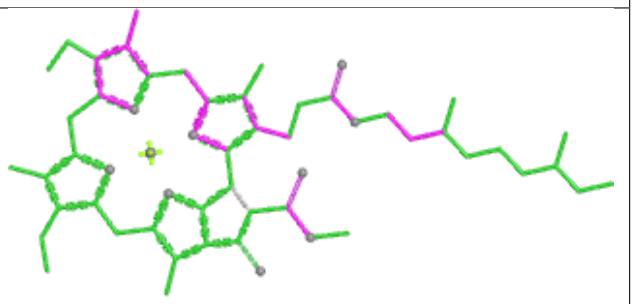


Rings

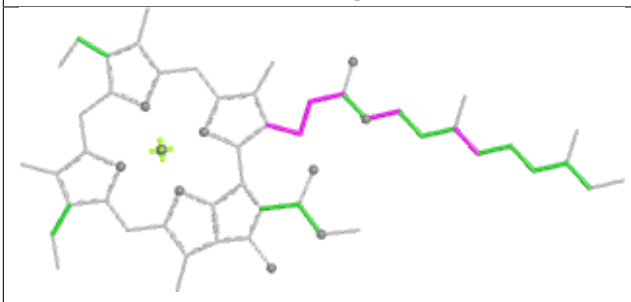
## Ligand CLA B 832



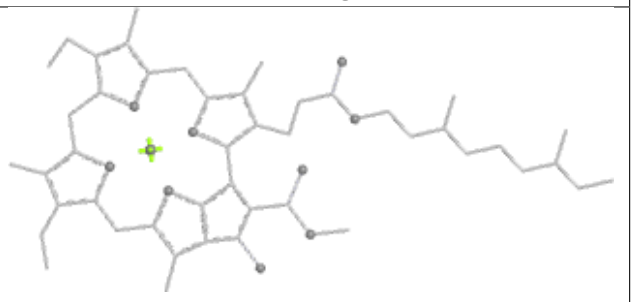
Bond lengths



Bond angles

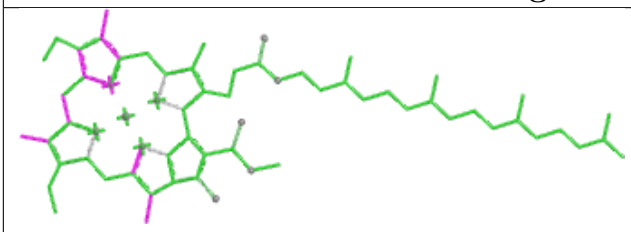


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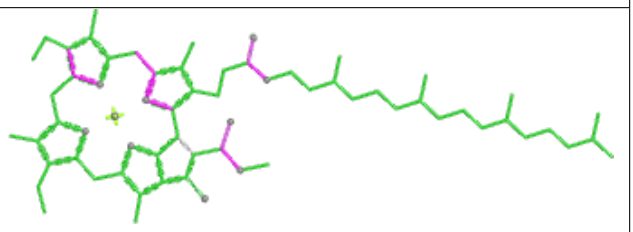


Rings

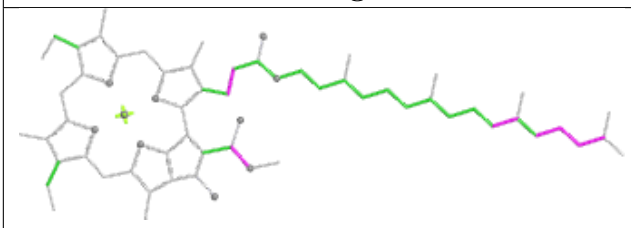
## Ligand CLA c 613



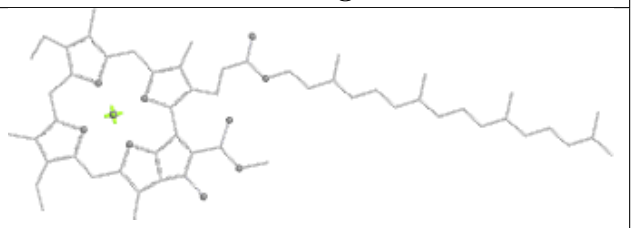
Bond lengths



Bond angles

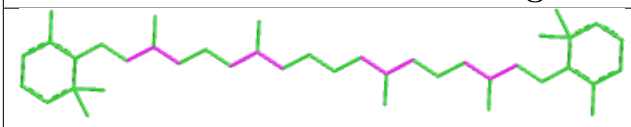


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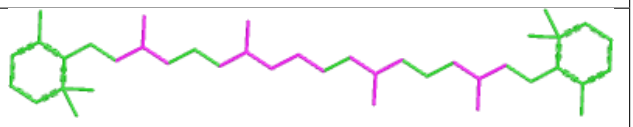


Rings

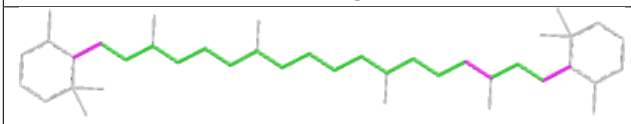
## Ligand BCR 8 616



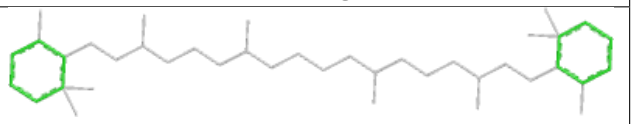
Bond lengths



Bond angles

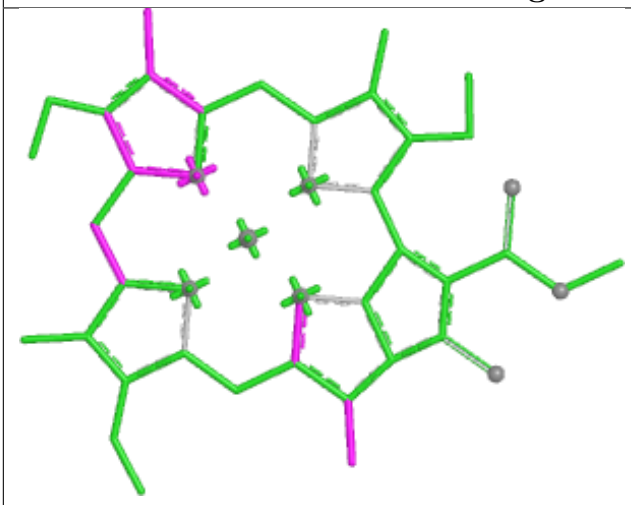


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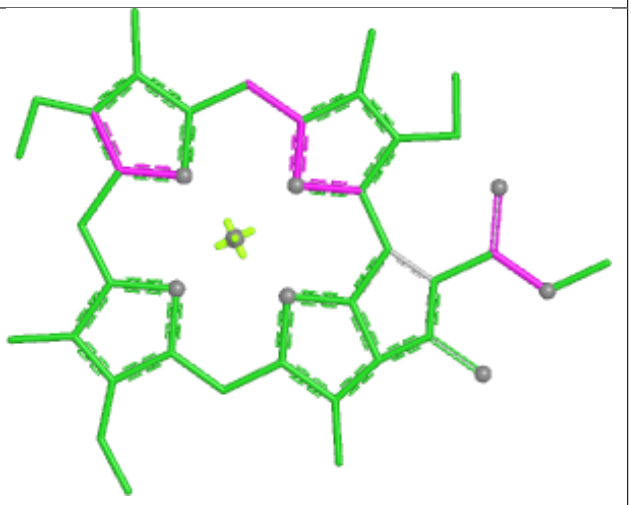


Rings

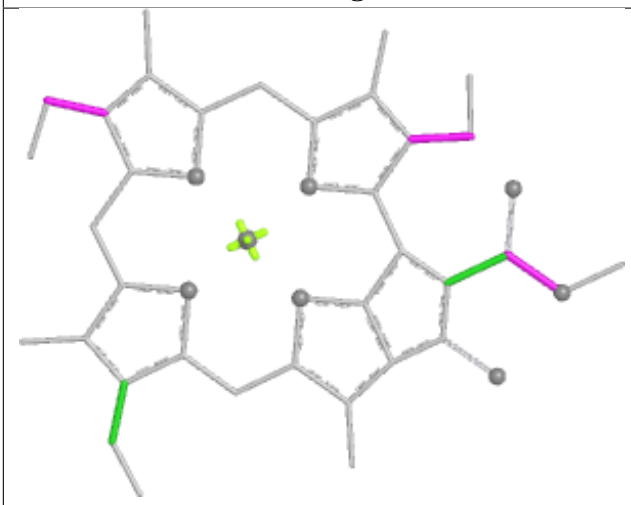
**Ligand CLA 6 613**



Bond lengths



Bond angles

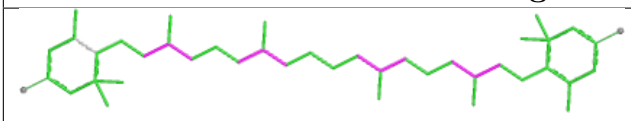


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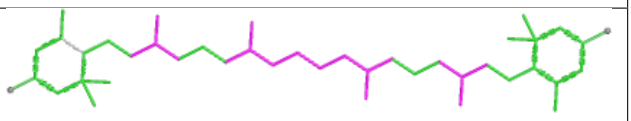


Rings

**Ligand LUT c 615**



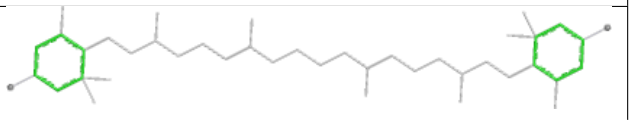
Bond lengths



Bond angles

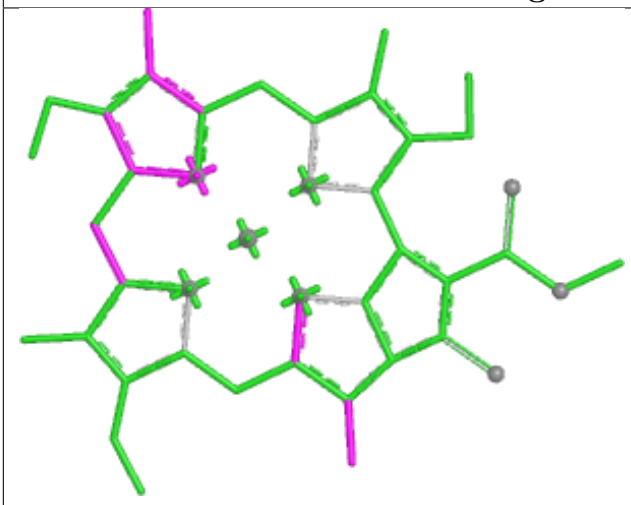


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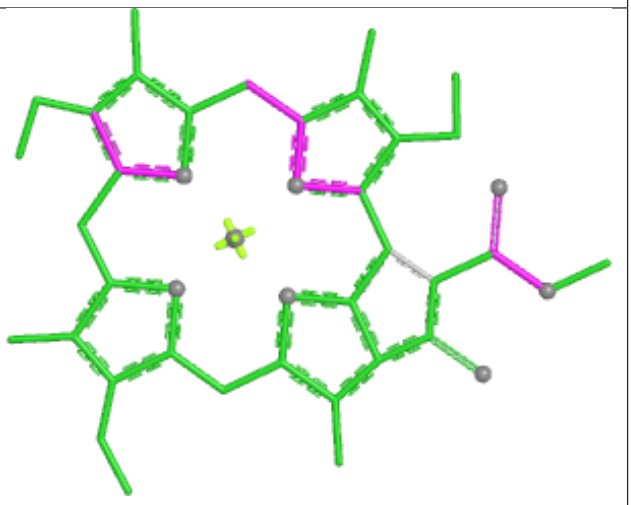


Rings

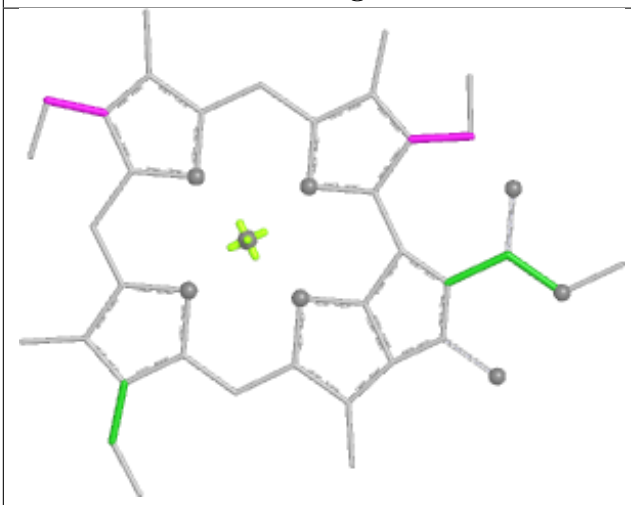
## Ligand CLA 2 613



Bond lengths



Bond angles

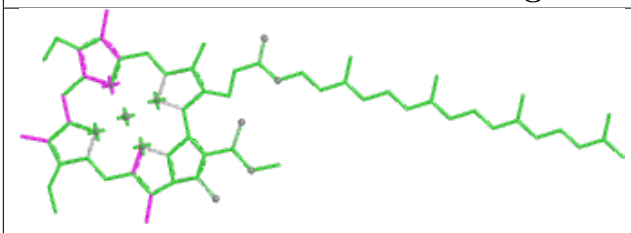


Torsions

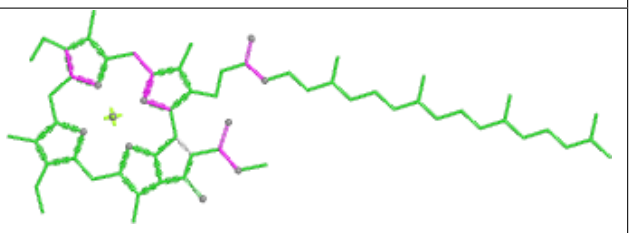


Rings

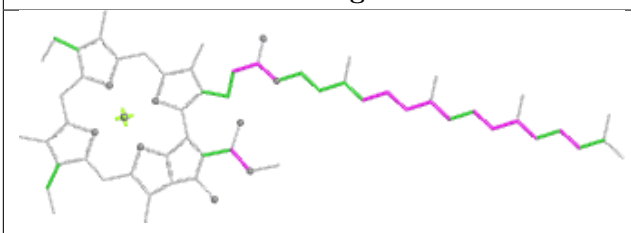
## Ligand CLA B 805



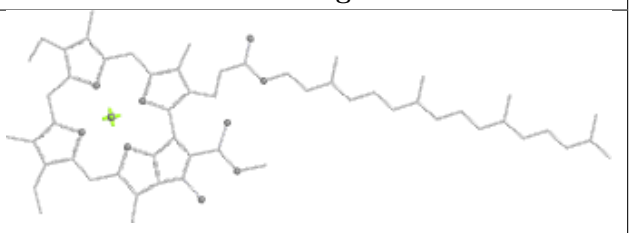
Bond lengths



Bond angles

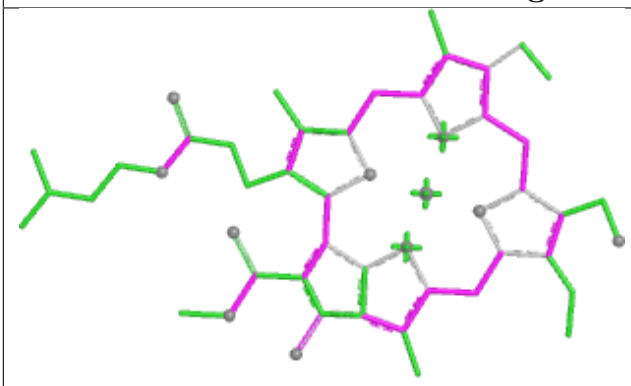


Torsions

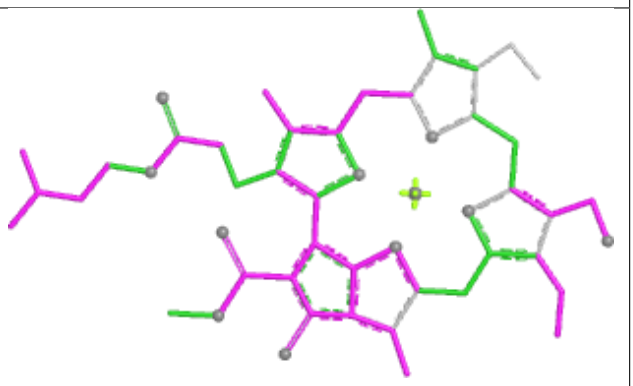


Rings

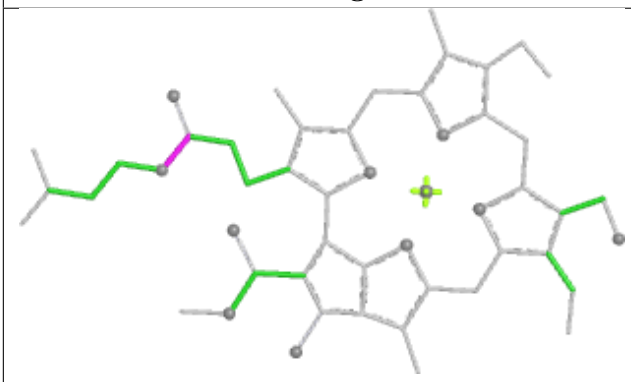
**Ligand CHL 1 307**



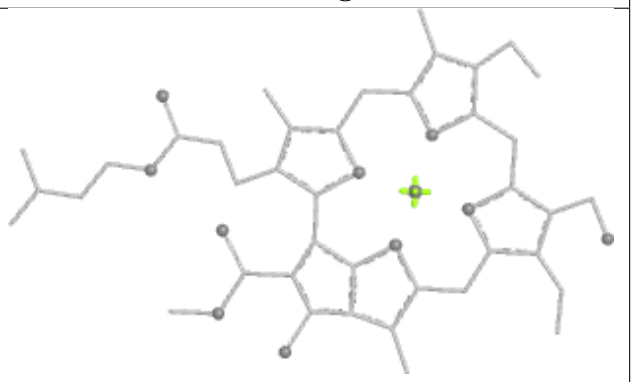
**Bond lengths**



**Bond angles**

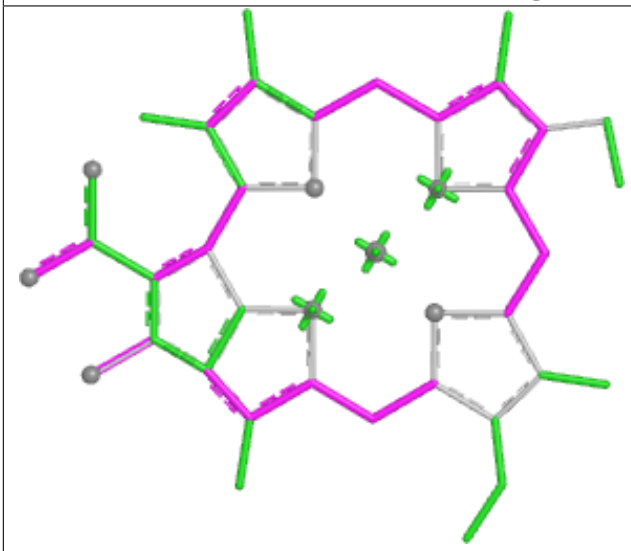


**Torsions**

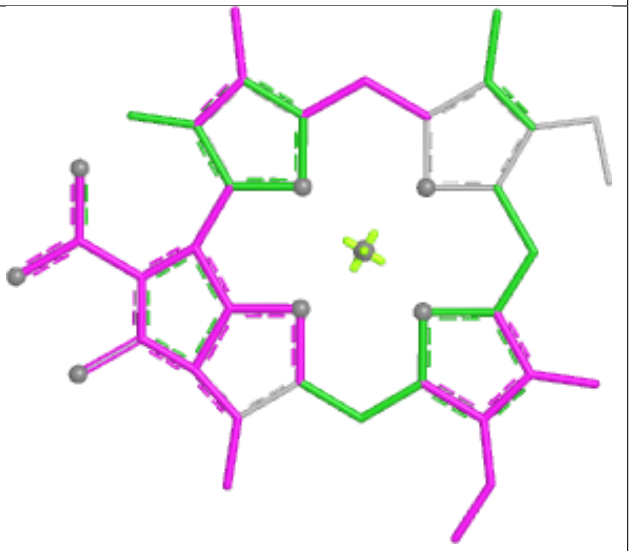


**Rings**

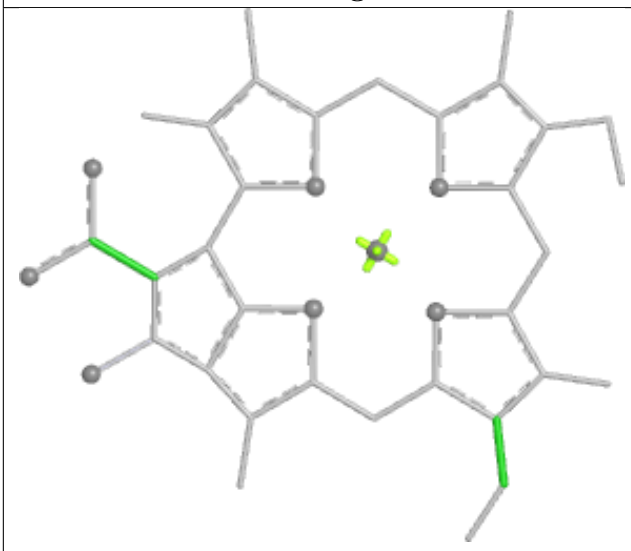
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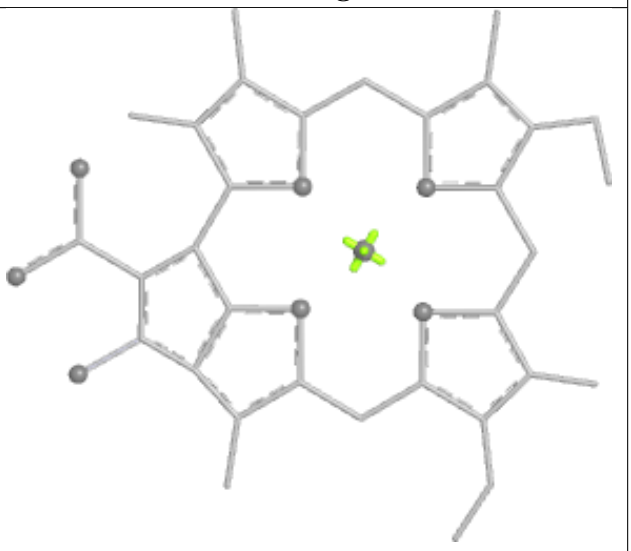
**Bond lengths**



**Bond angles**

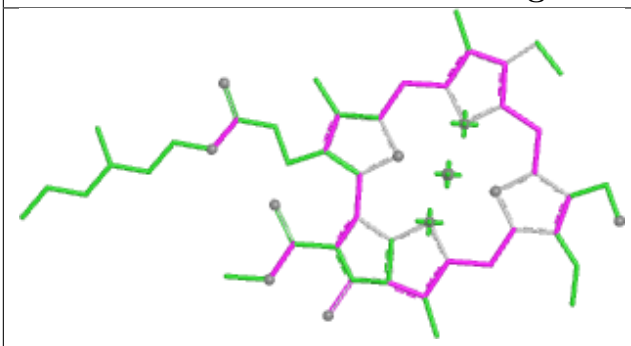


**Torsions**

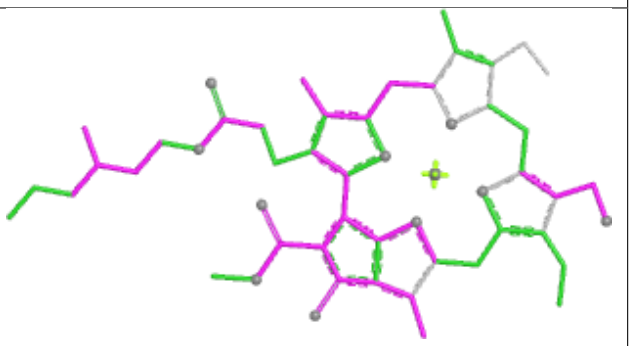


**Rings**

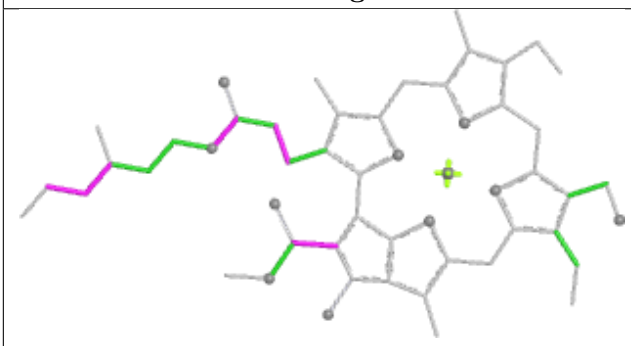
## Ligand CHL 2 601



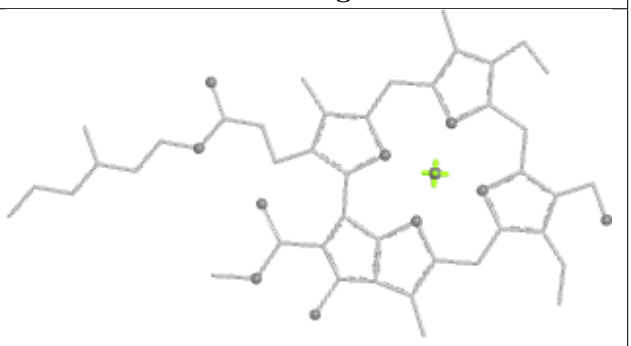
Bond lengths



Bond angles

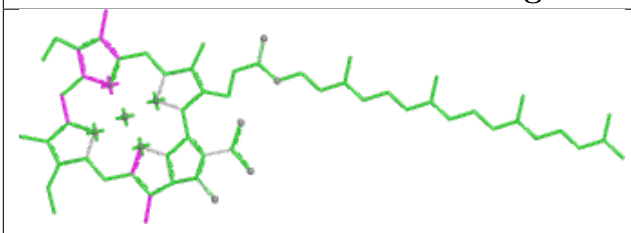


Torsions

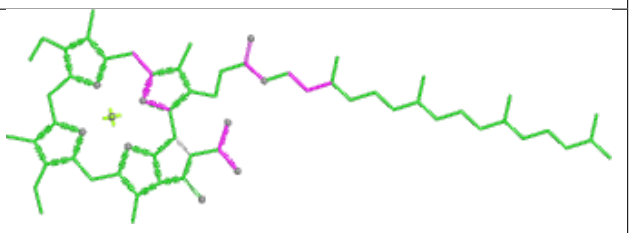


Rings

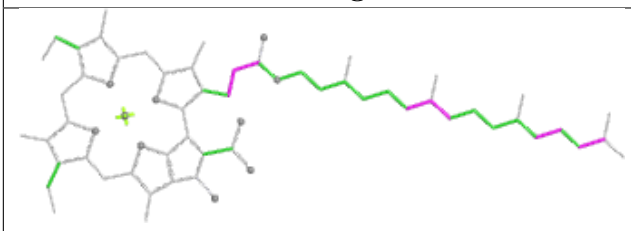
## Ligand CLA B 837



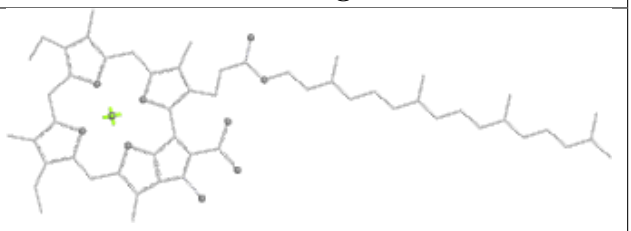
Bond lengths



Bond angles

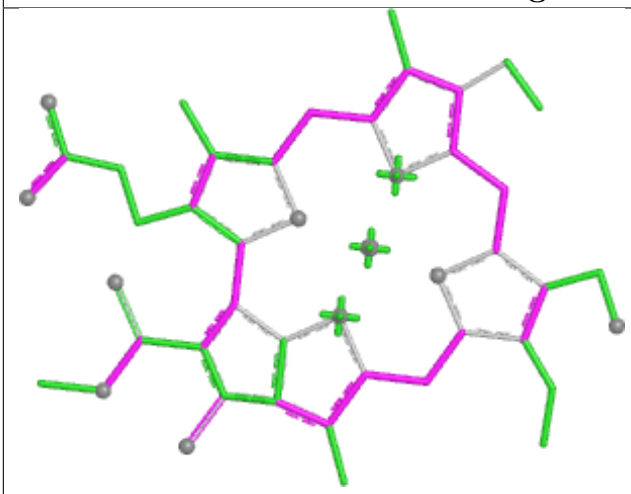


Torsions

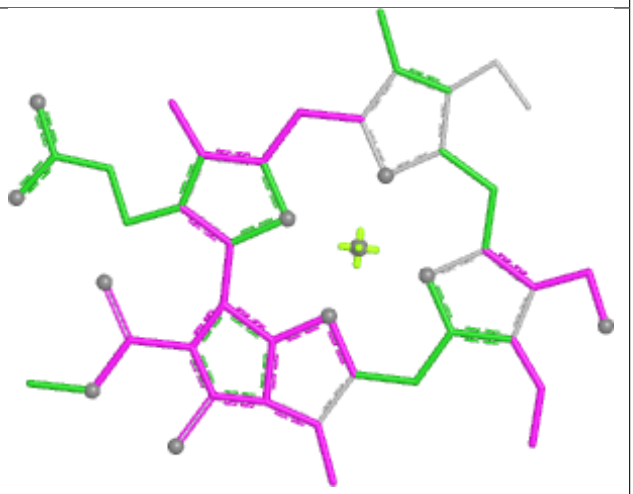


Rings

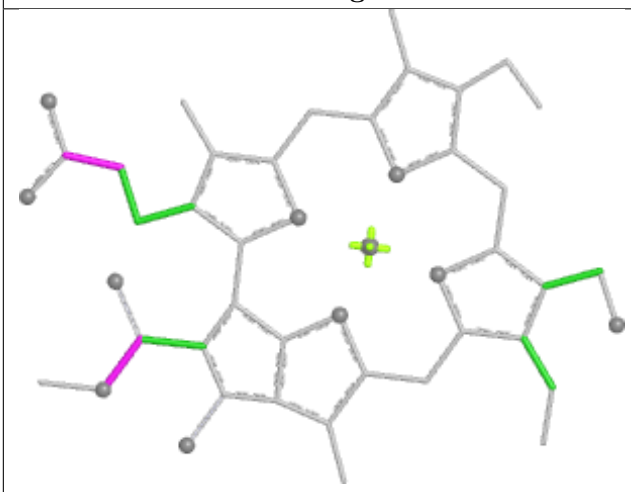
**Ligand CHL c 606**



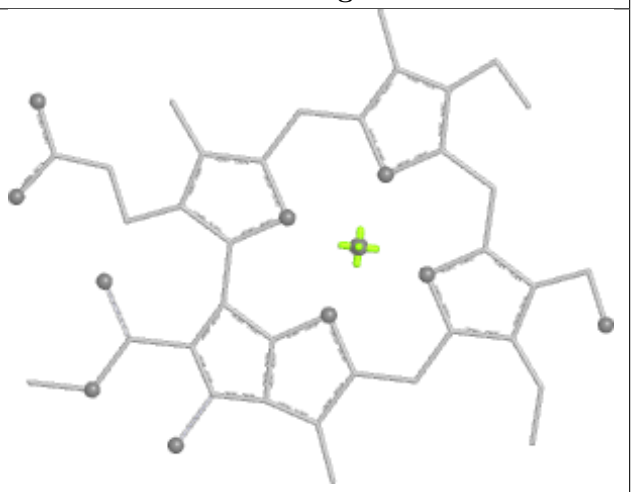
**Bond lengths**



**Bond angles**

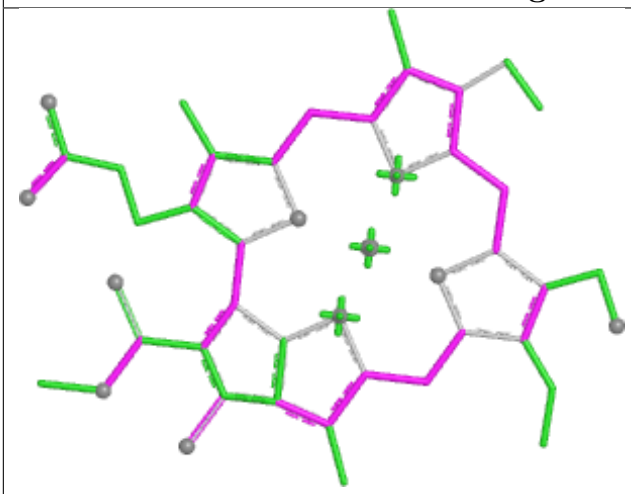


**Torsions**

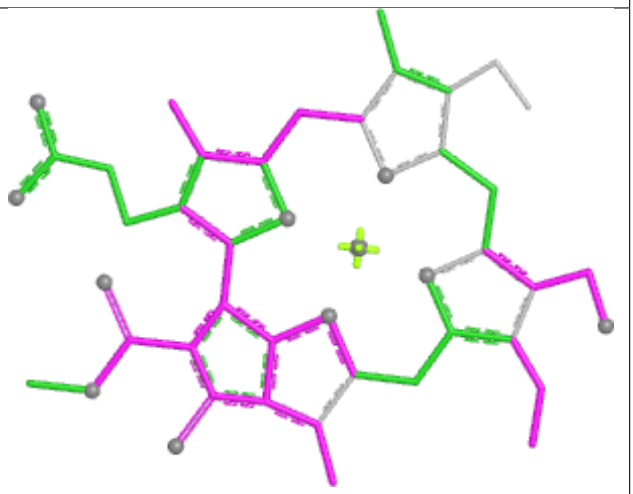


**Rings**

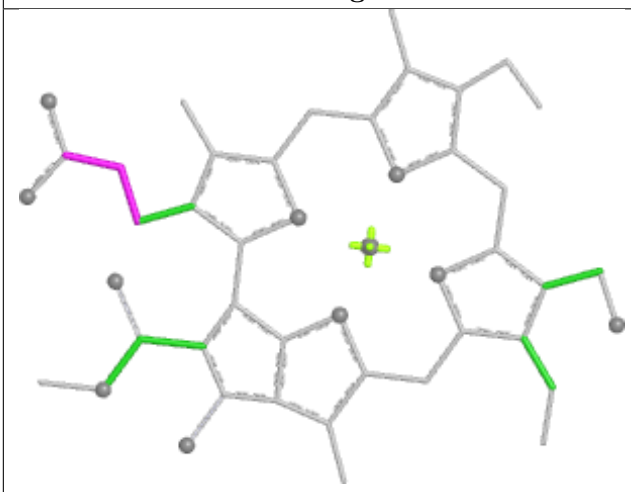
**Ligand CHL c 607**



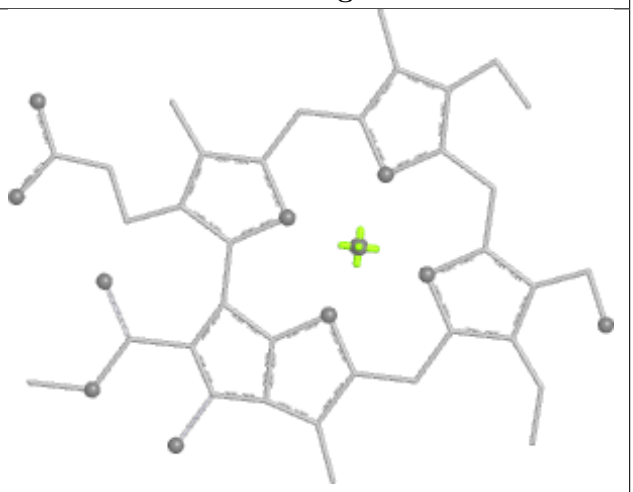
**Bond lengths**



**Bond angles**

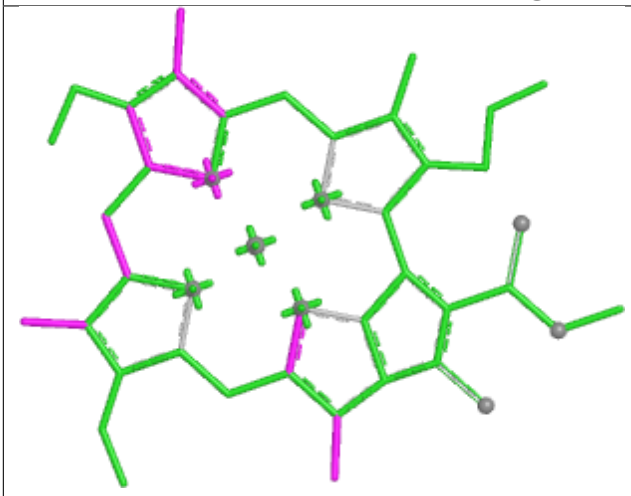


**Torsions**

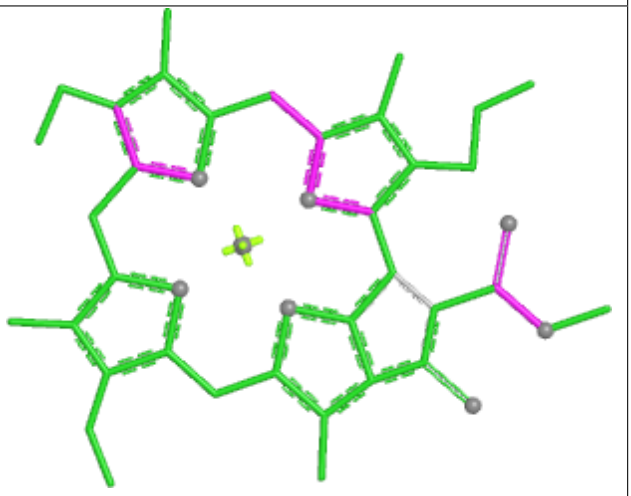


**Rings**

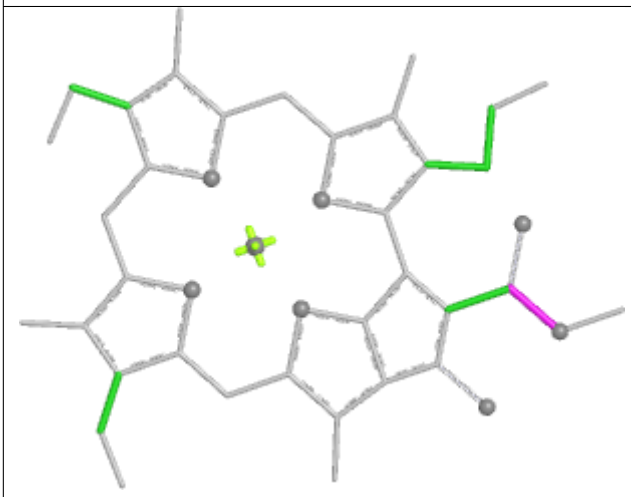
**Ligand CLA 3 411**



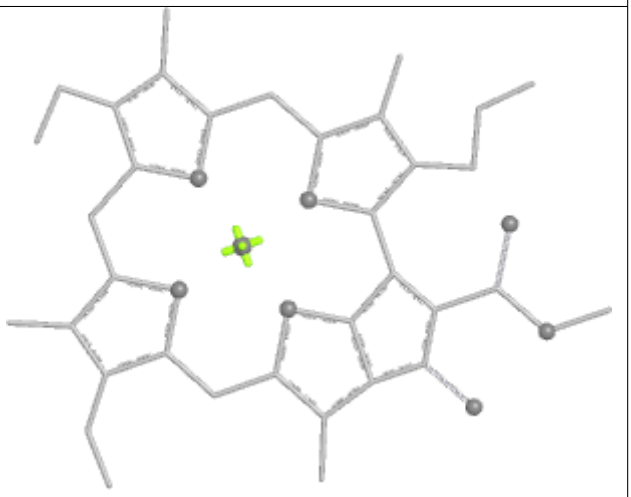
**Bond lengths**



**Bond angles**

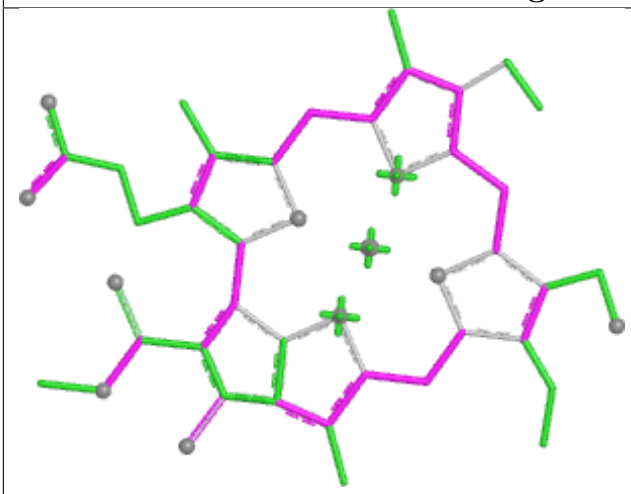


**Torsions**

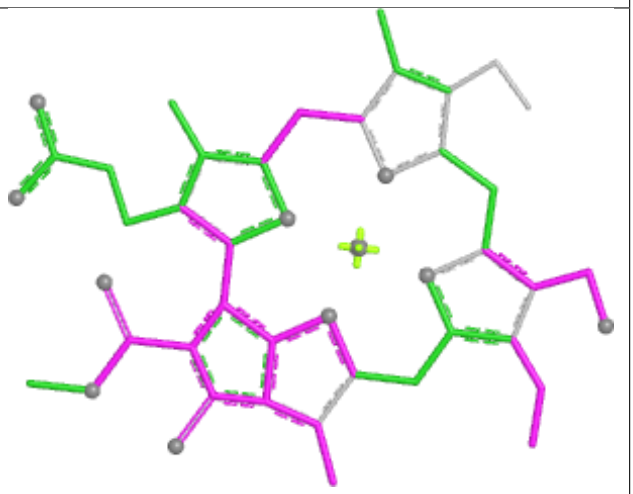


**Rings**

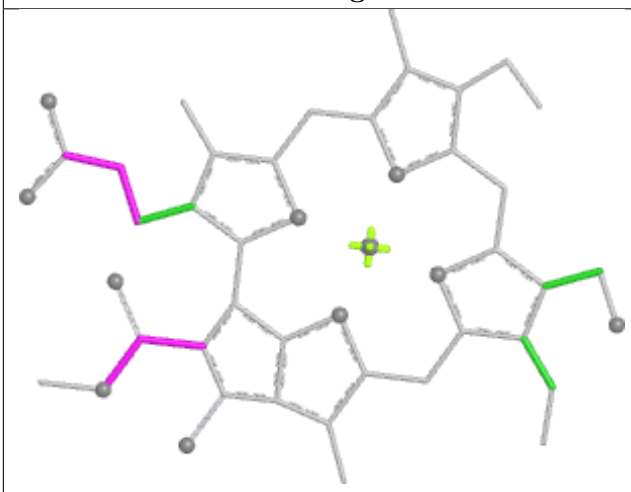
**Ligand CHL a 608**



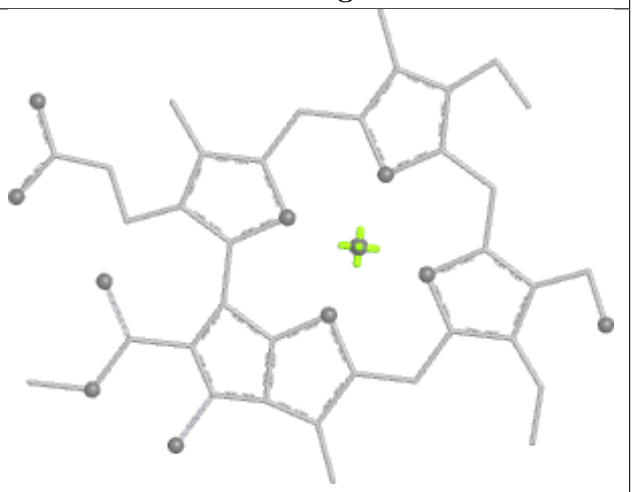
**Bond lengths**



**Bond angles**

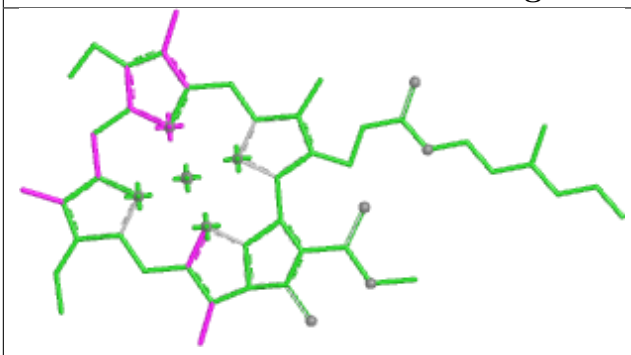


**Torsions**

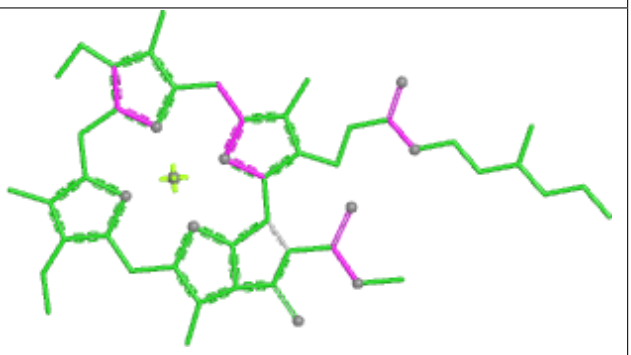


**Rings**

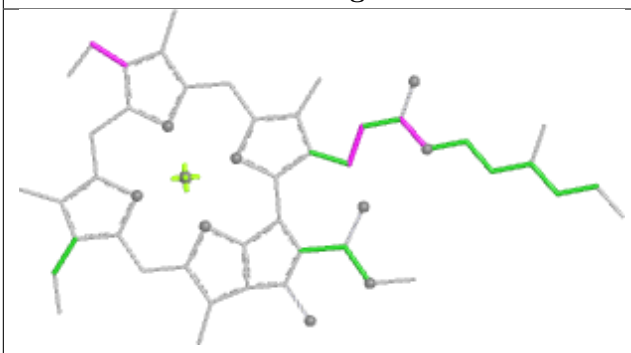
**Ligand CLA B 816**



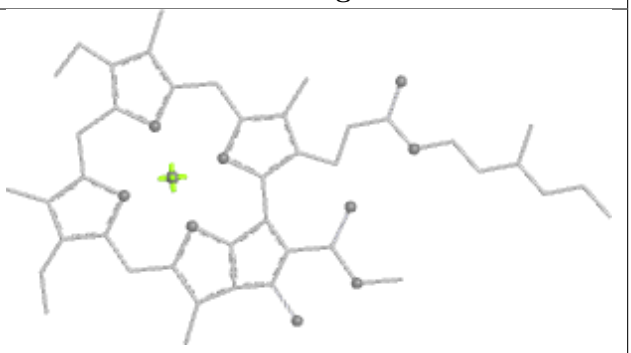
**Bond lengths**



**Bond angles**

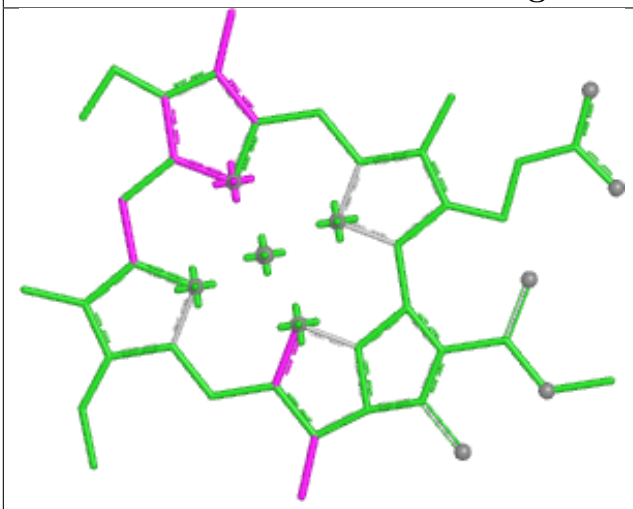


**Torsions**

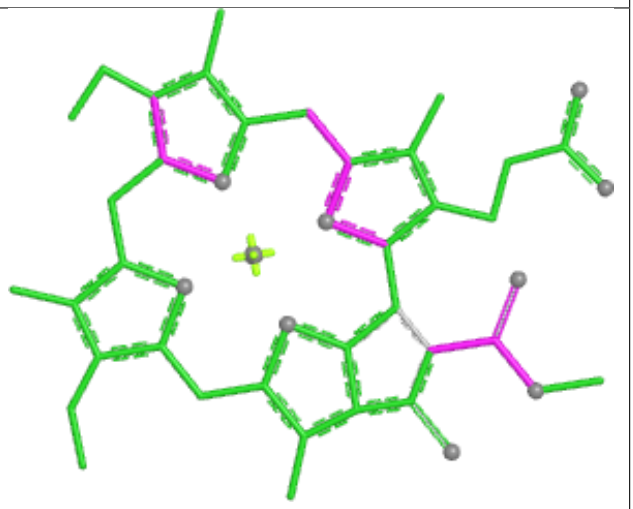


**Rings**

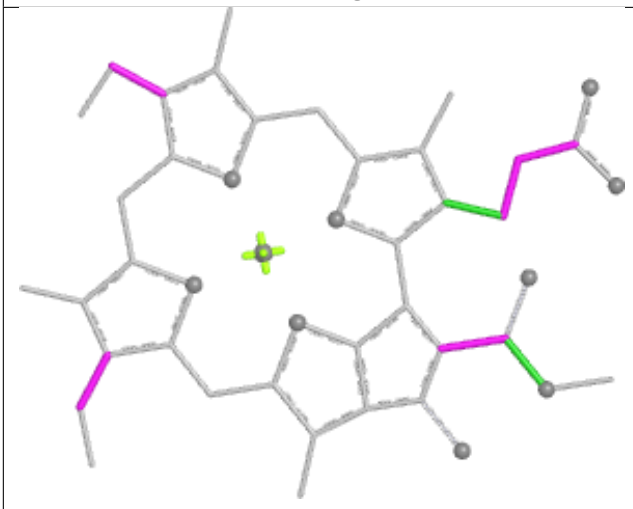
**Ligand CLA 7 401**



**Bond lengths**



**Bond angles**

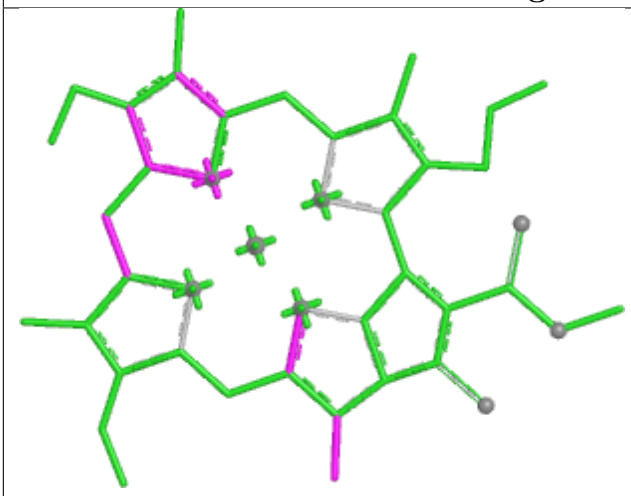


**Torsions**

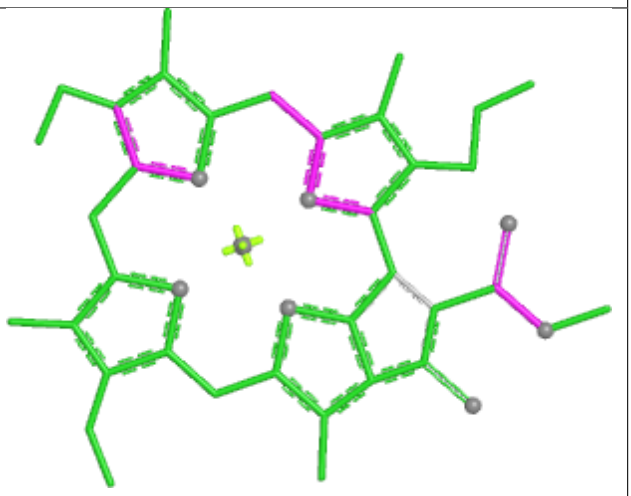


**Rings**

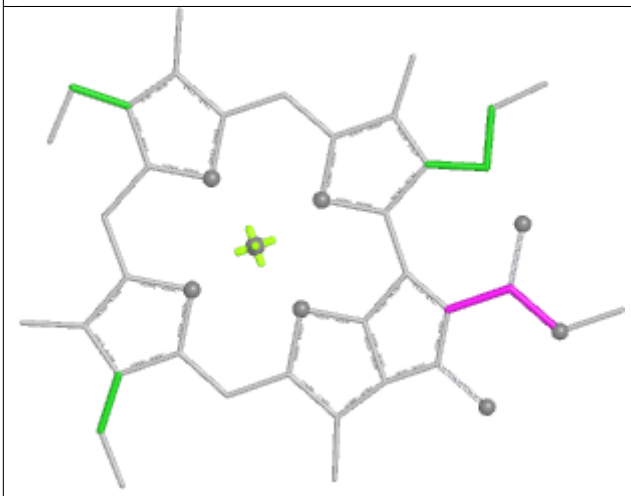
**Ligand CLA 8 612**



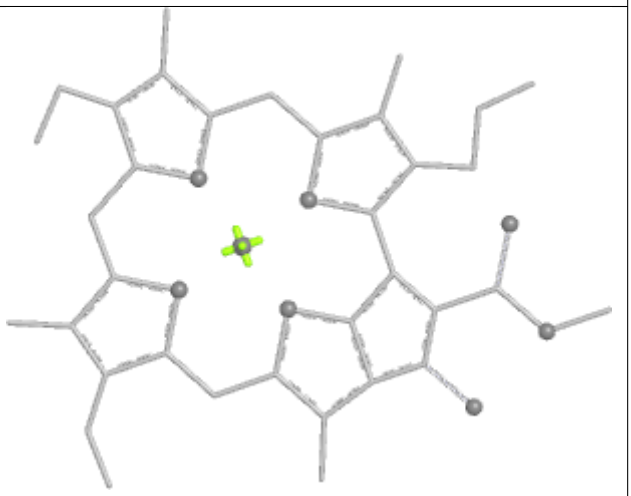
**Bond lengths**



**Bond angles**

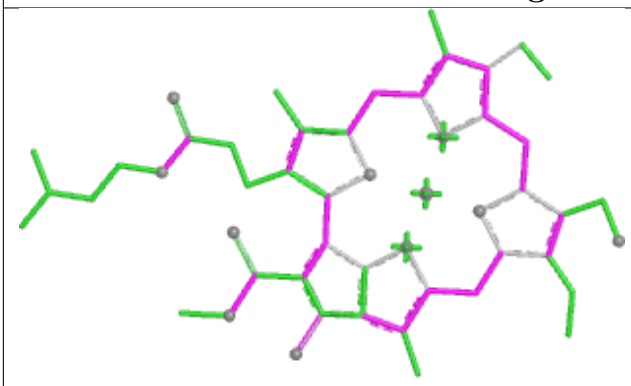


**Torsions**

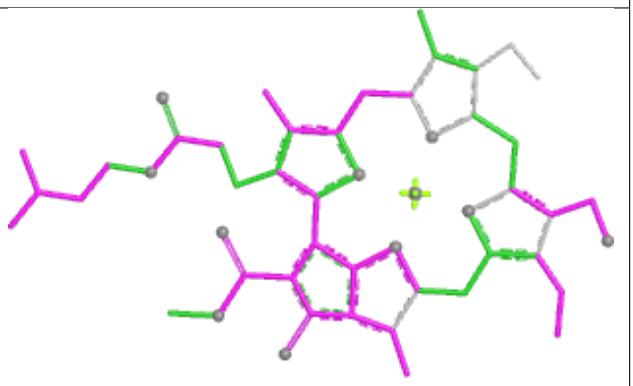


**Rings**

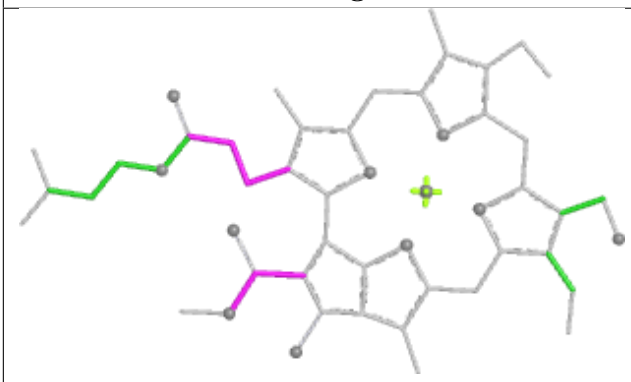
**Ligand CHL 8 607**



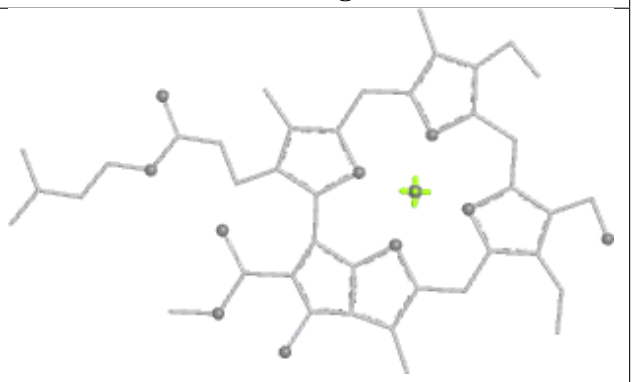
**Bond lengths**



**Bond angles**

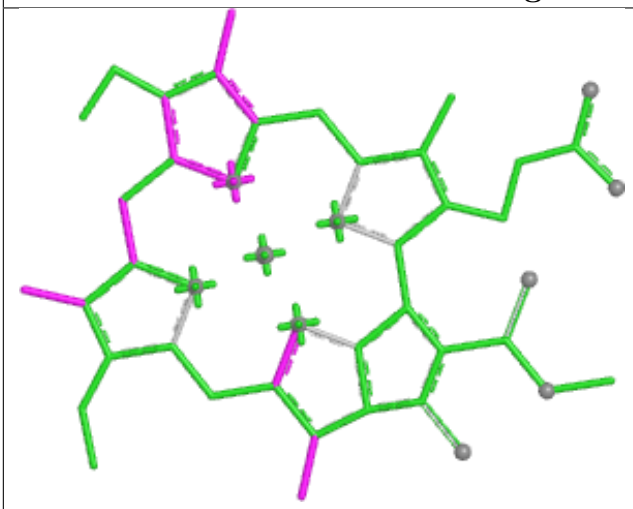


**Torsions**

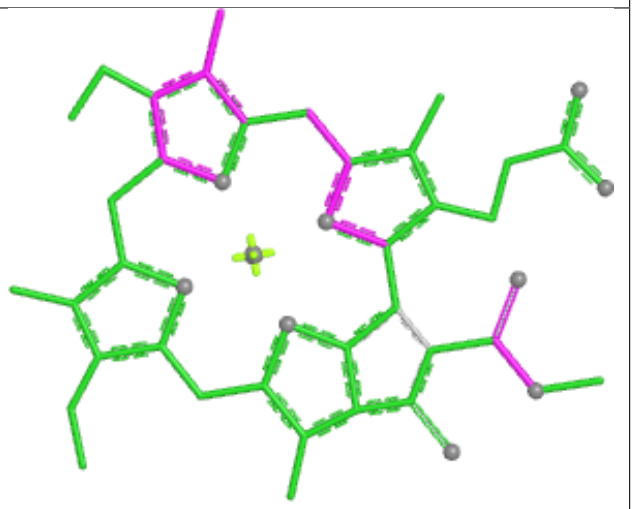


**Rings**

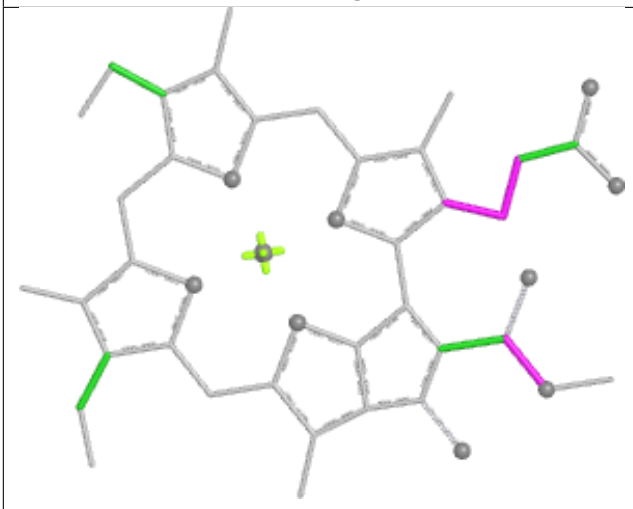
**Ligand CLA B 834**



**Bond lengths**



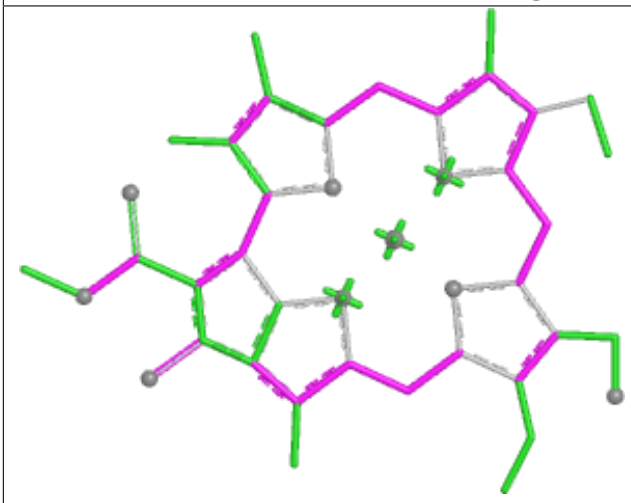
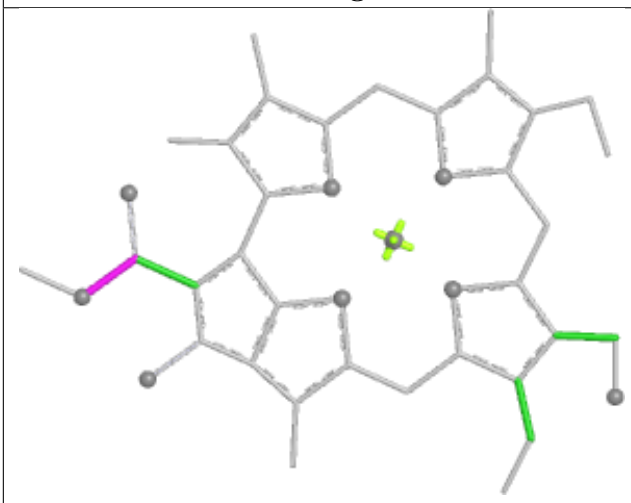
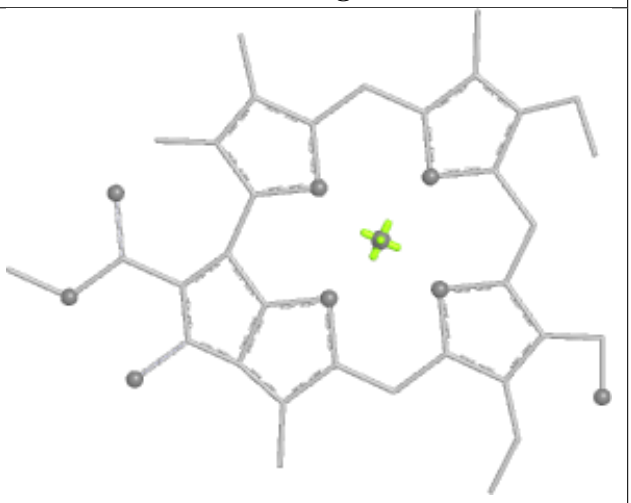
**Bond angles**

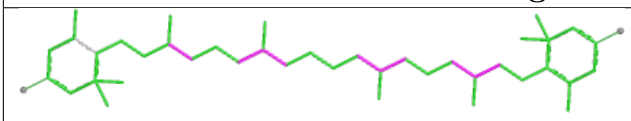
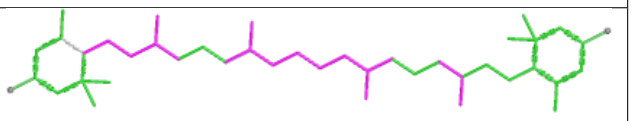
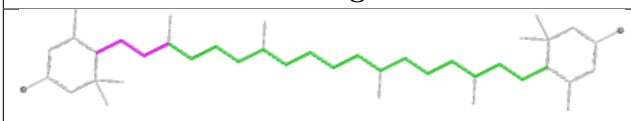
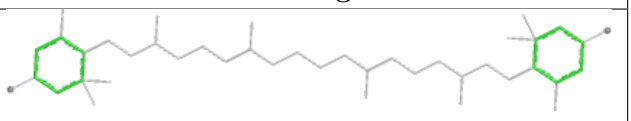


**Torsions**

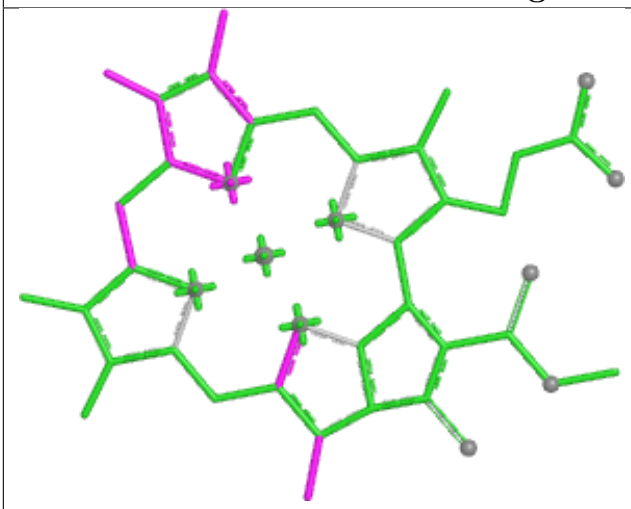


**Rings**

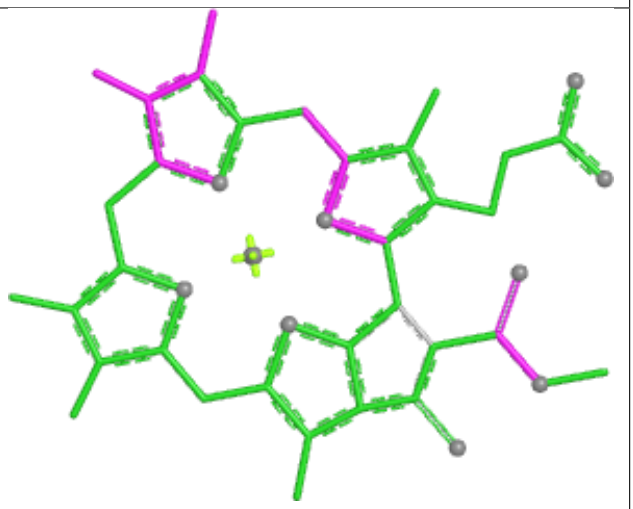
| Ligand CHL 8 613 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand LUT a 615 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

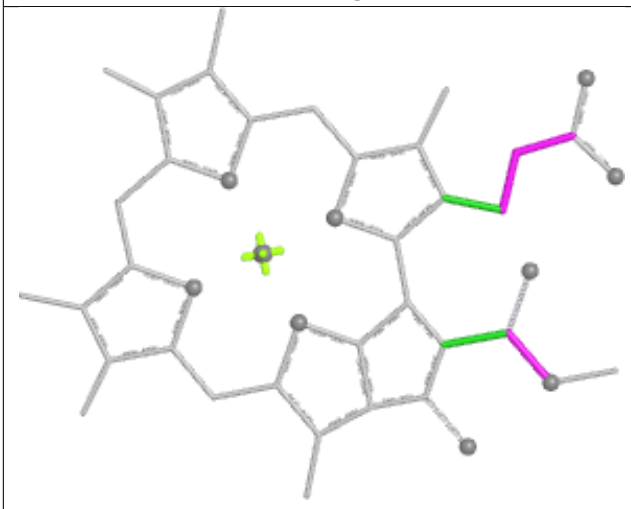
## Ligand CLA 5 614



Bond lengths



Bond angles



Torsions



Rings

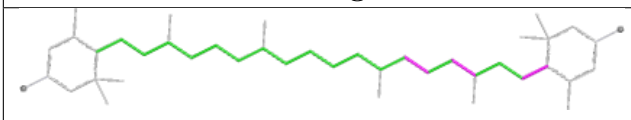
## Ligand LUT 3 416



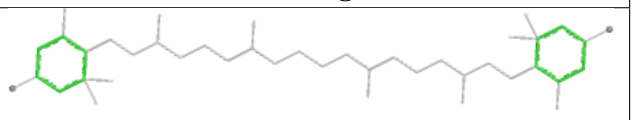
Bond lengths



Bond angles

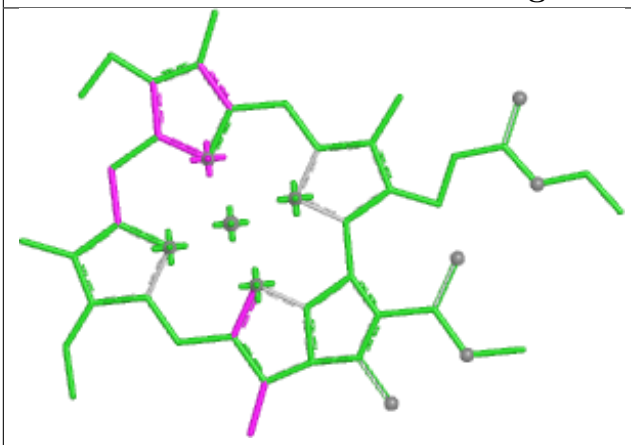


Torsions

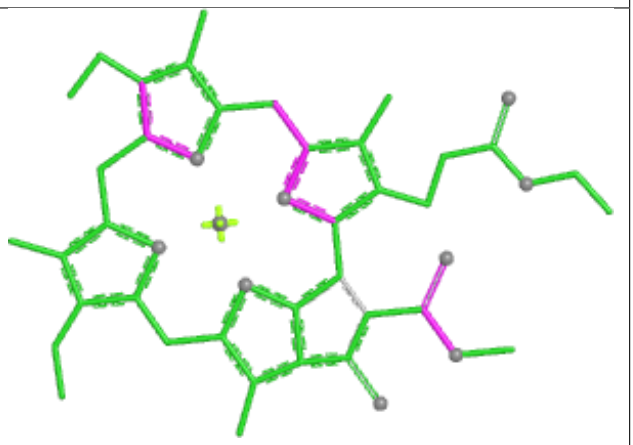


Rings

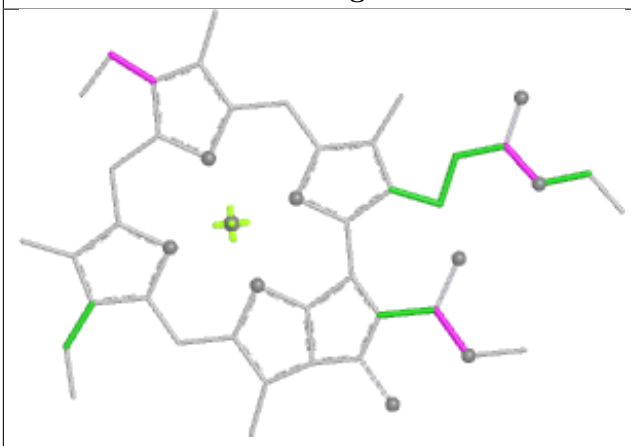
**Ligand CLA a 611**



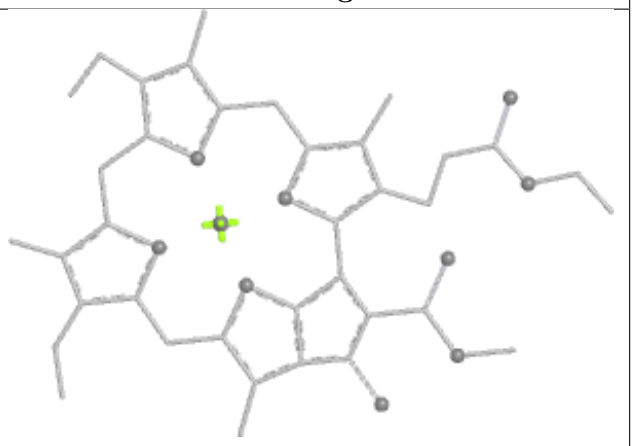
**Bond lengths**



**Bond angles**

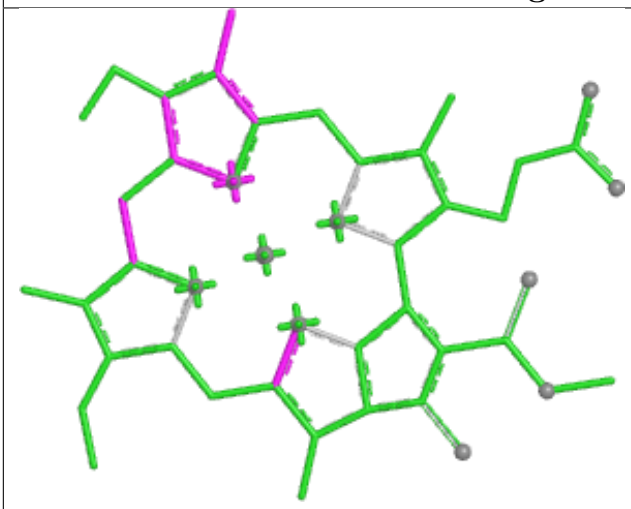


**Torsions**

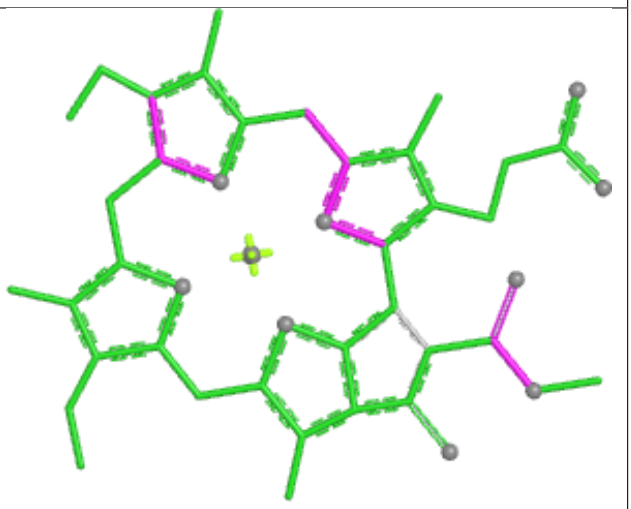


**Rings**

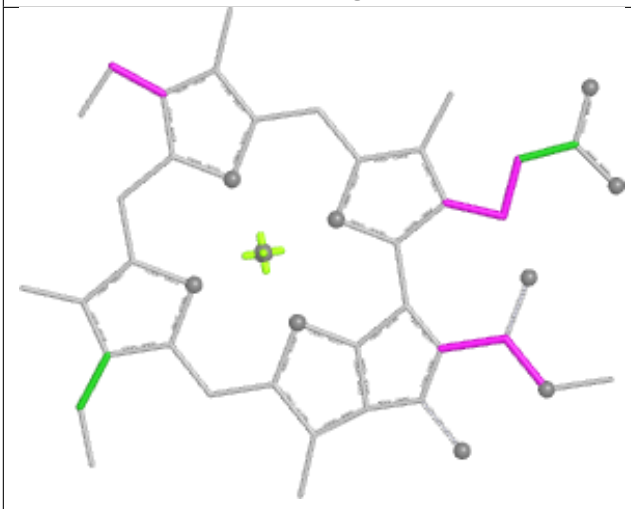
**Ligand CLA 8 601**



**Bond lengths**



**Bond angles**

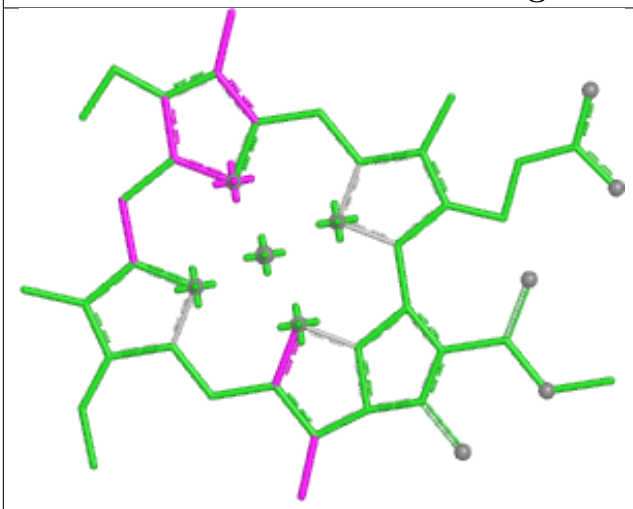


**Torsions**

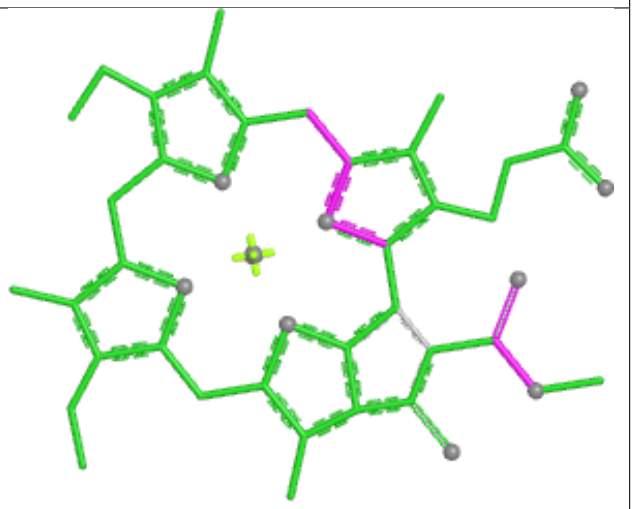


**Rings**

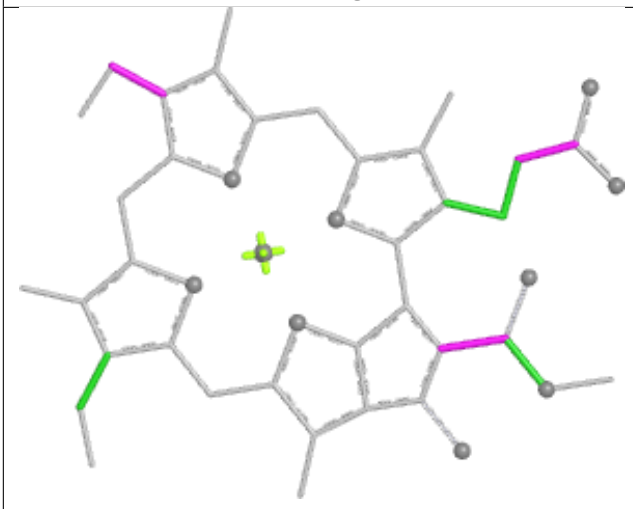
**Ligand CLA 5 603**



**Bond lengths**



**Bond angles**

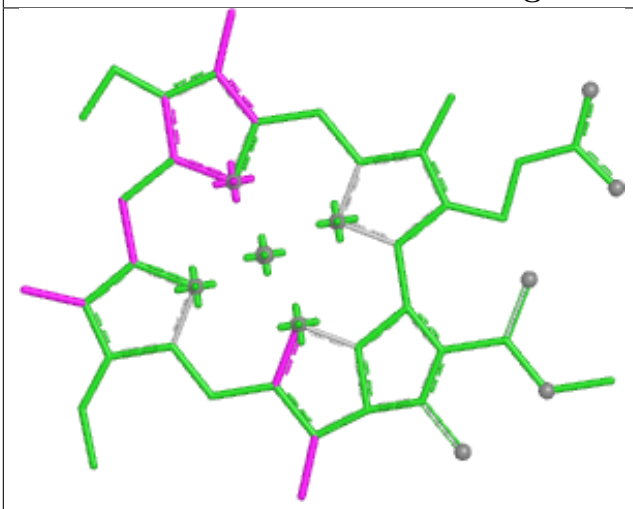


**Torsions**

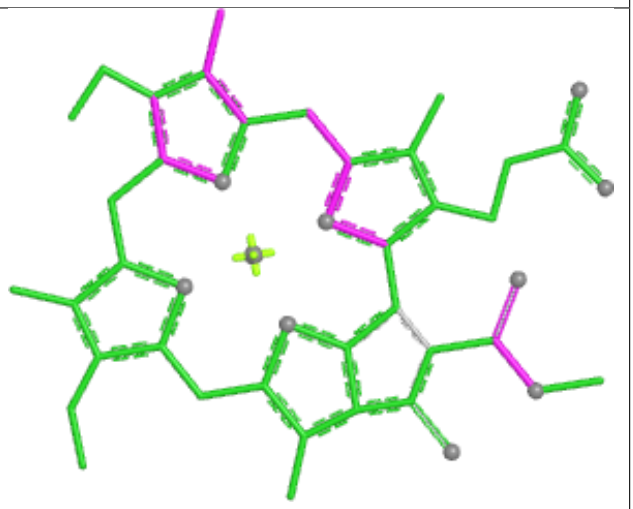


**Rings**

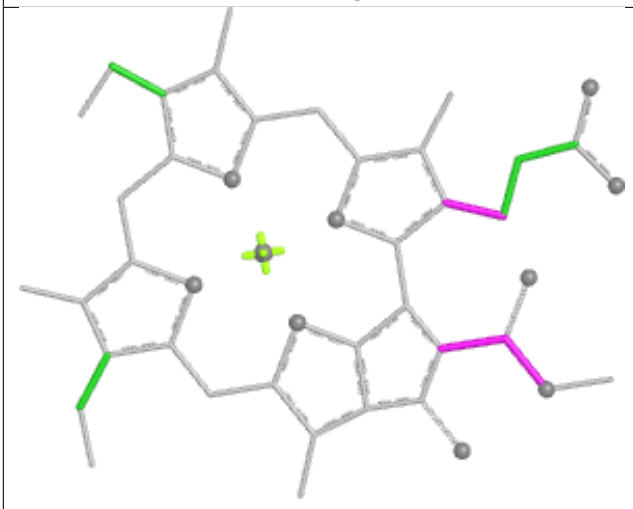
**Ligand CLA A 815**



**Bond lengths**



**Bond angles**

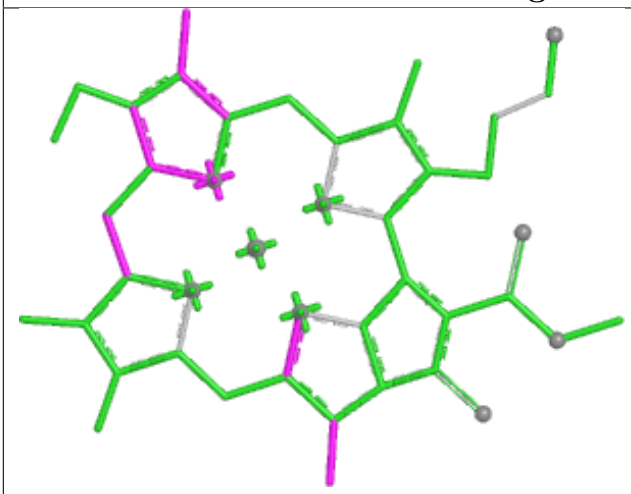


**Torsions**

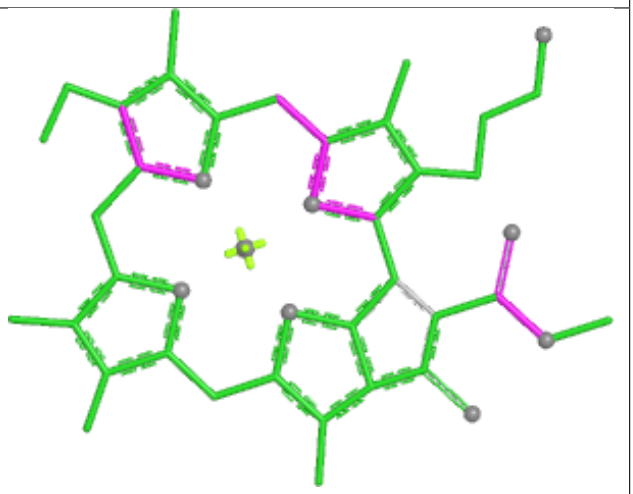


**Rings**

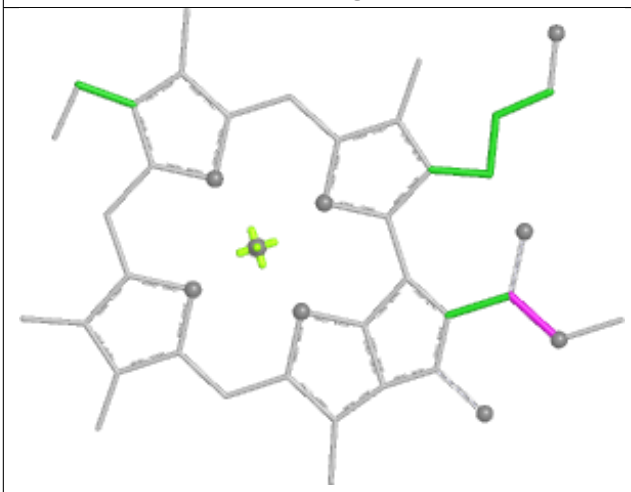
## Ligand CLA 4 604



Bond lengths



Bond angles

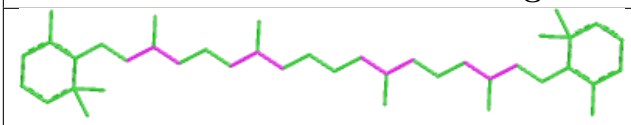


Torsions



Rings

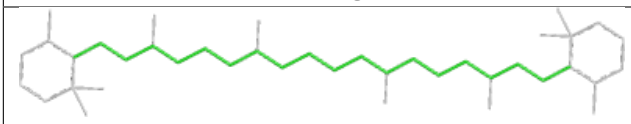
## Ligand BCR F 303



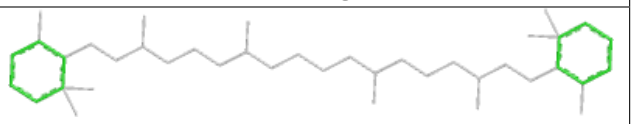
Bond lengths



Bond angles

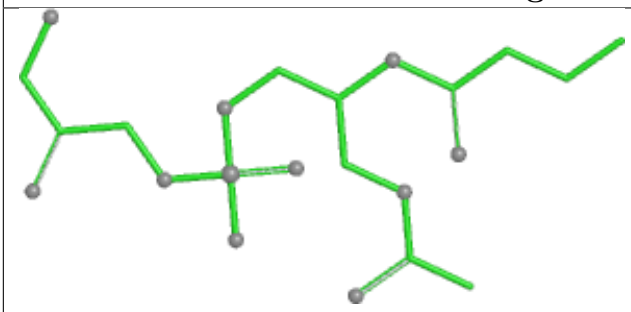


Torsions

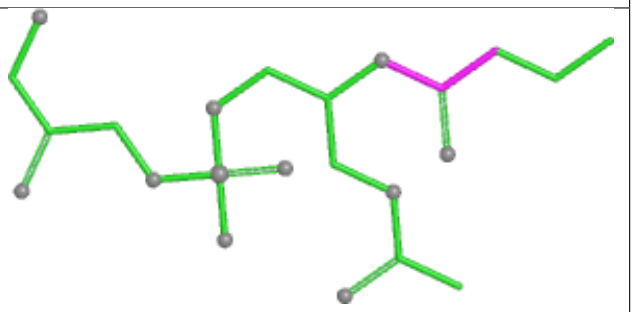


Rings

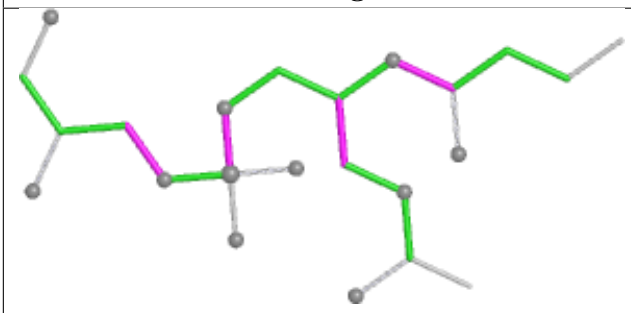
**Ligand LHG 1 301**



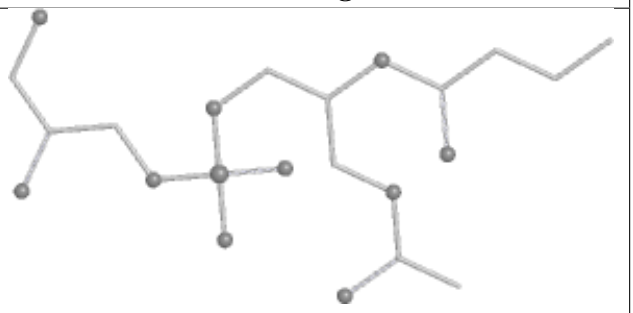
Bond lengths



Bond angles

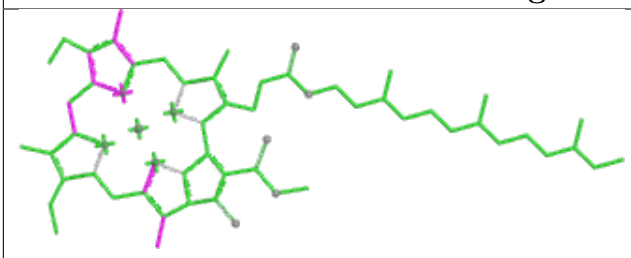


Torsions

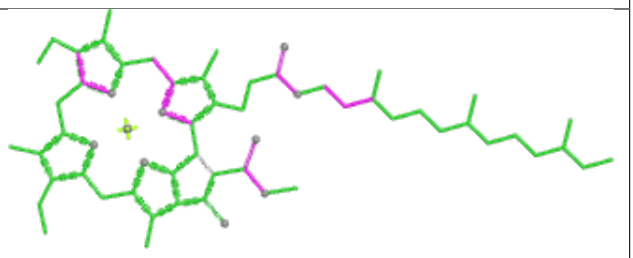


Rings

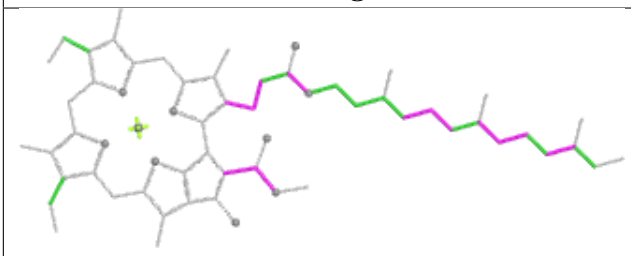
**Ligand CLA 5 602**



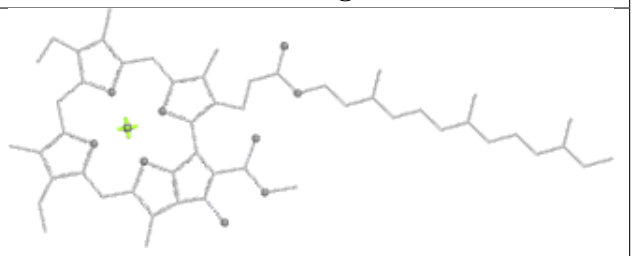
Bond lengths



Bond angles

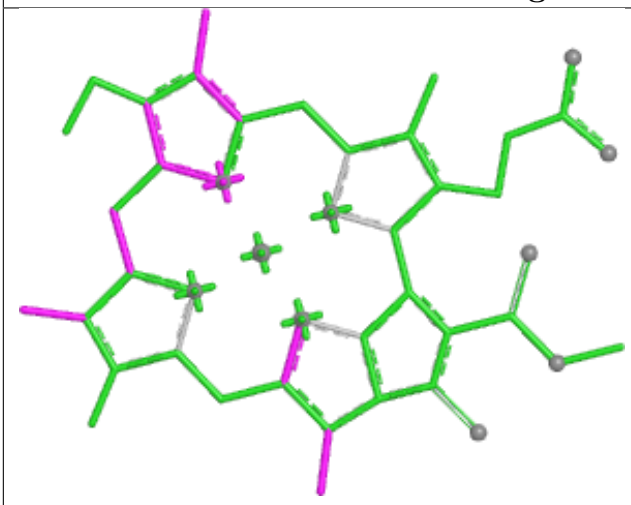


Torsions

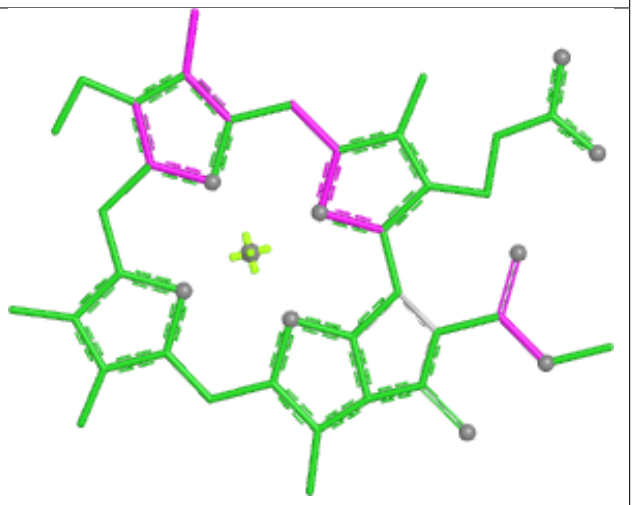


Rings

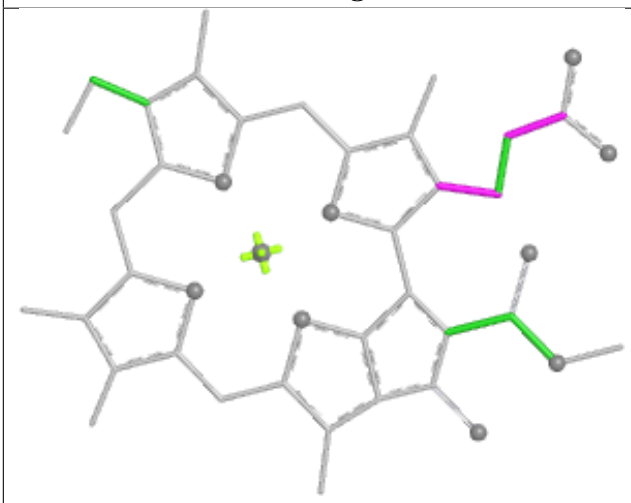
**Ligand CLA 4 611**



Bond lengths



Bond angles

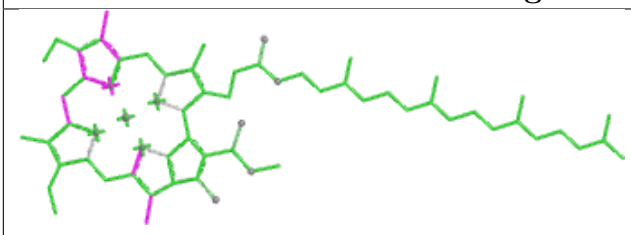


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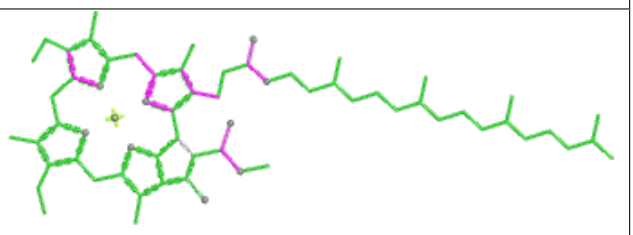


Rings

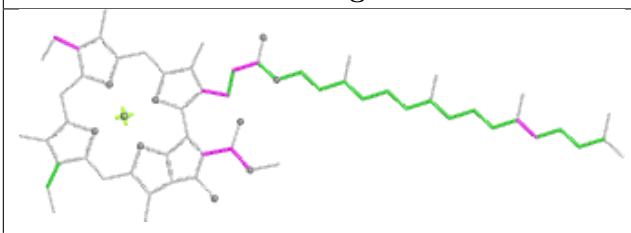
**Ligand CLA B 839**



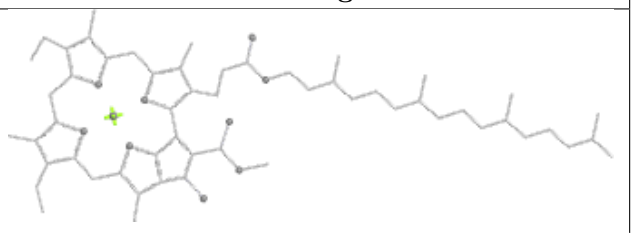
Bond lengths



Bond angles

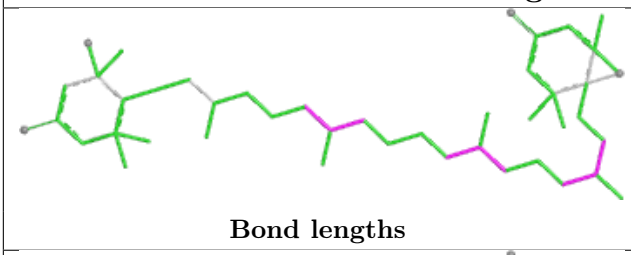


Torsions

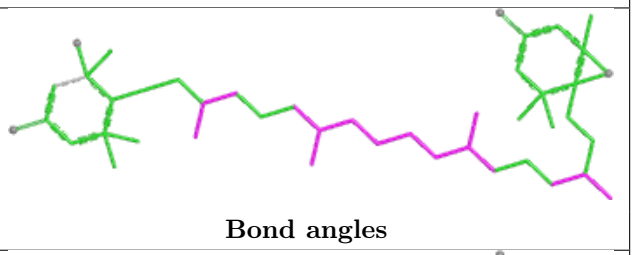


Rings

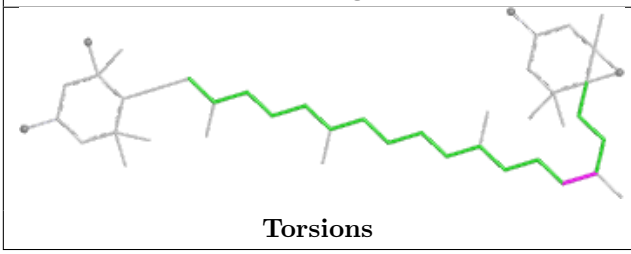
**Ligand NEX b 318**



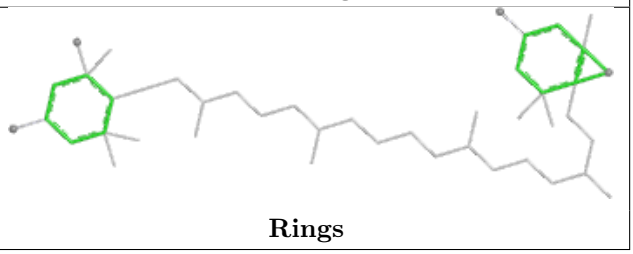
Bond lengths



Bond angles

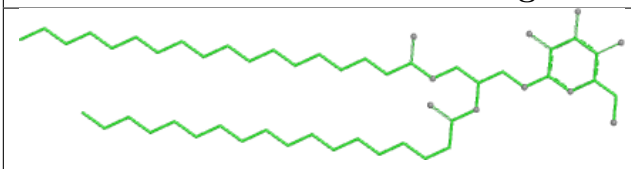


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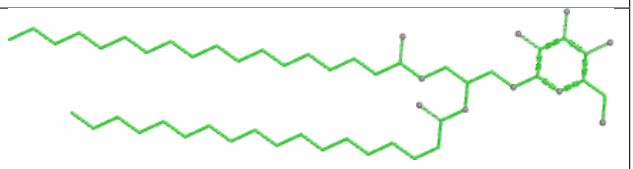


Rings

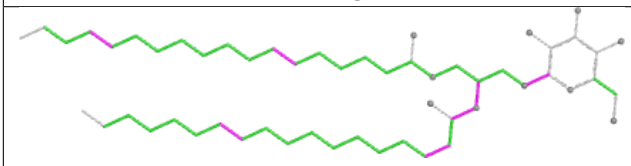
**Ligand LMG G 206**



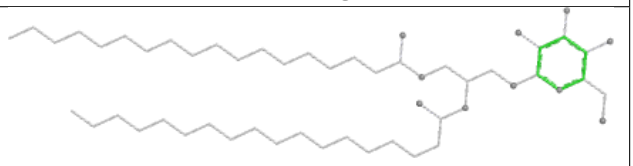
Bond lengths



Bond angles

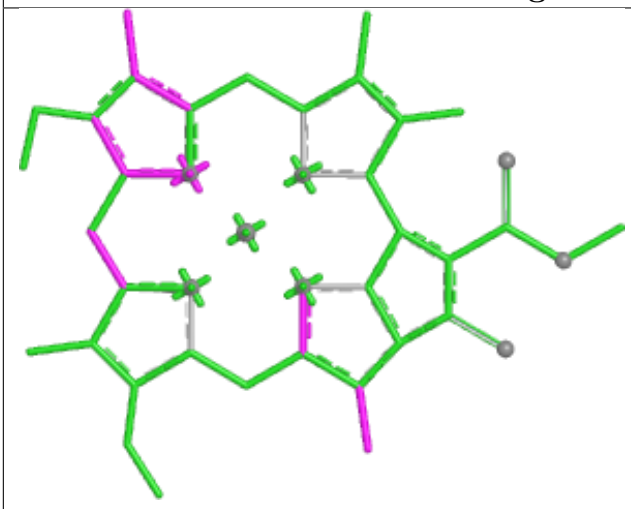


Torsions

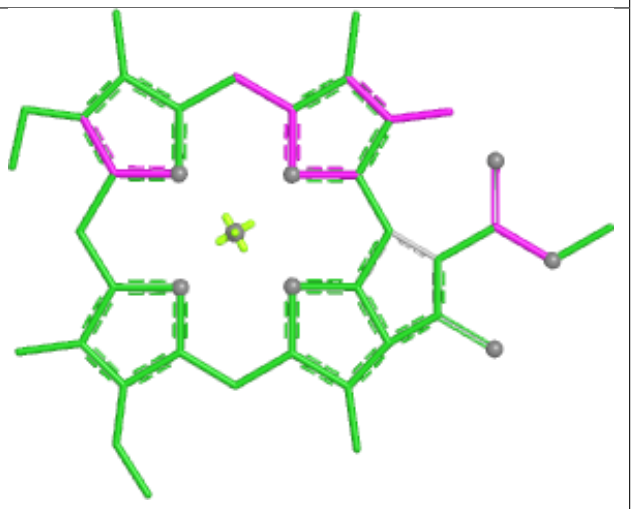


Rings

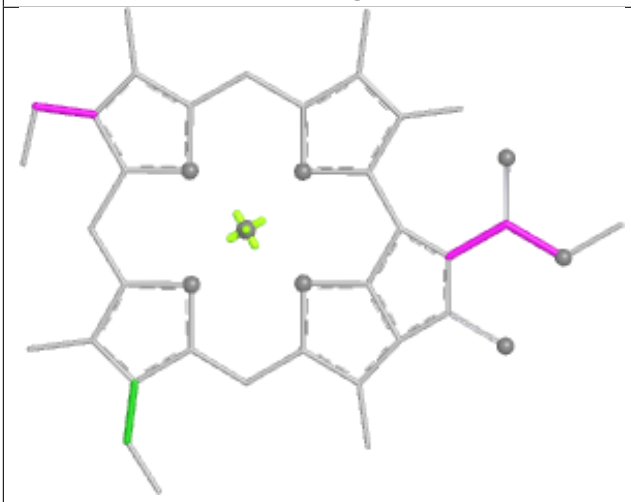
## Ligand CLA 6 611



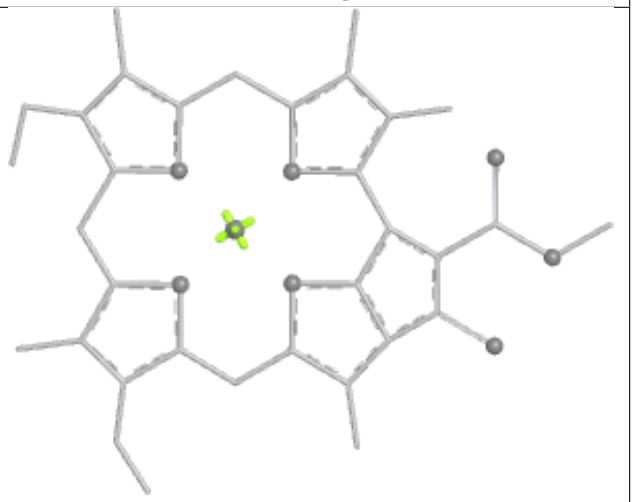
Bond lengths



Bond angles

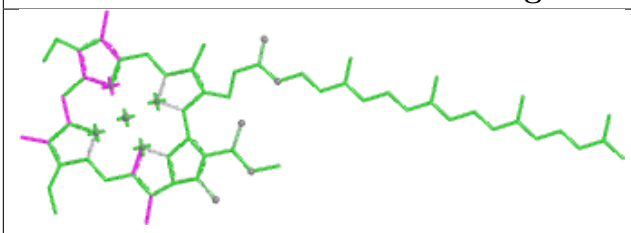


Torsions

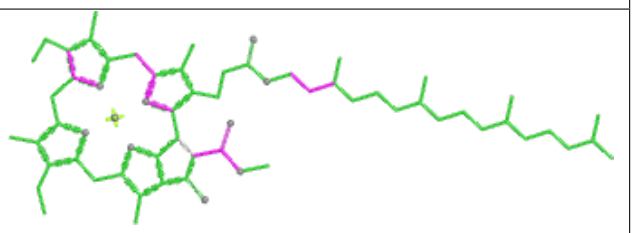


Rings

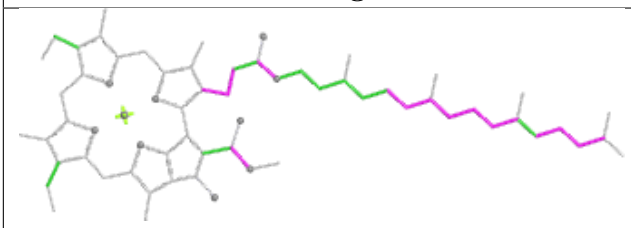
## Ligand CLA B 817



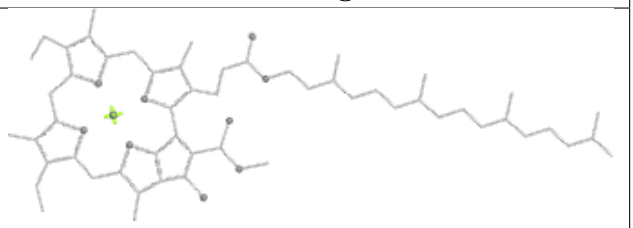
Bond lengths



Bond angles

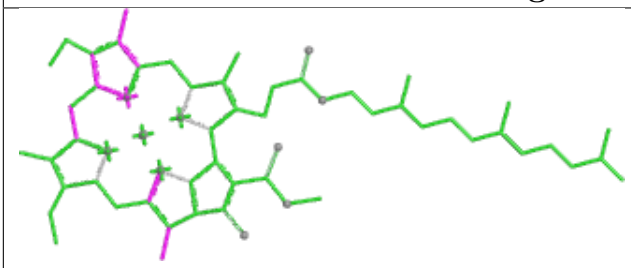


Torsions

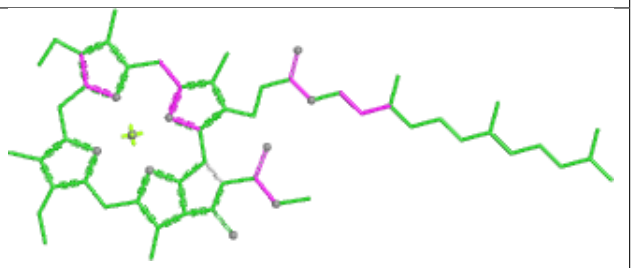


Rings

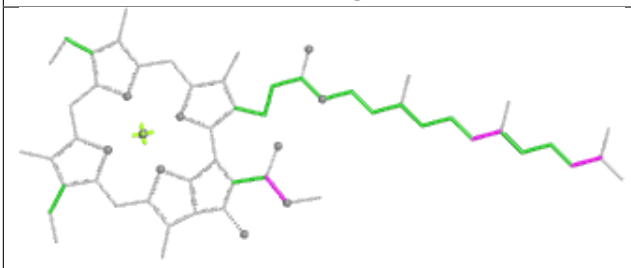
## Ligand CLA 3 402



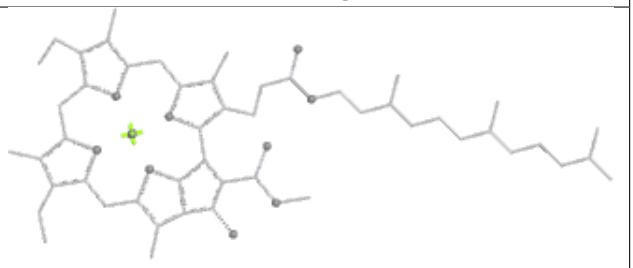
Bond lengths



Bond angles

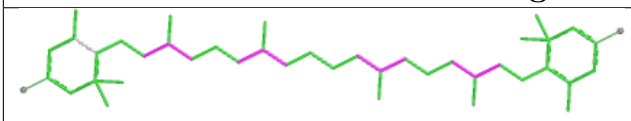


Torsions

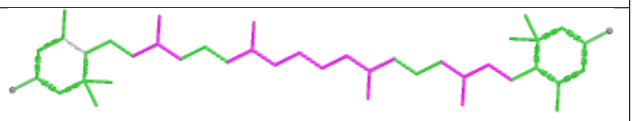


Rings

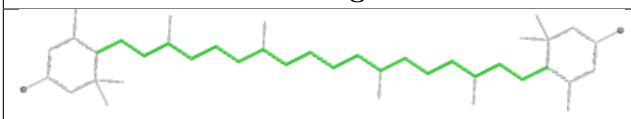
## Ligand LUT c 616



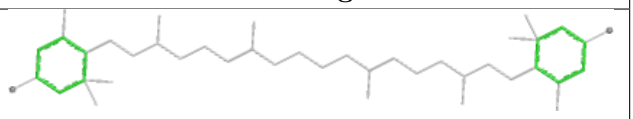
Bond lengths



Bond angles

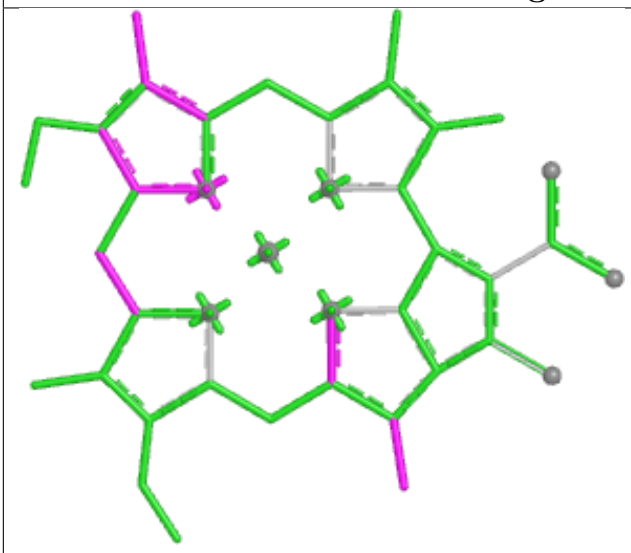


Torsions

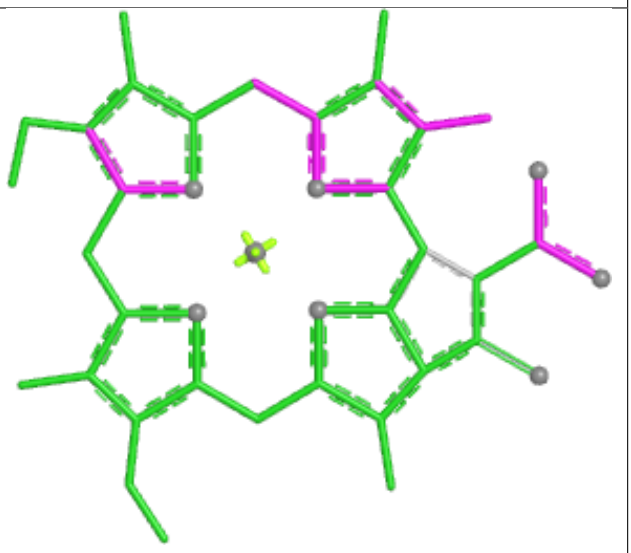


Rings

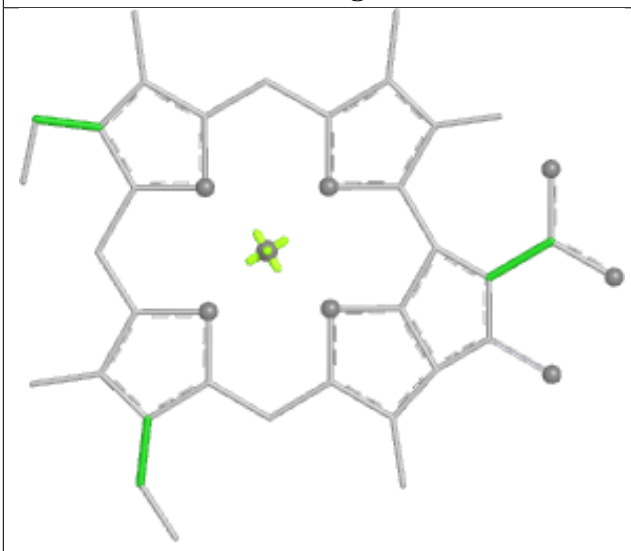
**Ligand CLA 3 415**



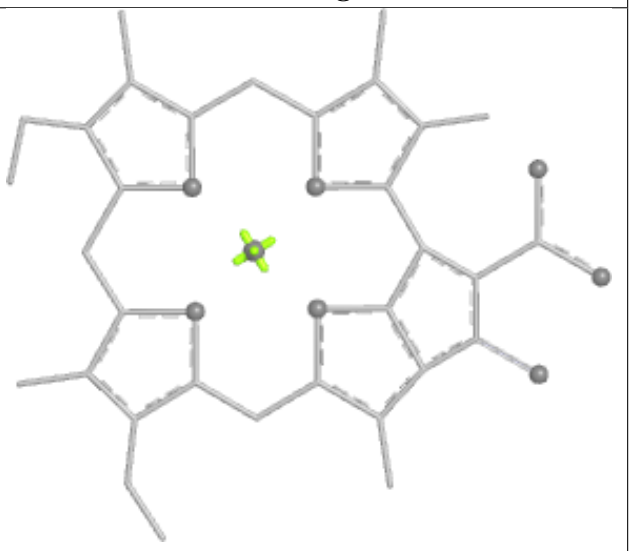
**Bond lengths**



**Bond angles**

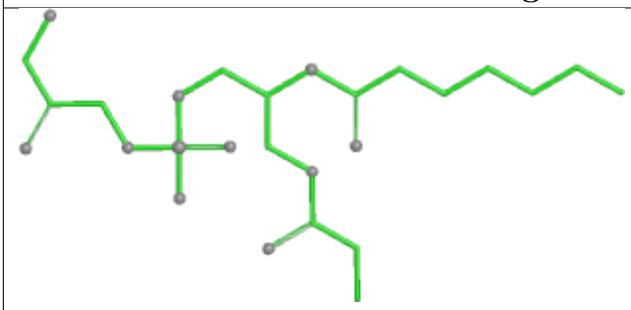


**Torsions**

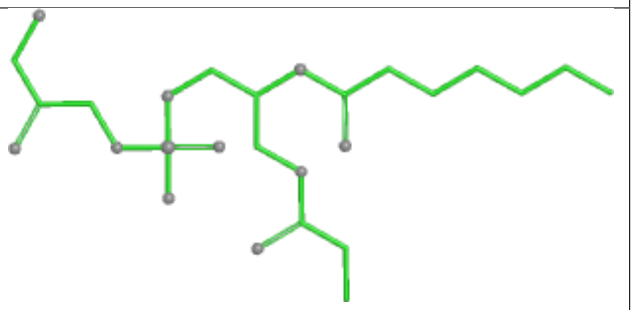


**Rings**

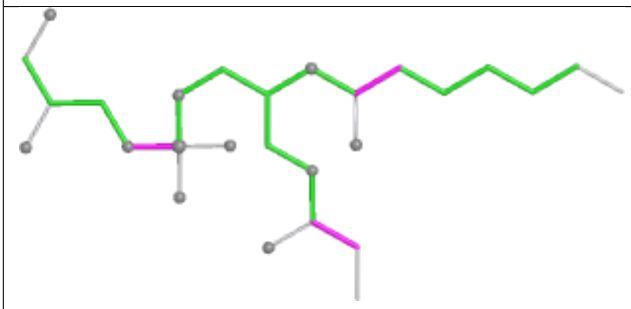
**Ligand LHG A 845**



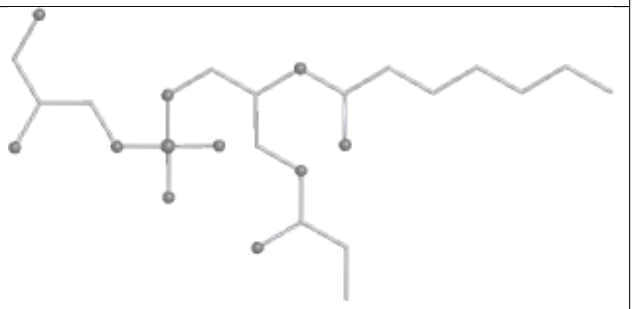
**Bond lengths**



**Bond angles**

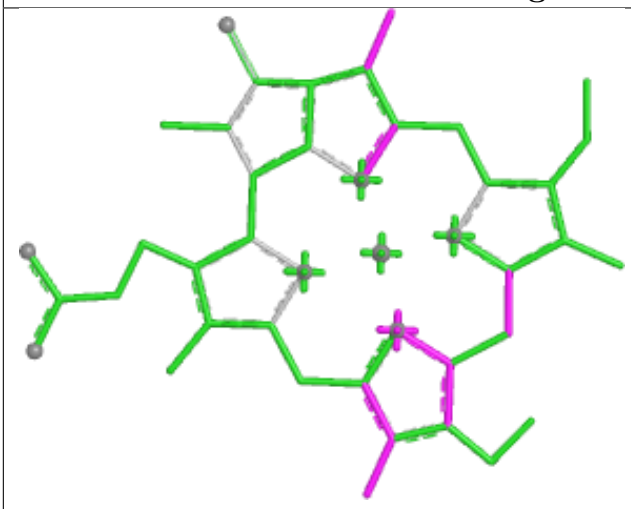


**Torsions**

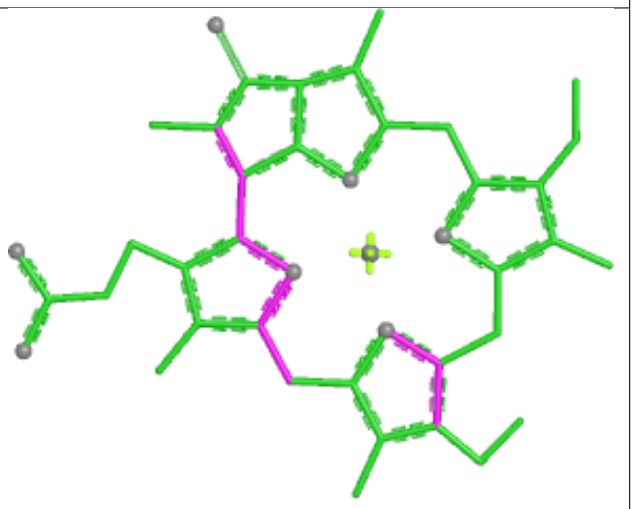


**Rings**

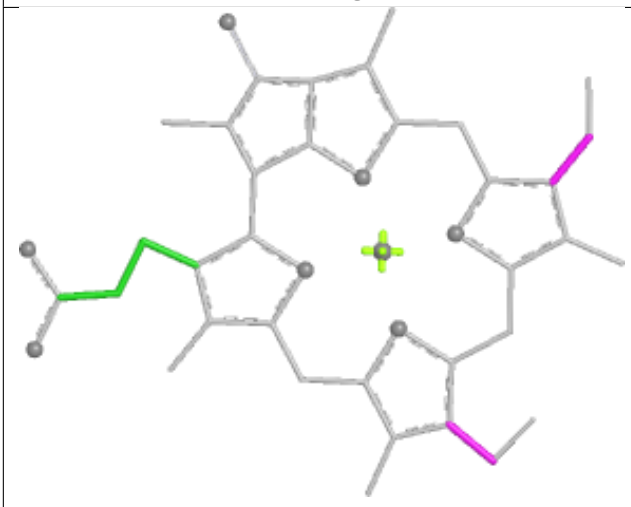
## Ligand CLA 2 610



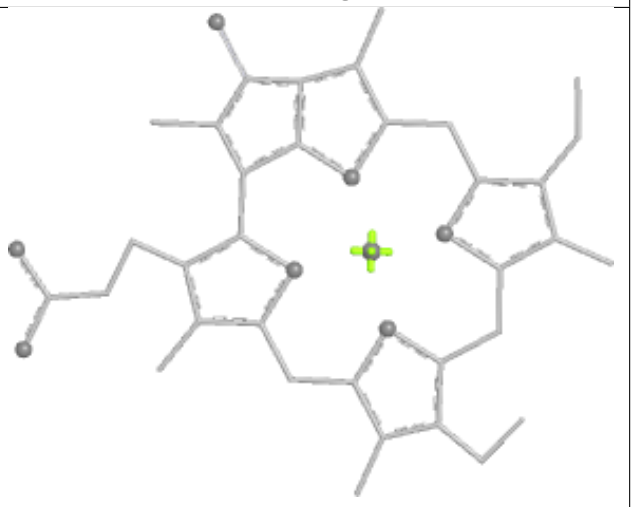
Bond lengths



Bond angles

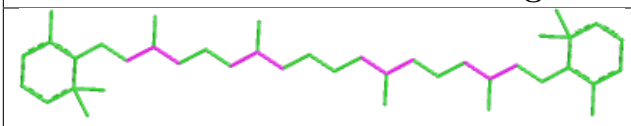


Torsions

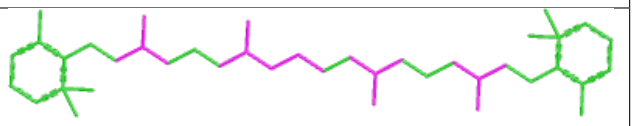


Rings

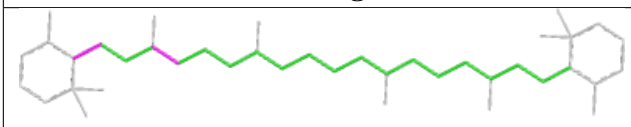
## Ligand BCR L 301



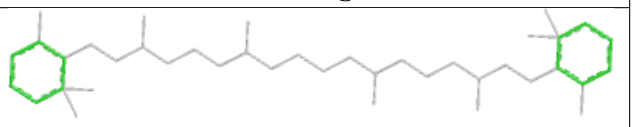
Bond lengths



Bond angles

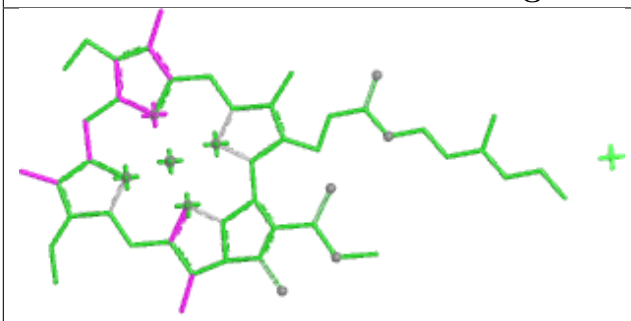


Torsions

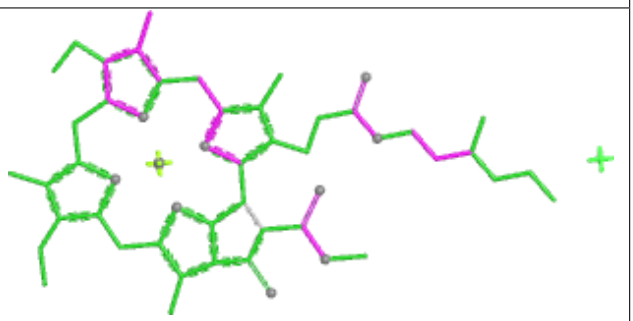


Rings

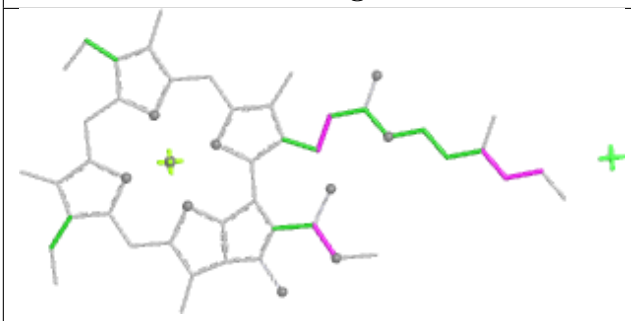
**Ligand CLA A 852**



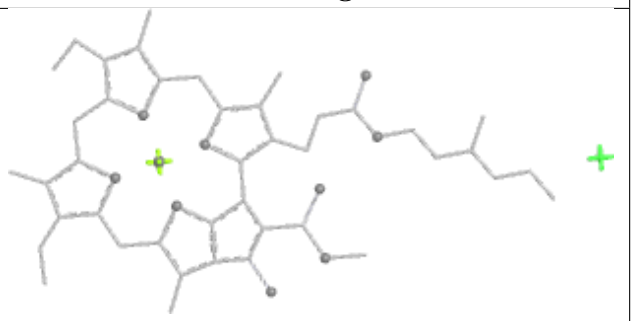
**Bond lengths**



**Bond angles**

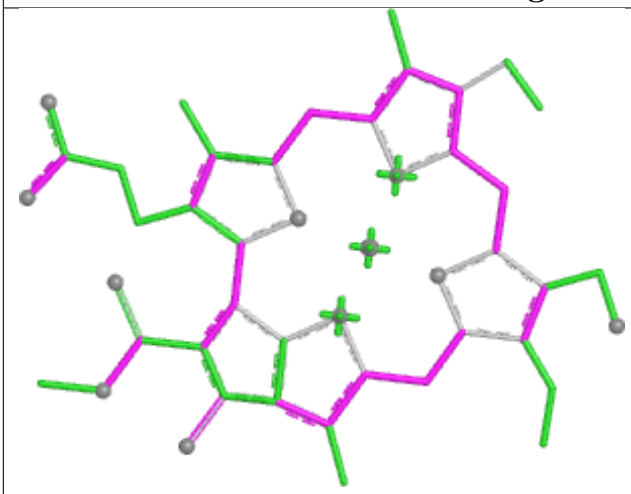


**Torsions**

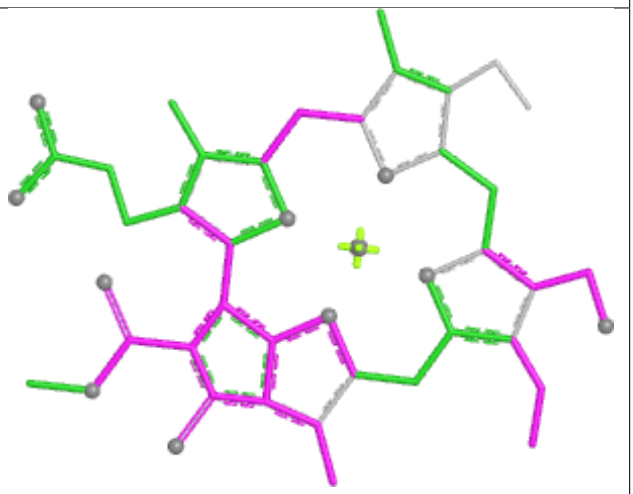


**Rings**

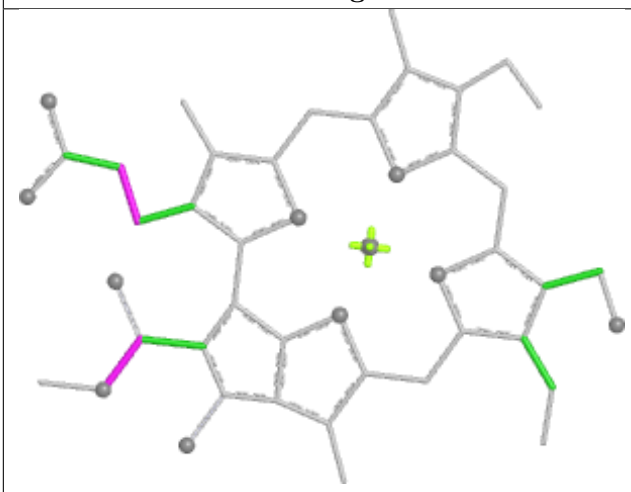
**Ligand CHL 2 605**



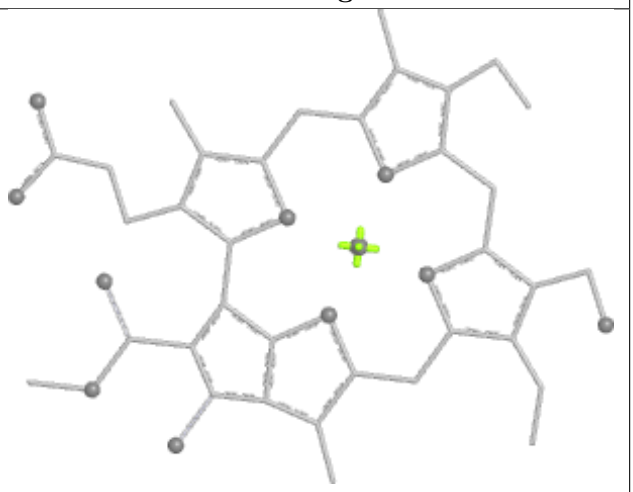
**Bond lengths**



**Bond angles**

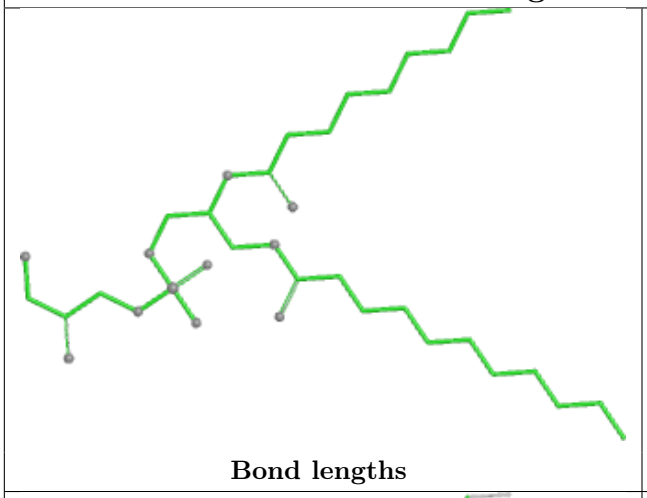


**Torsions**

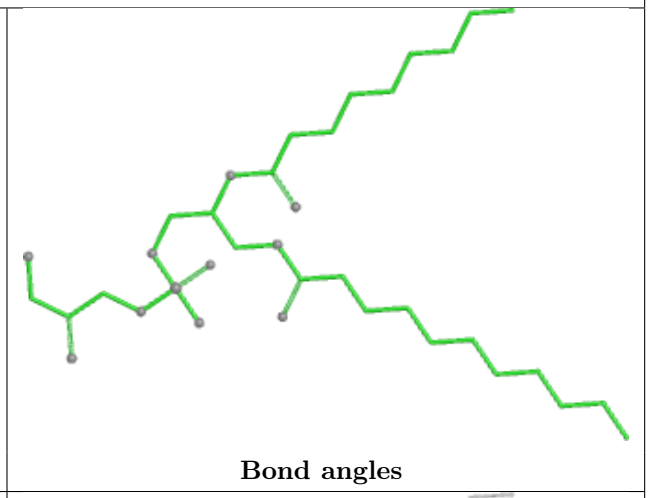


**Rings**

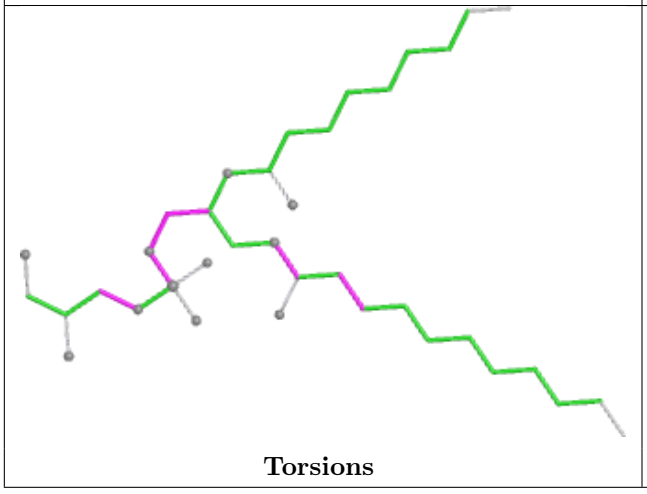
## Ligand LHG 8 617



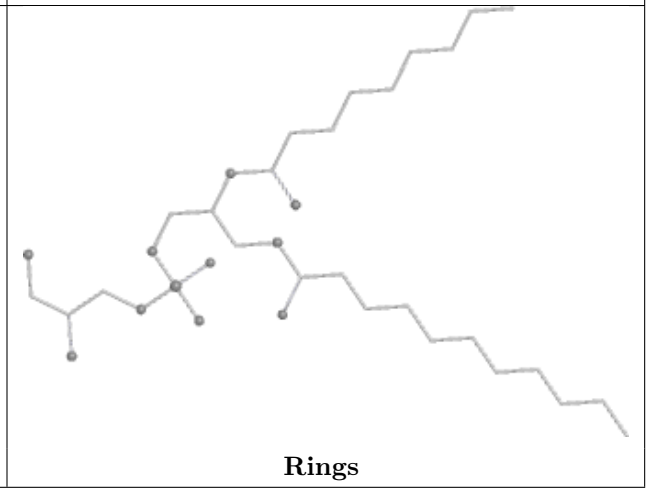
Bond lengths



Bond angles

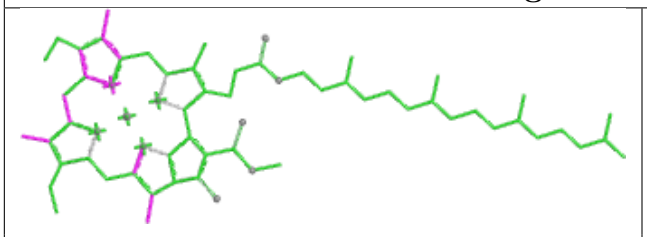


Torsions

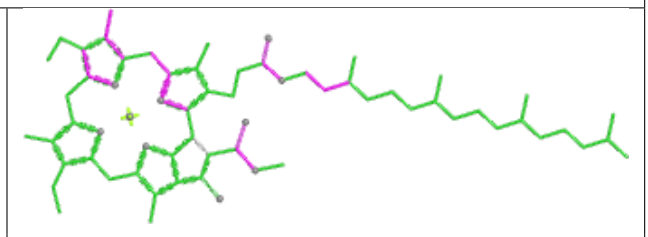


Rings

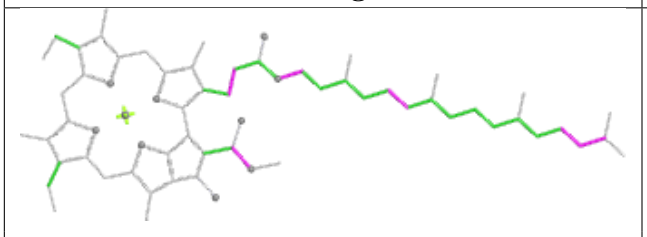
## Ligand CLA A 814



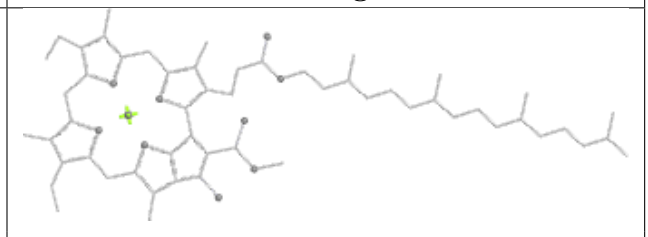
Bond lengths



Bond angles

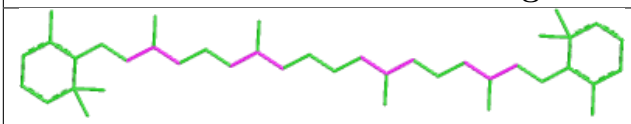


Torsions

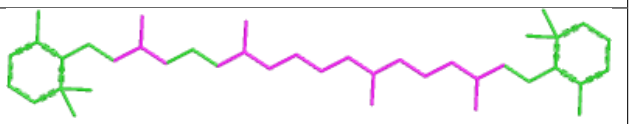


Rings

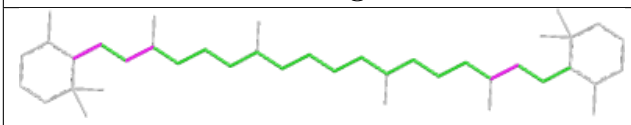
**Ligand BCR O 205**



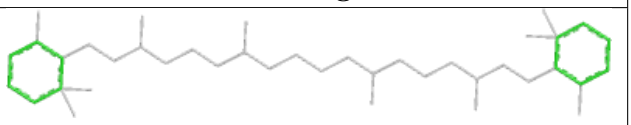
Bond lengths



Bond angles

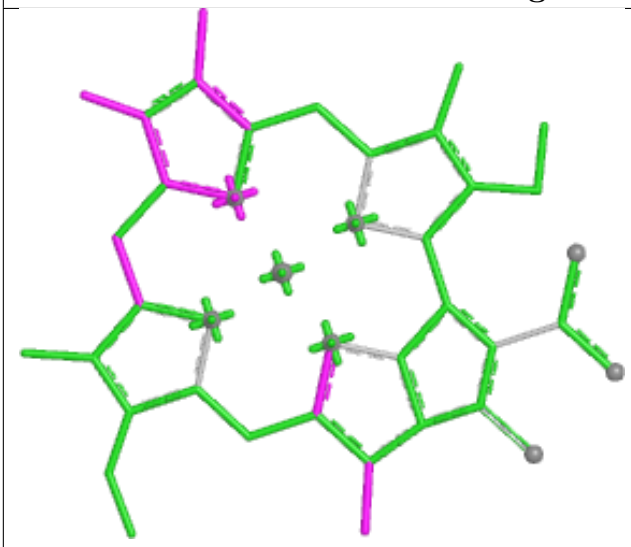


Torsions

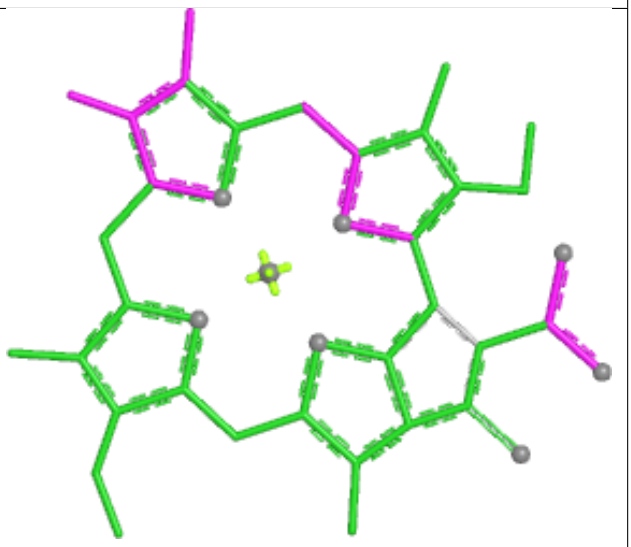


Rings

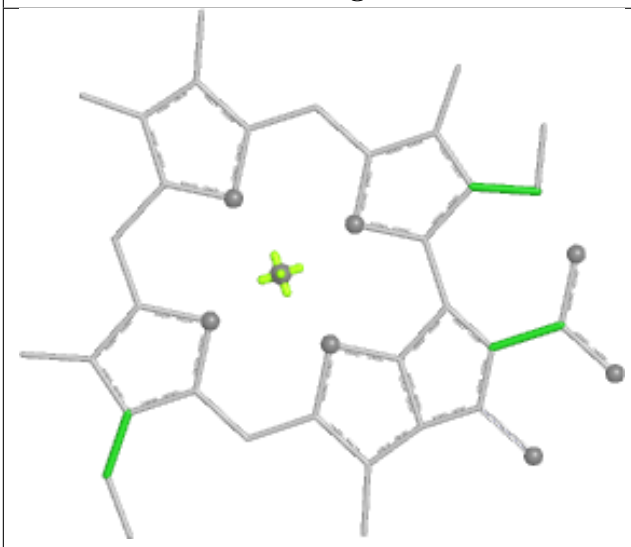
**Ligand CLA 3 406**



Bond lengths



Bond angles

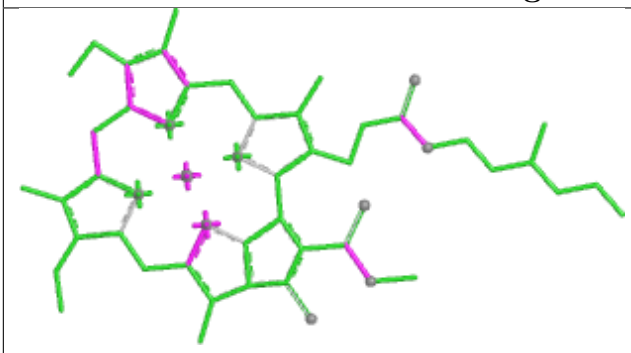


Torsions

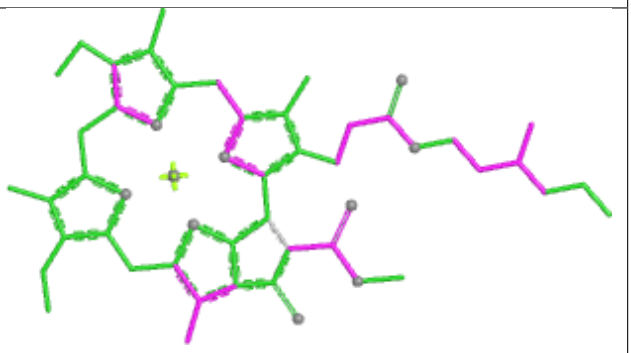


Rings

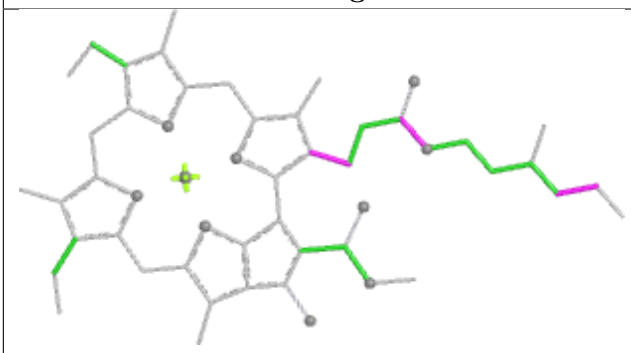
## Ligand CLA A 830



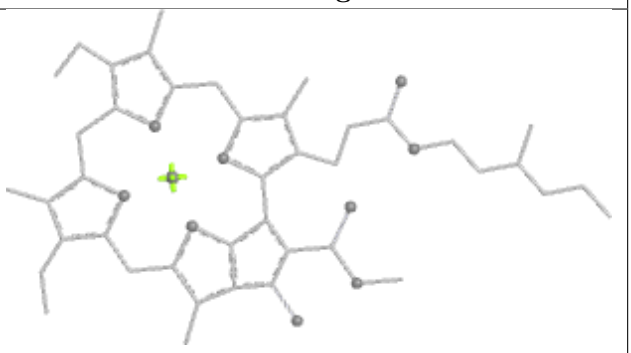
Bond lengths



Bond angles

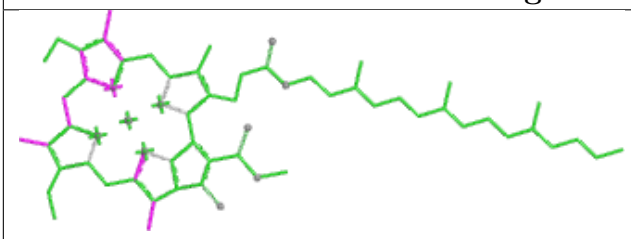


Torsions

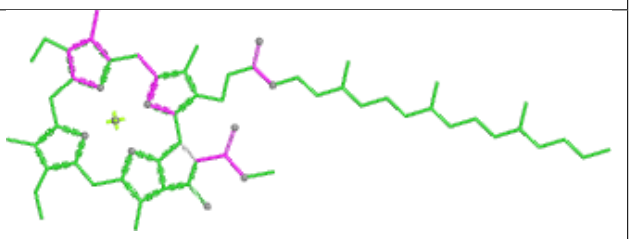


Rings

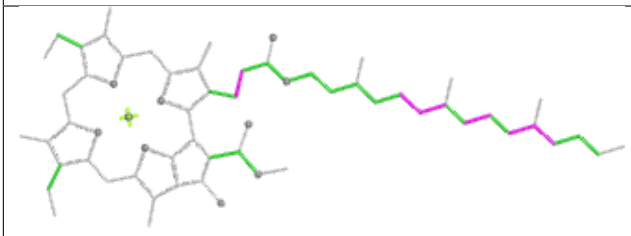
## Ligand CLA B 806



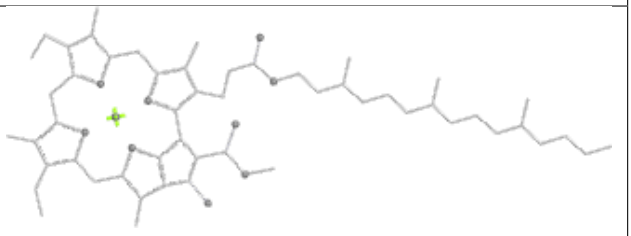
Bond lengths



Bond angles

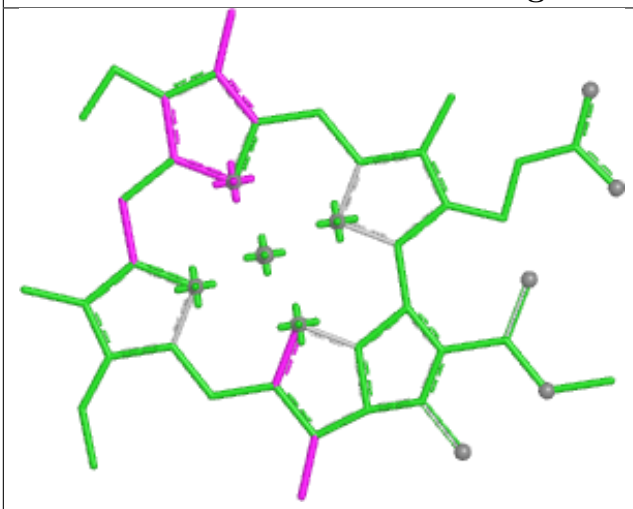


Torsions

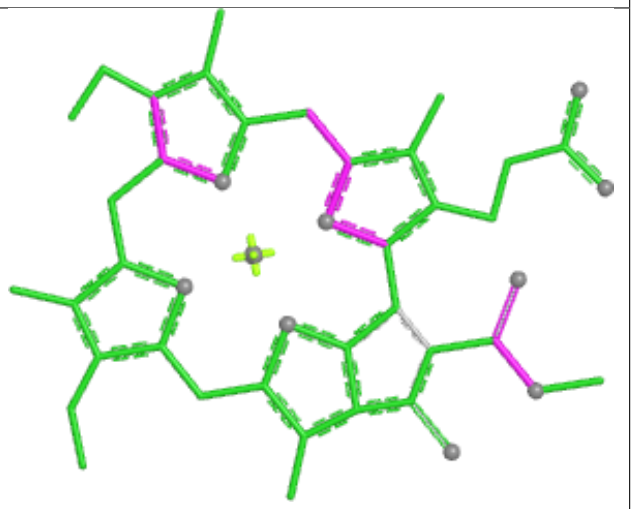


Rings

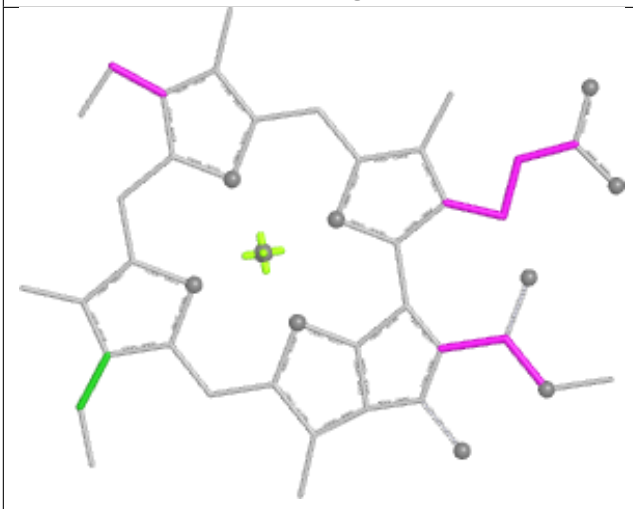
**Ligand CLA b 315**



**Bond lengths**



**Bond angles**

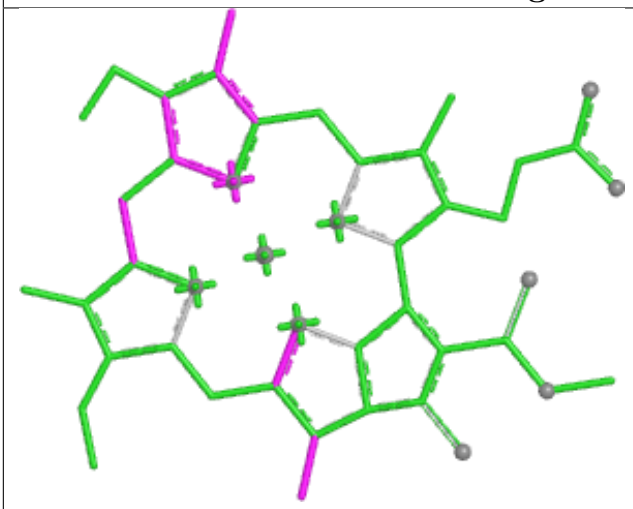


**Torsions**

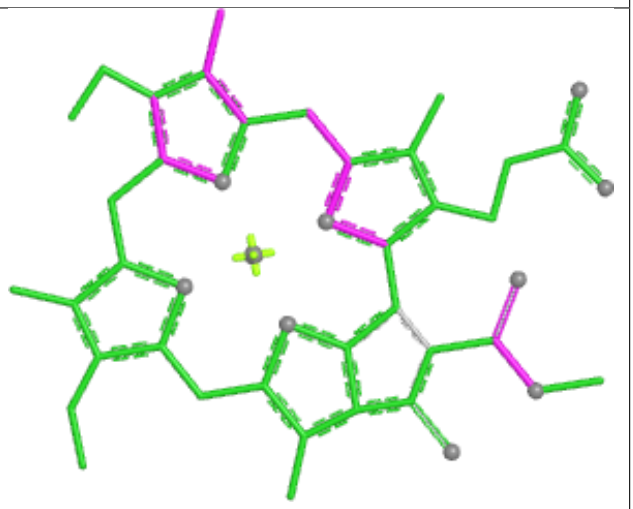


**Rings**

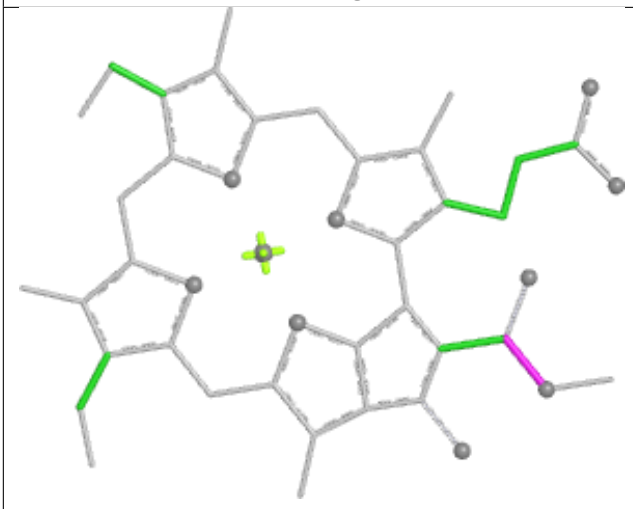
**Ligand CLA 2 604**



**Bond lengths**



**Bond angles**

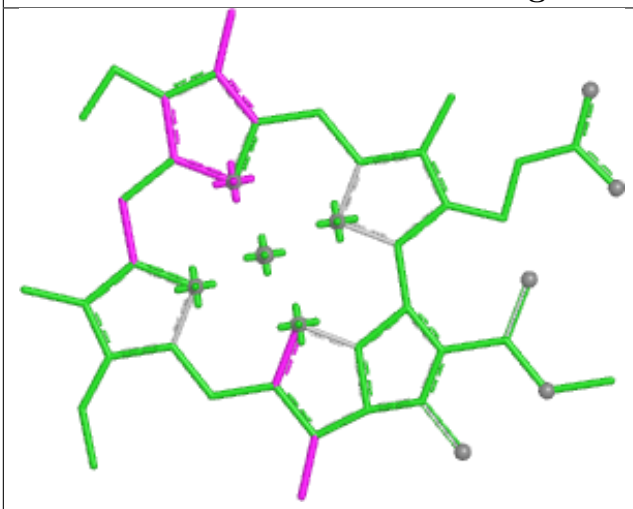


**Torsions**

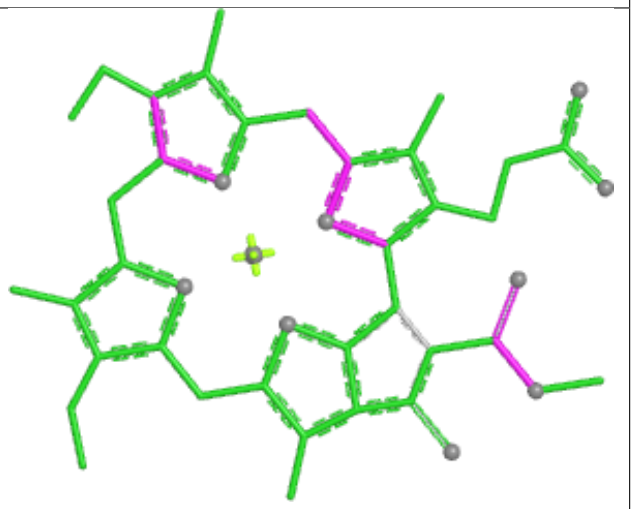


**Rings**

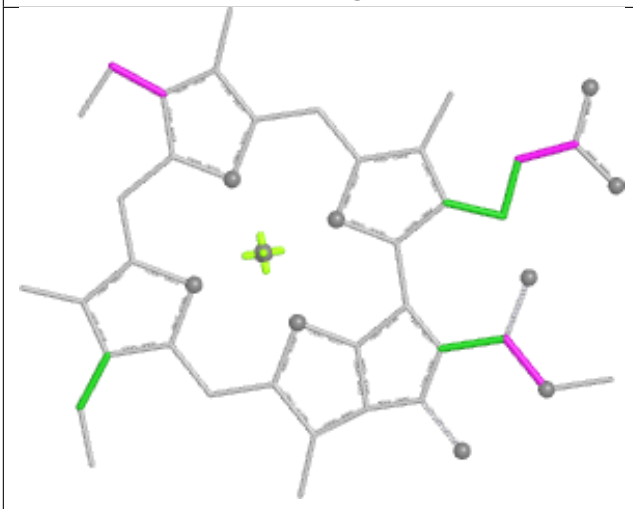
**Ligand CLA a 612**



**Bond lengths**



**Bond angles**

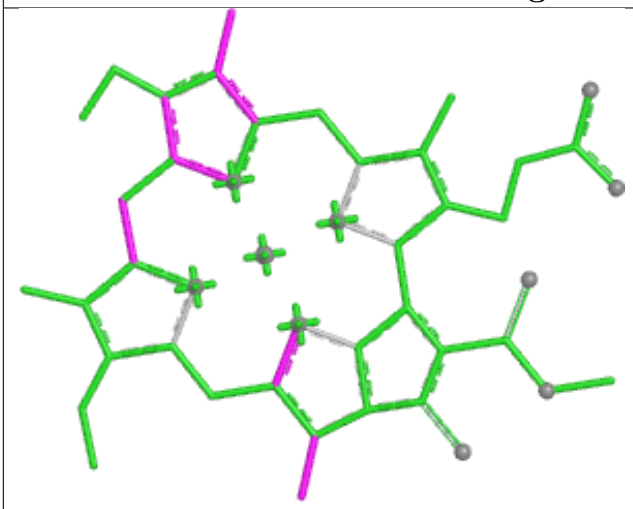


**Torsions**

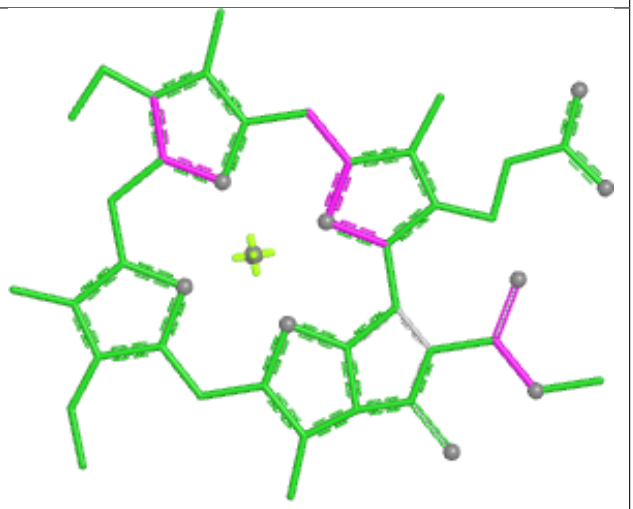


**Rings**

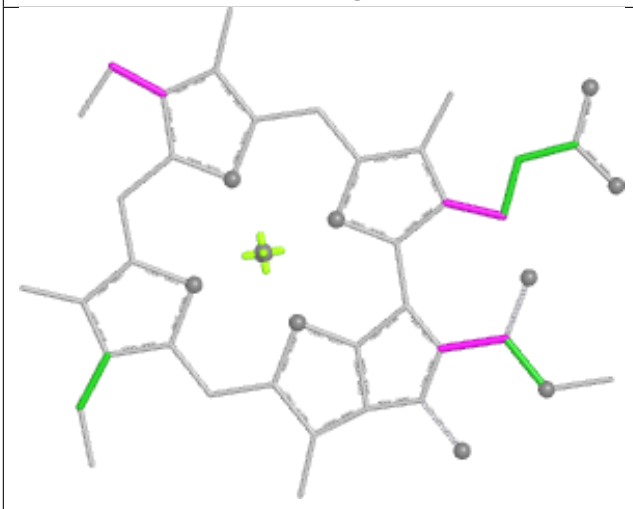
**Ligand CLA 9 603**



**Bond lengths**



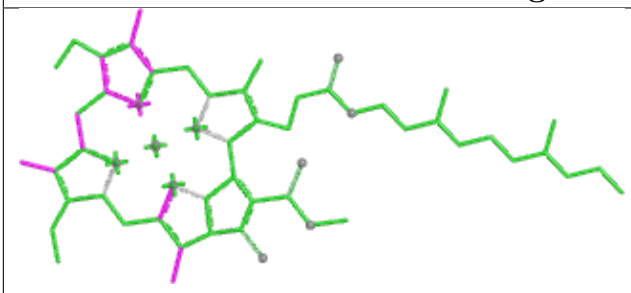
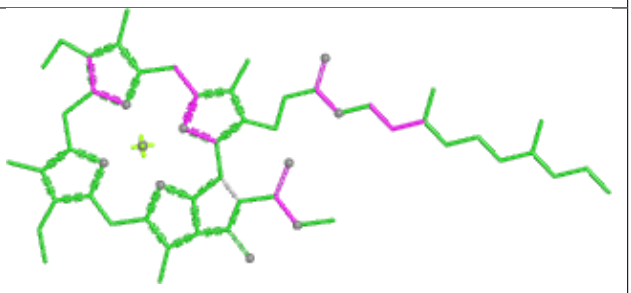
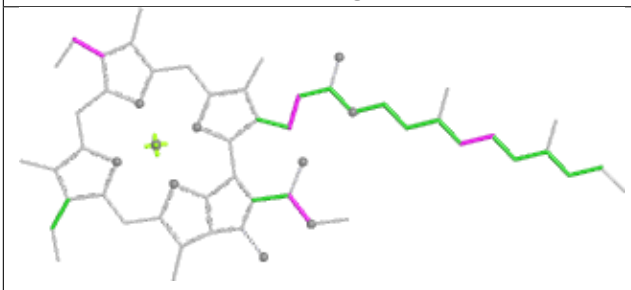
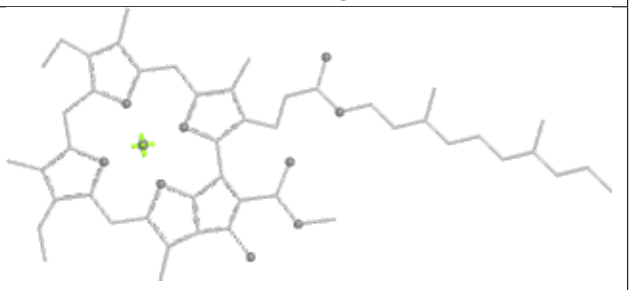
**Bond angles**

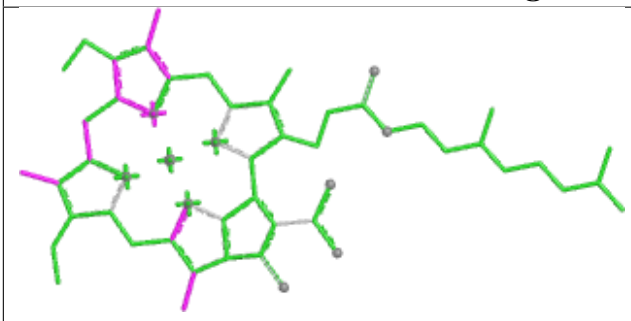
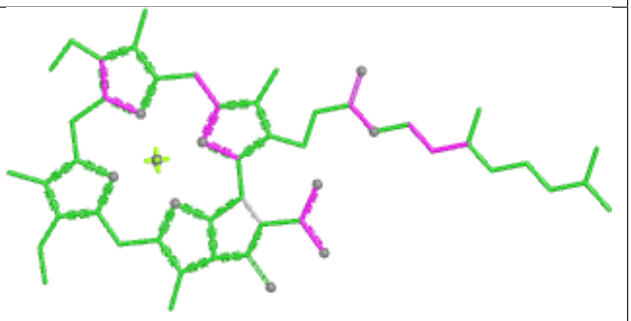
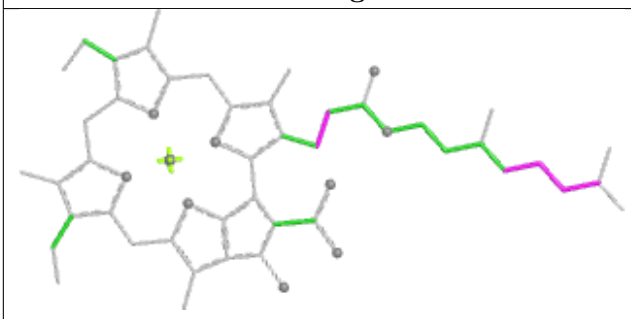
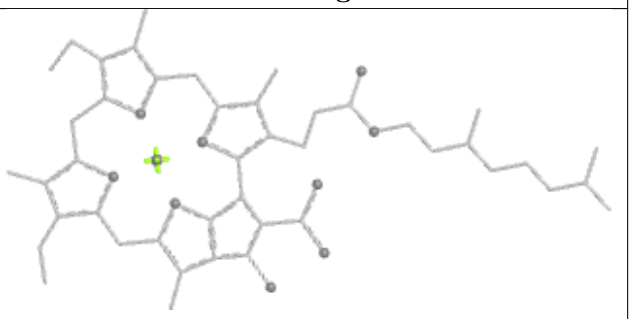


**Torsions**

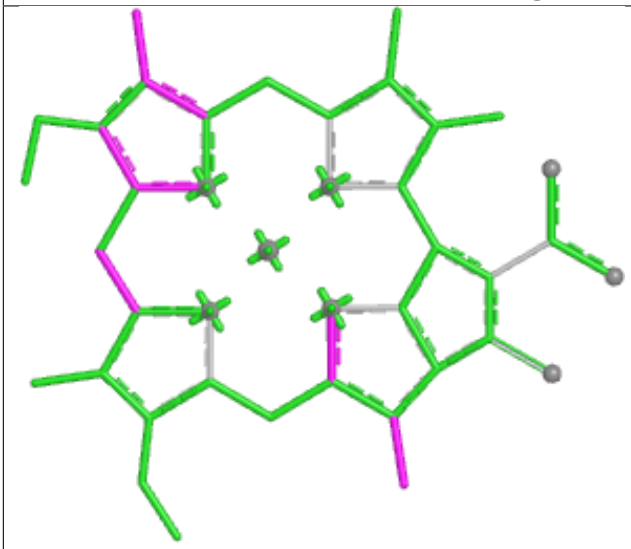


**Rings**

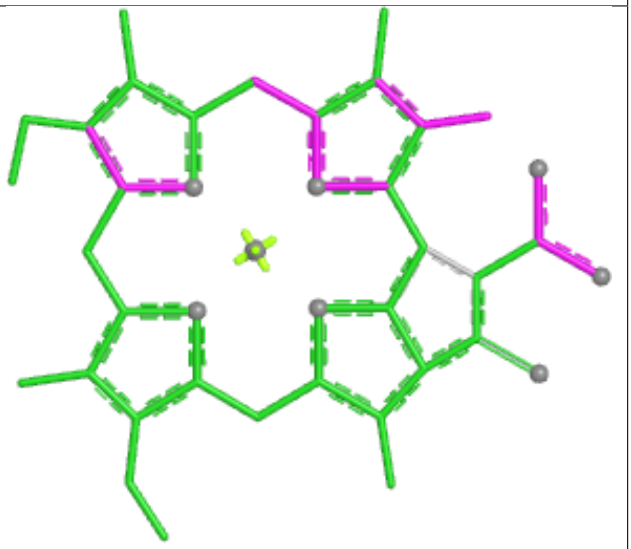
| Ligand CLA a 613 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

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

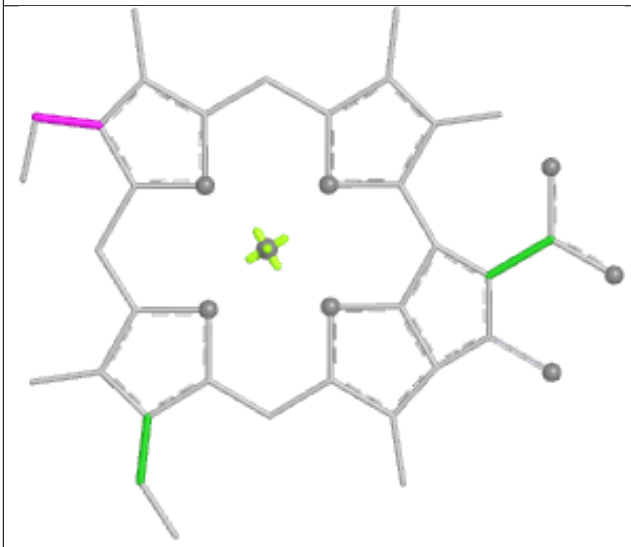
**Ligand CLA 7 412**



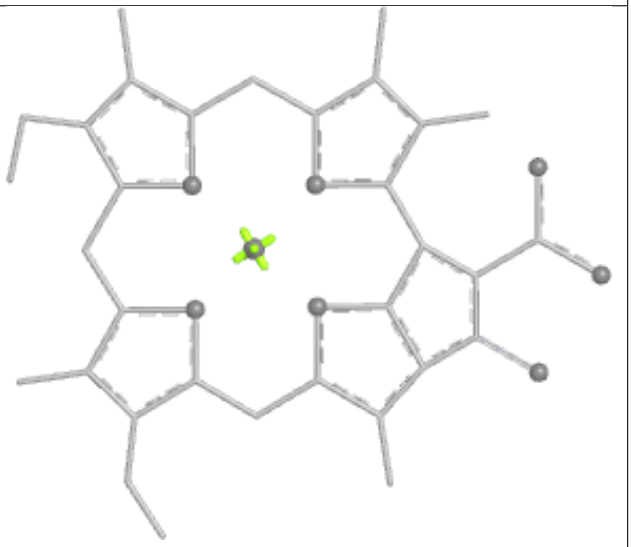
**Bond lengths**



**Bond angles**

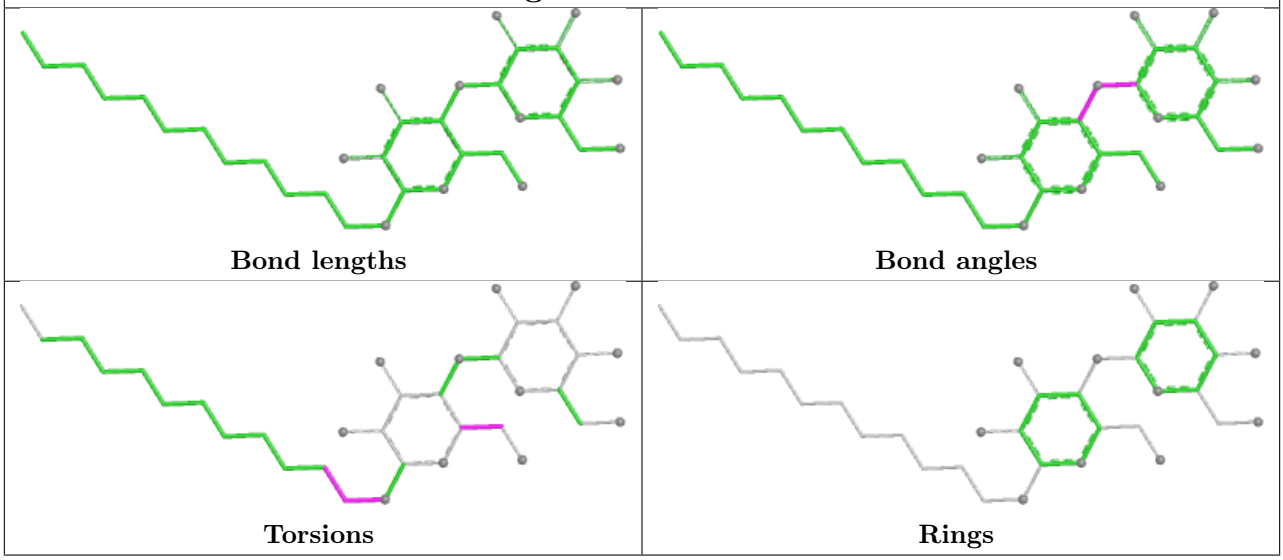


**Torsions**

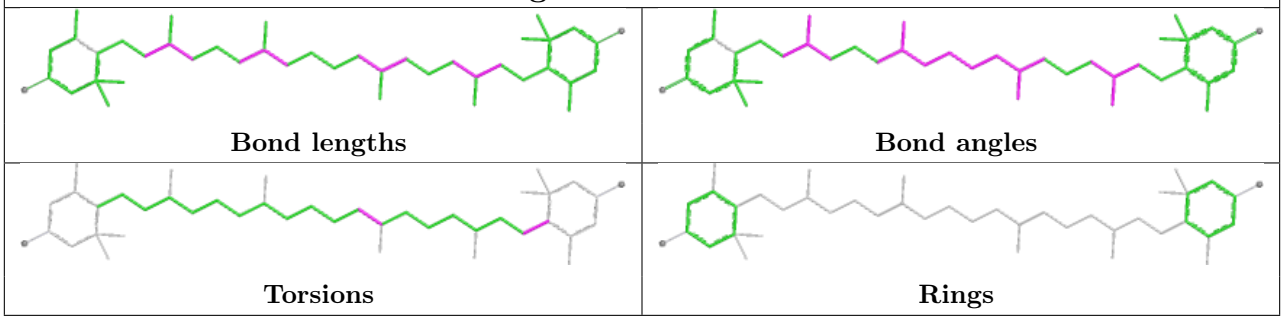


**Rings**

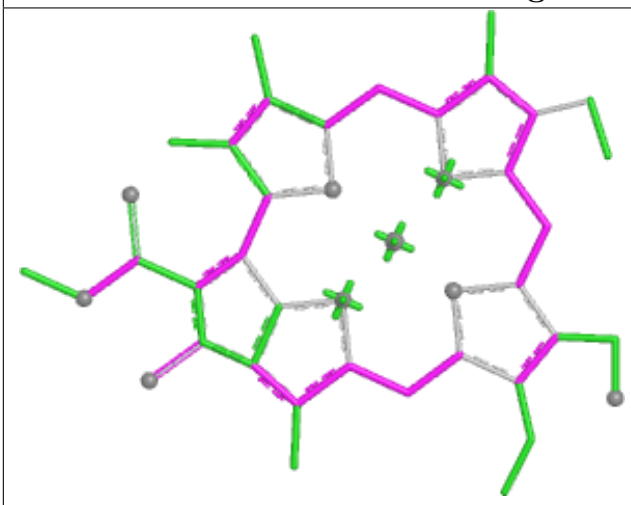
**Ligand LMU 3 420**




**Ligand LUT 4 615**



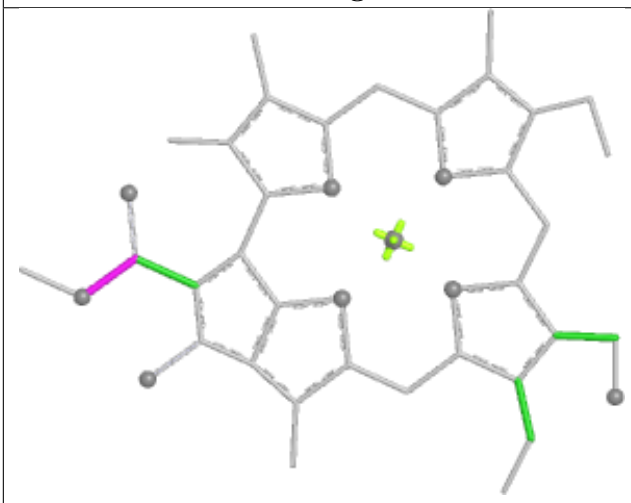
**Ligand CHL 4 614**



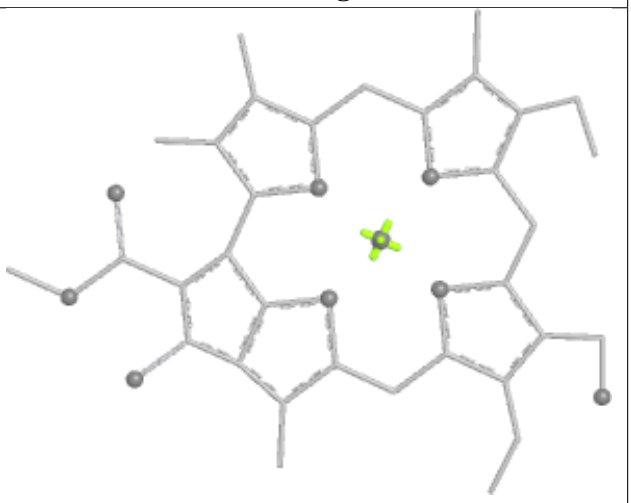
**Bond lengths**



**Bond angles**

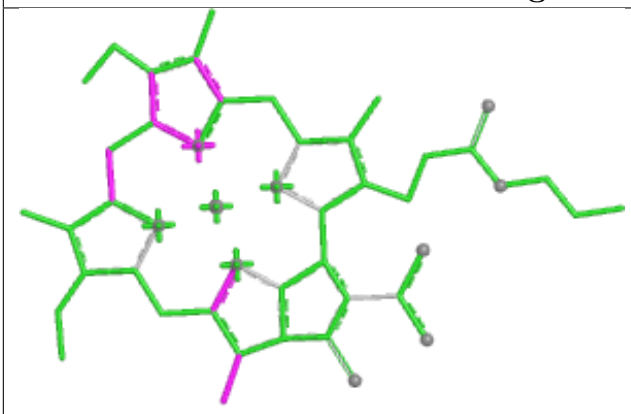


**Torsions**

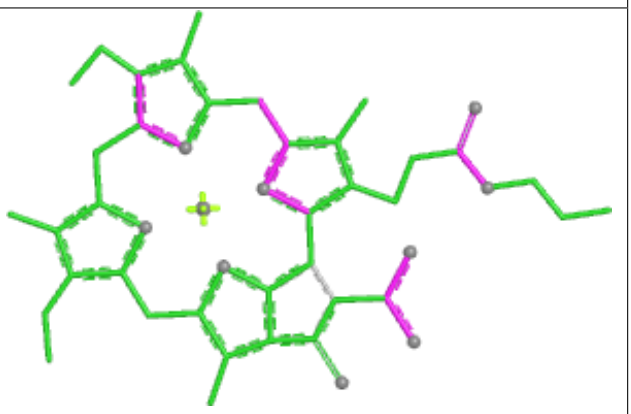


**Rings**

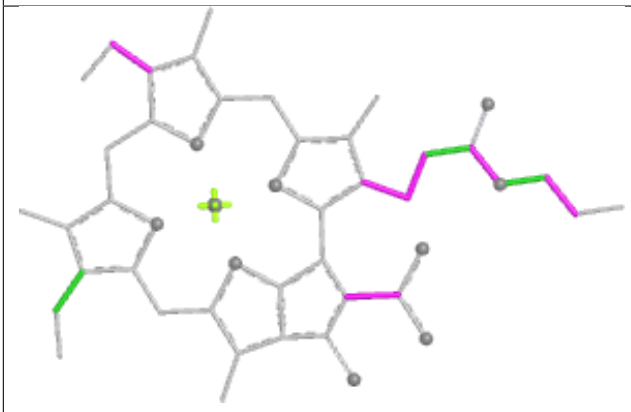
## Ligand CLA a 604



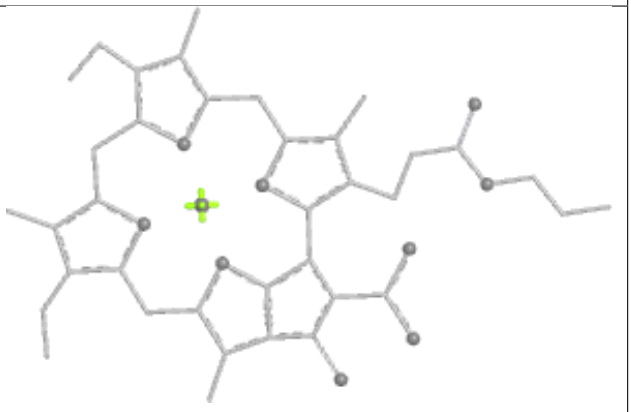
Bond lengths



Bond angles

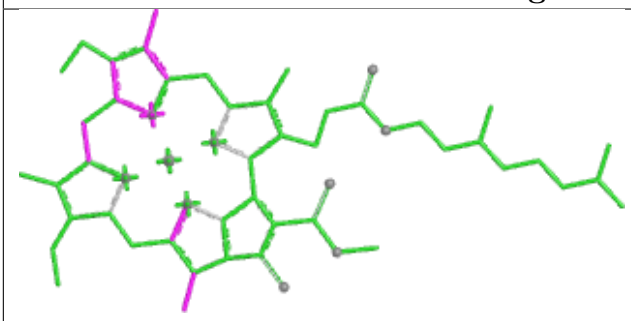


Torsions

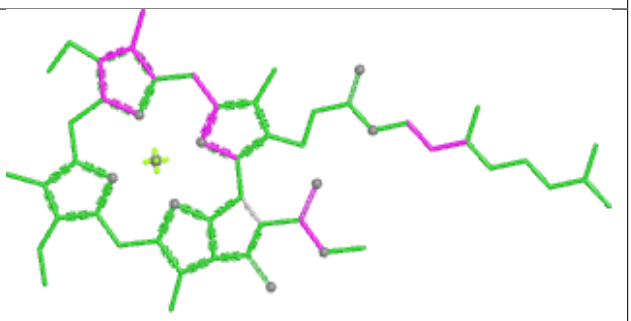


Rings

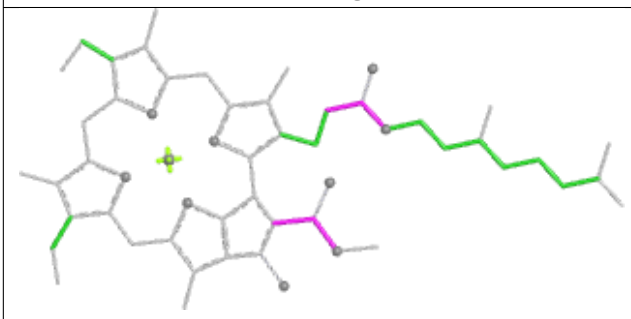
## Ligand CLA 1 304



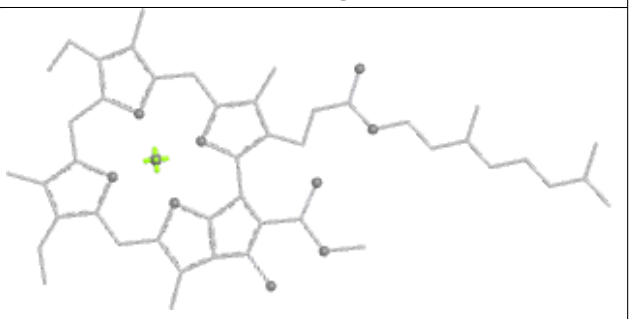
Bond lengths



Bond angles

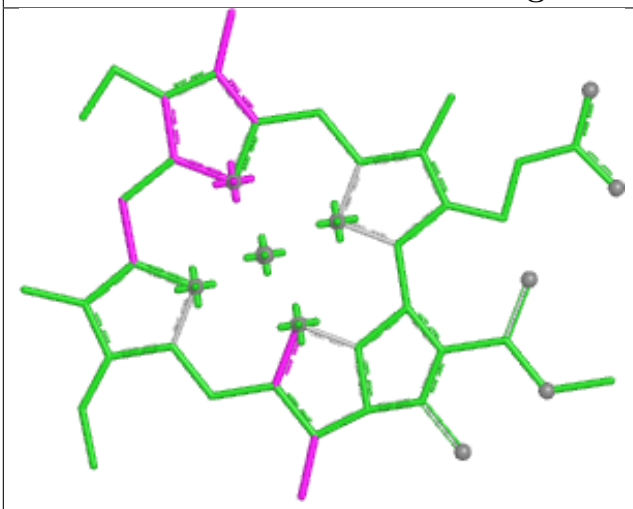


Torsions

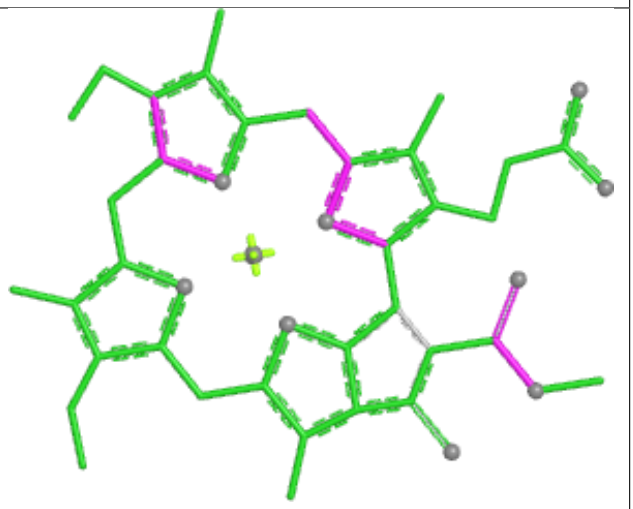


Rings

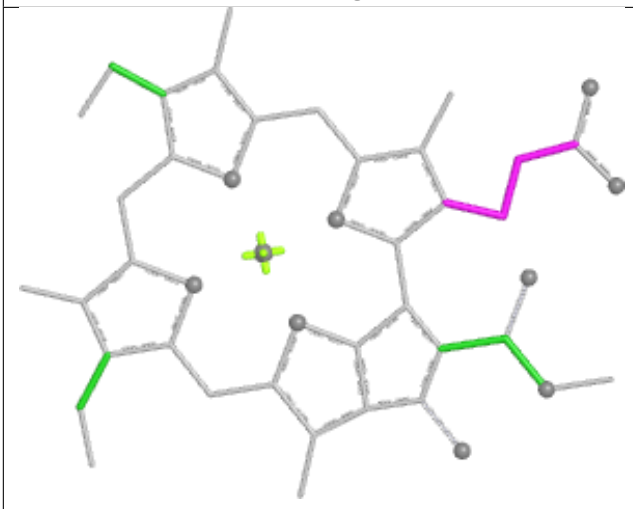
## Ligand CLA b 305



Bond lengths



Bond angles

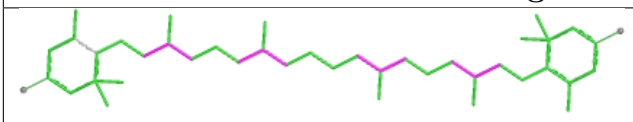


Torsions

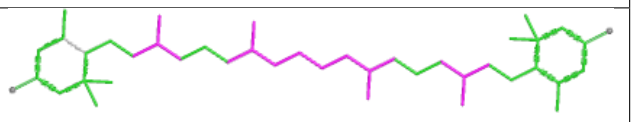


Rings

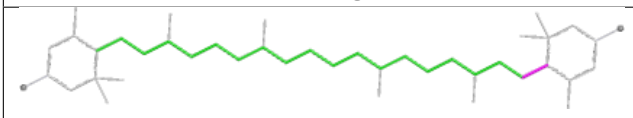
## Ligand LUT b 317



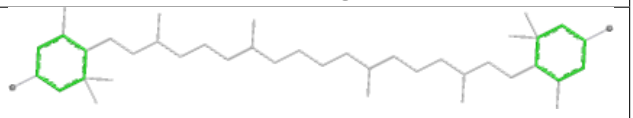
Bond lengths



Bond angles

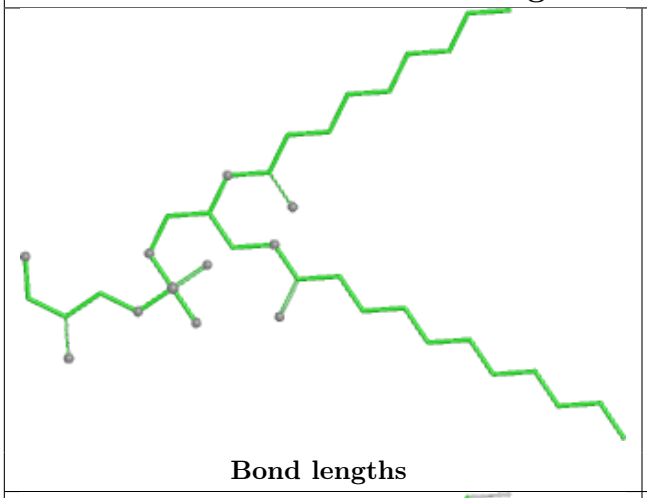


Torsions

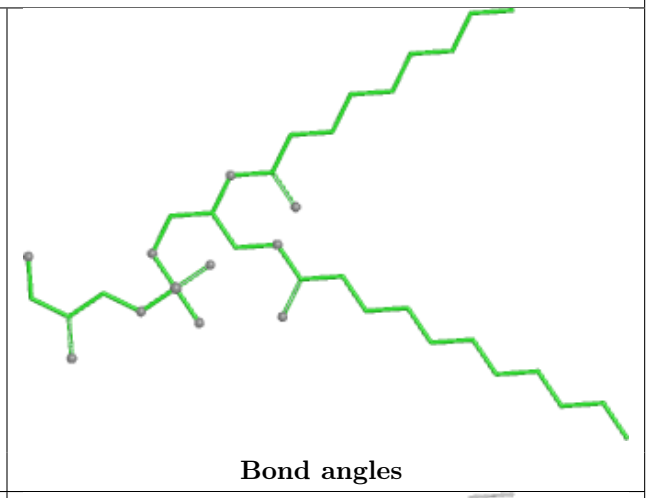


Rings

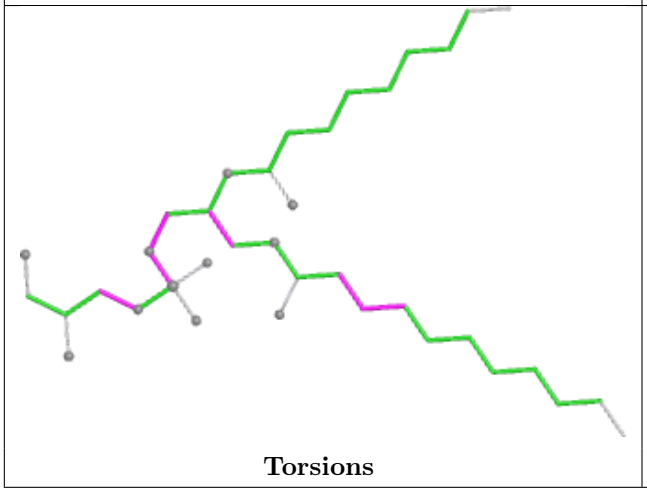
**Ligand LHG 4 618**



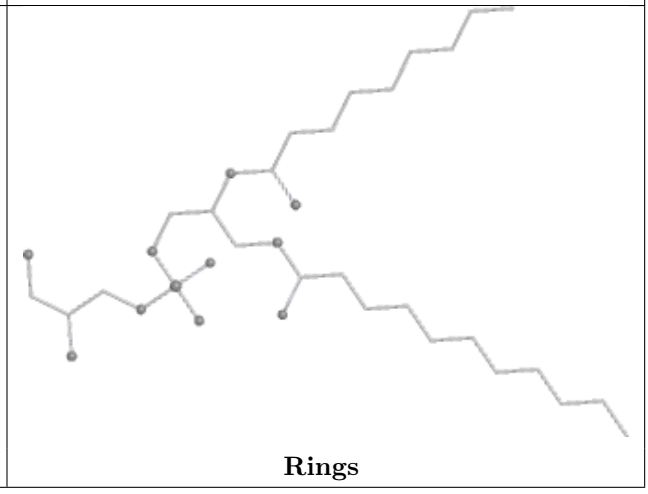
**Bond lengths**



**Bond angles**

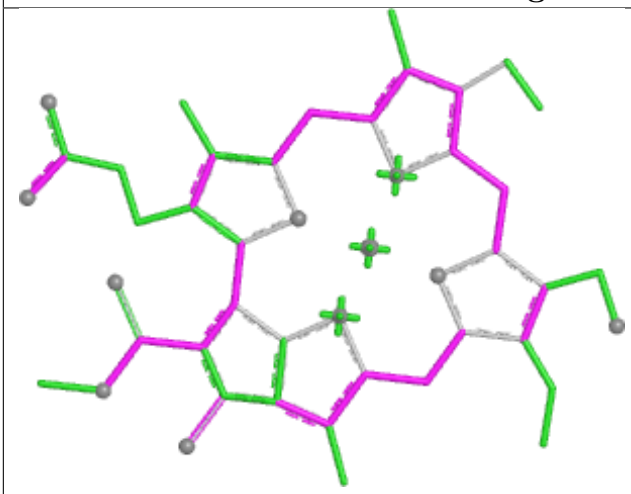


**Torsions**

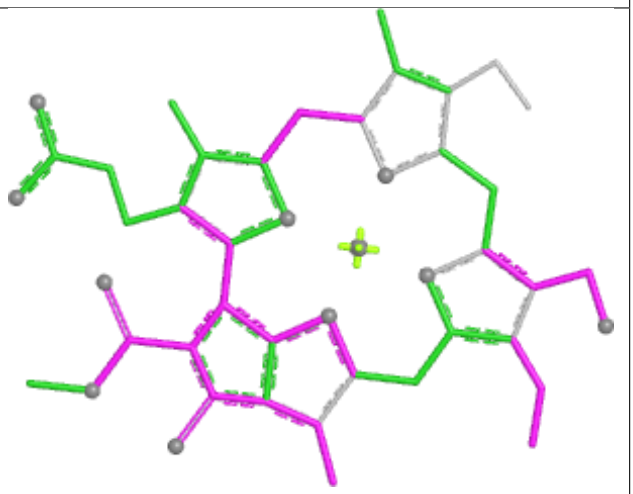


**Rings**

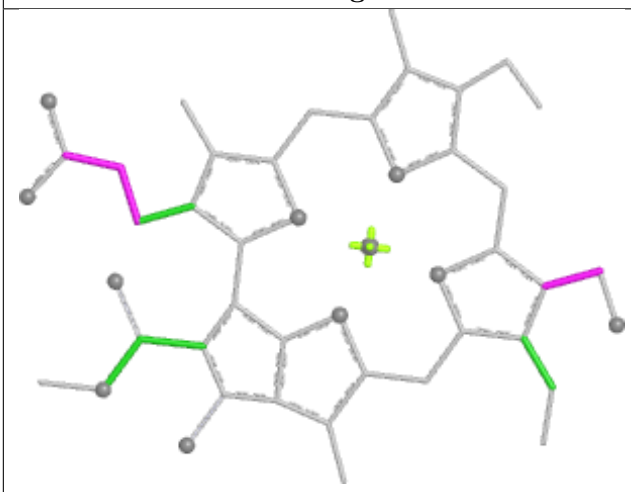
**Ligand CHL 5 601**



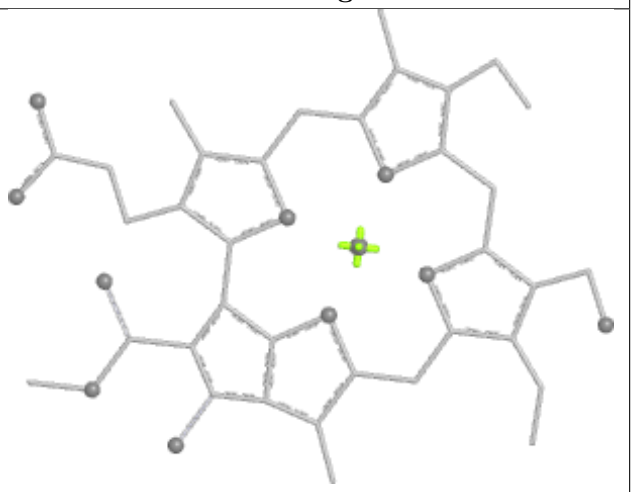
**Bond lengths**



**Bond angles**

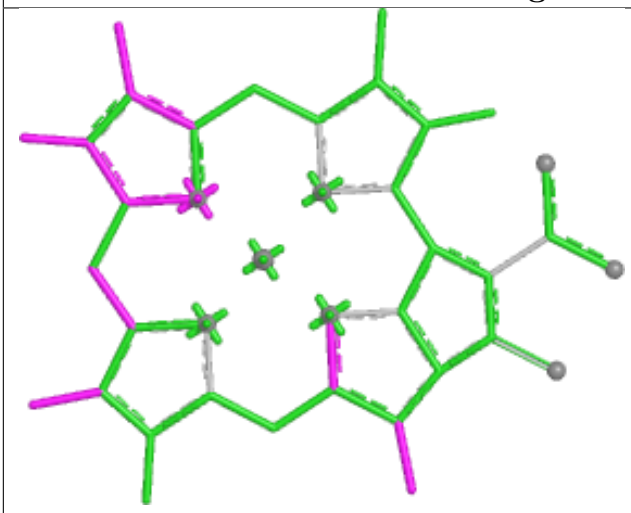


**Torsions**

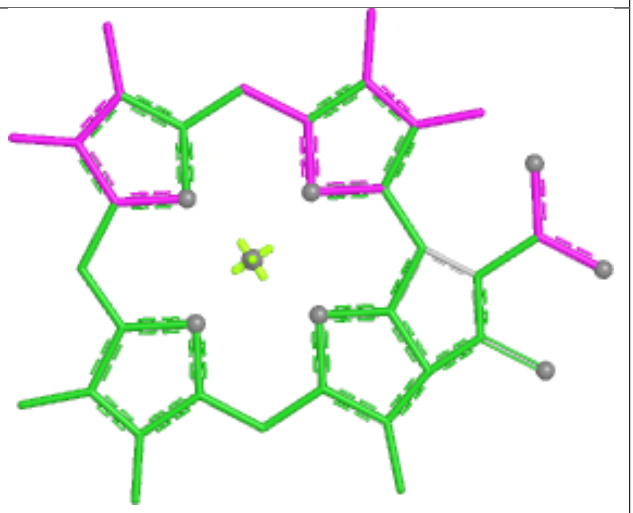


**Rings**

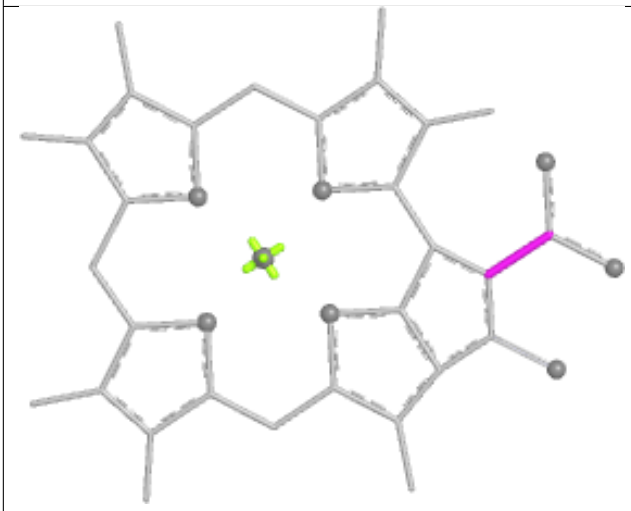
## Ligand CLA 1 311



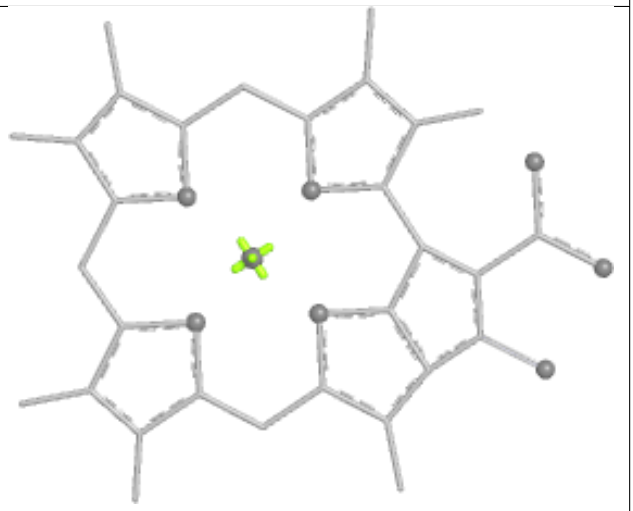
Bond lengths



Bond angles

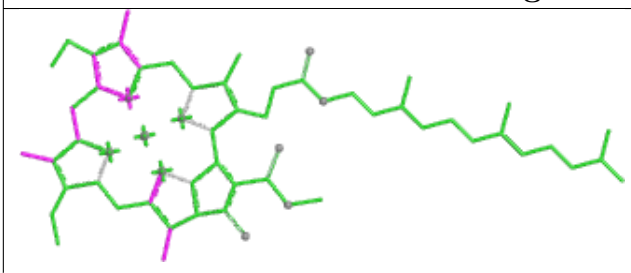


Torsions

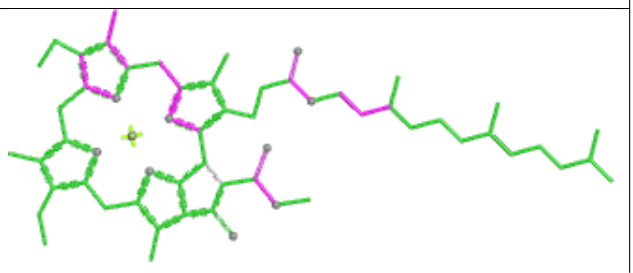


Rings

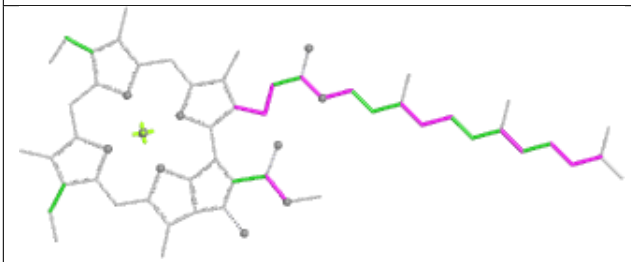
## Ligand CLA A 828



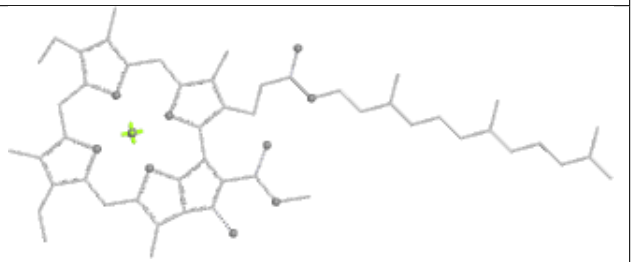
Bond lengths



Bond angles

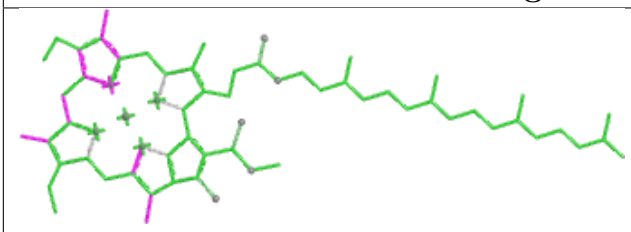


Torsions

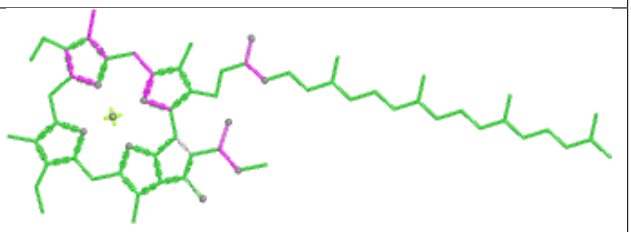


Rings

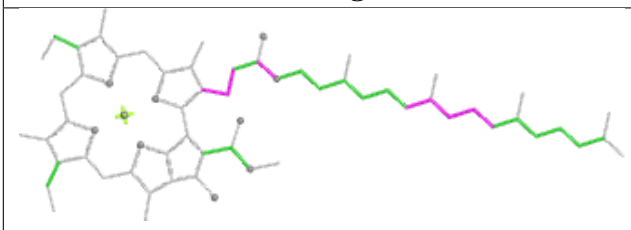
## Ligand CLA B 827



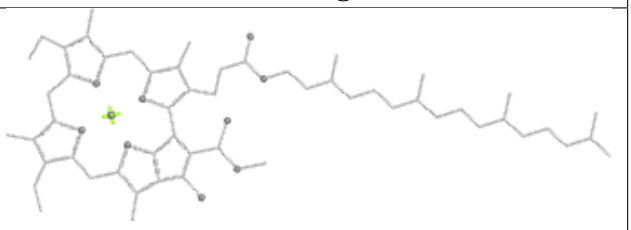
Bond lengths



Bond angles



Torsions



Rings

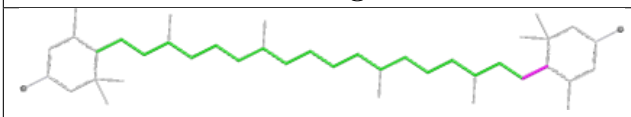
## Ligand LUT b 316



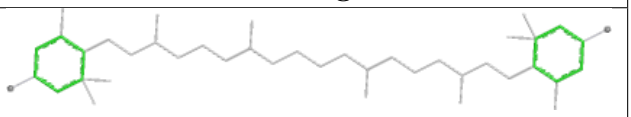
Bond lengths



Bond angles

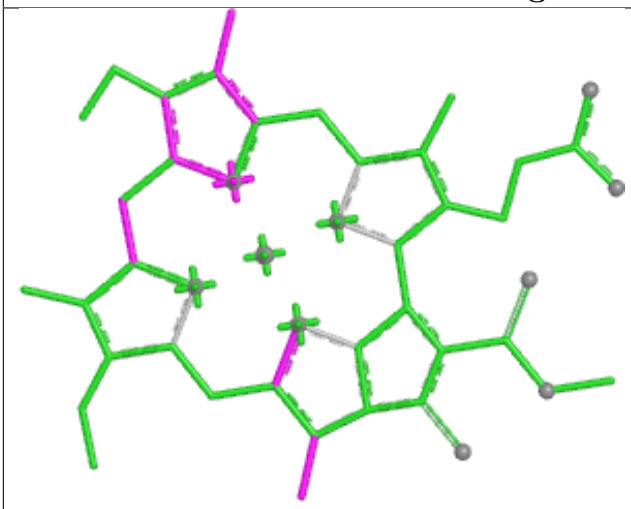


Torsions

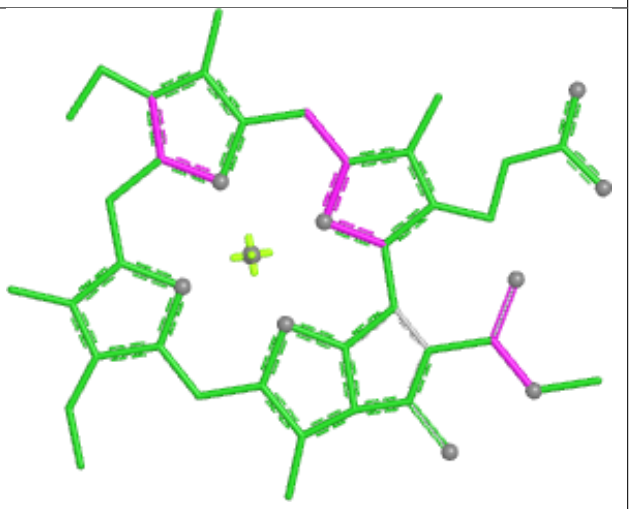


Rings

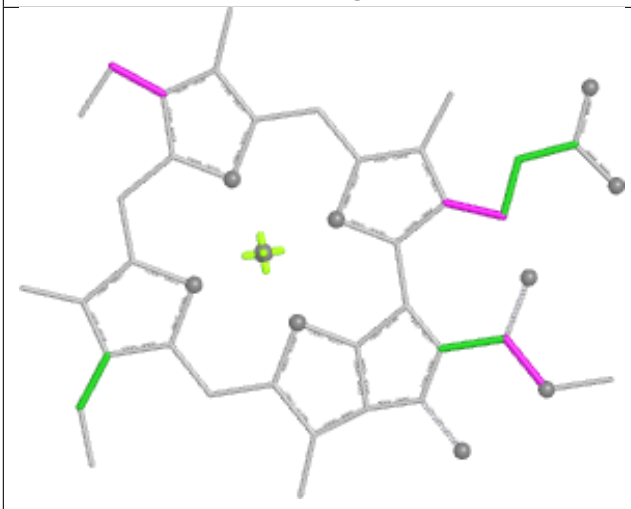
**Ligand CLA 5 612**



**Bond lengths**



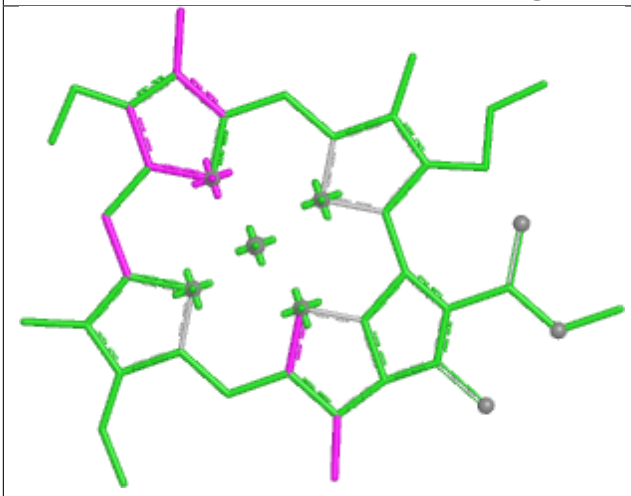
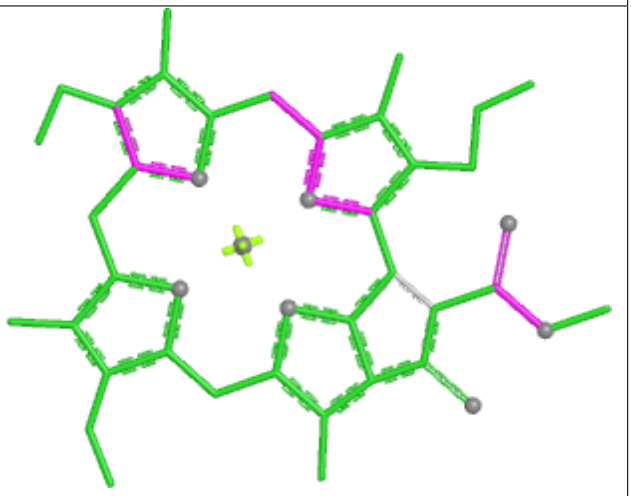
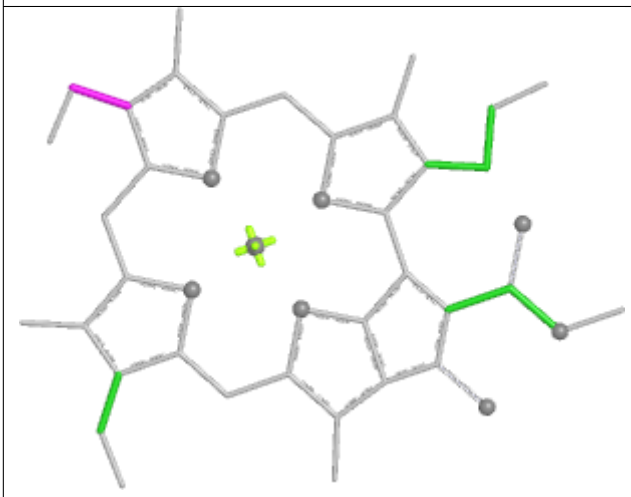
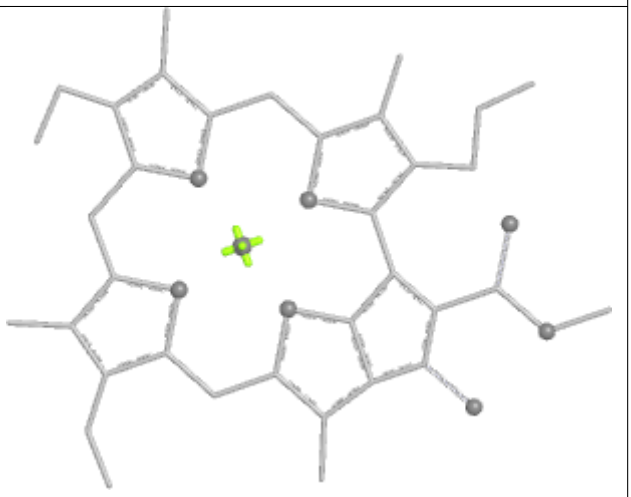
**Bond angles**

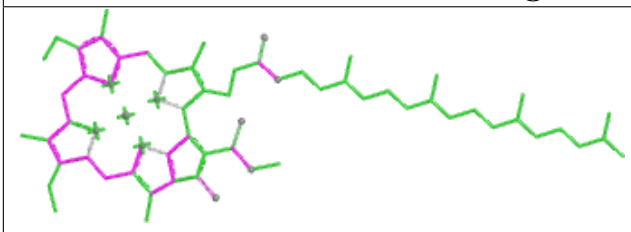
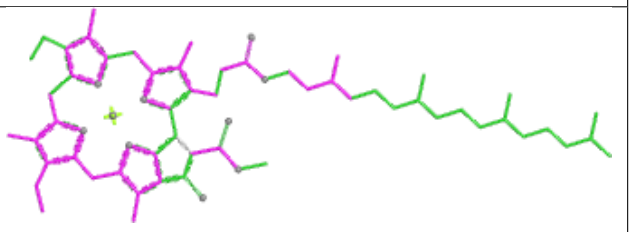
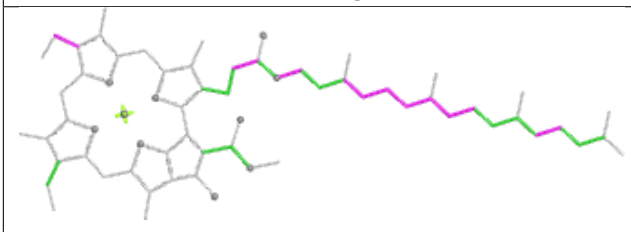
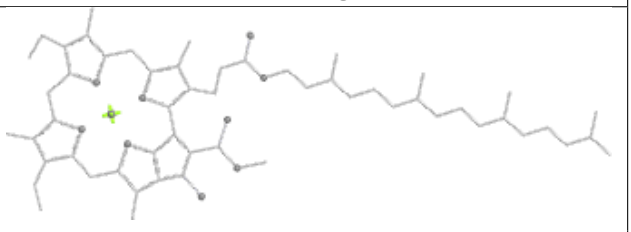


**Torsions**

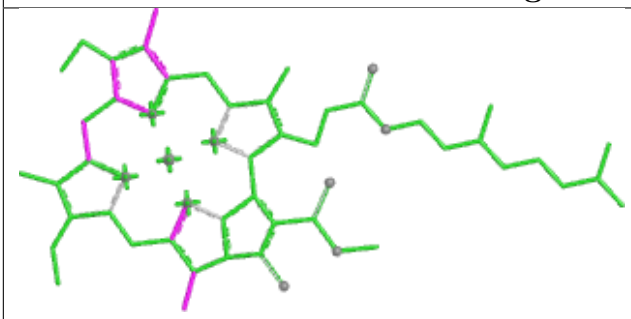


**Rings**

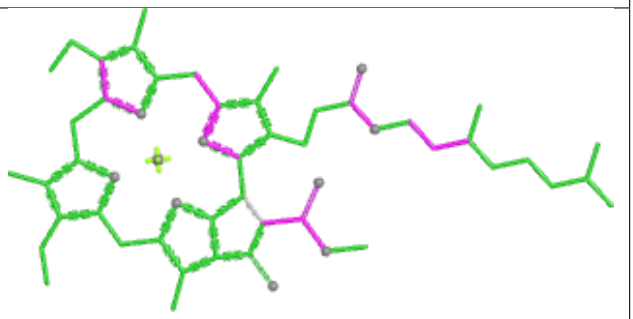
| Ligand CLA 4 613 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA B 801 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

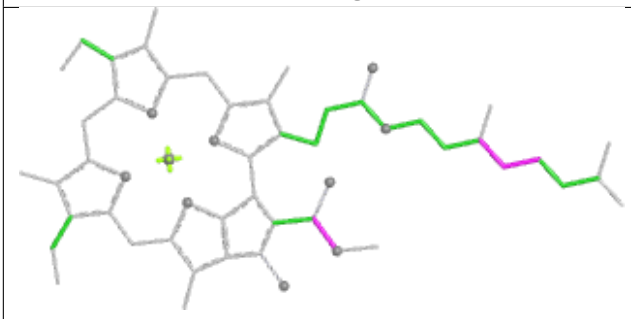
**Ligand CLA B 821**



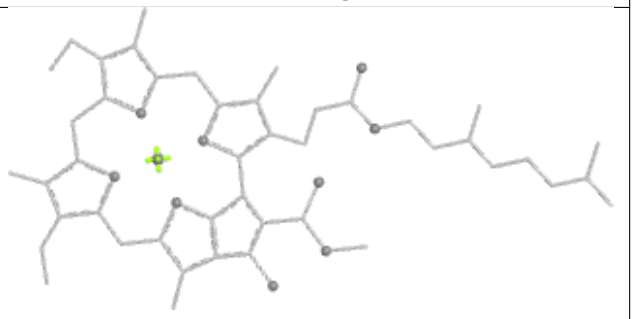
**Bond lengths**



**Bond angles**

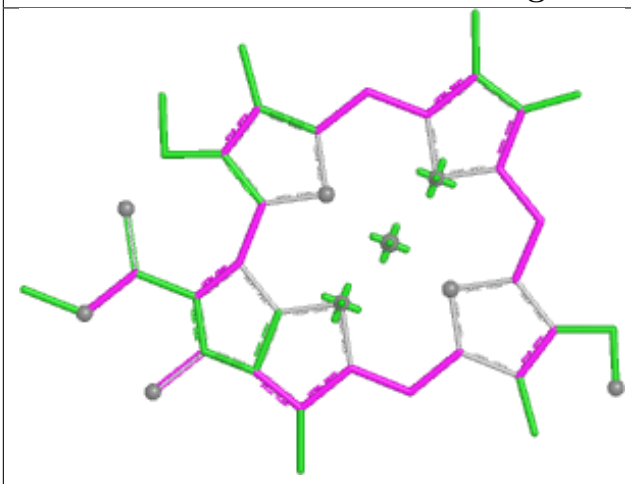


**Torsions**

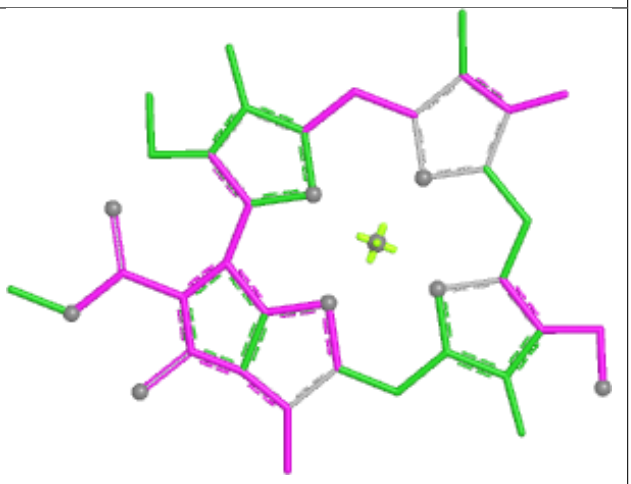


**Rings**

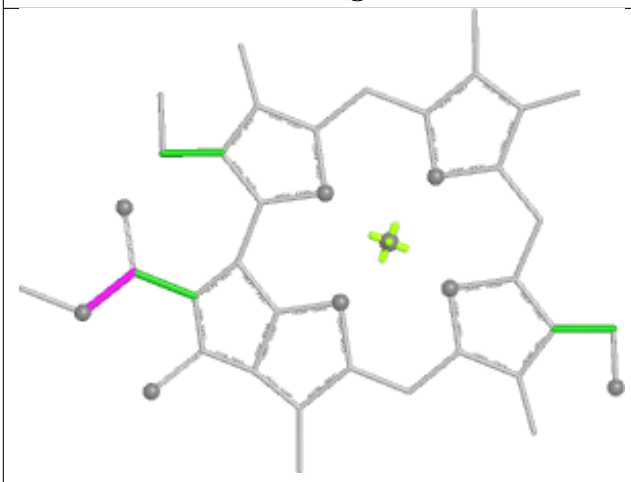
**Ligand CHL 8 605**



**Bond lengths**



**Bond angles**

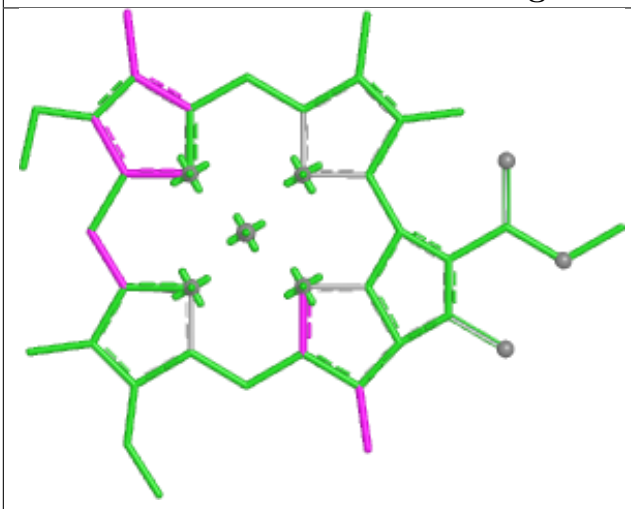


**Torsions**

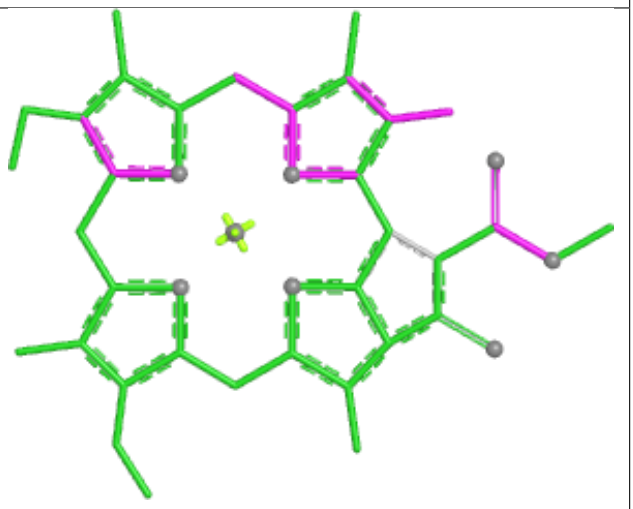


**Rings**

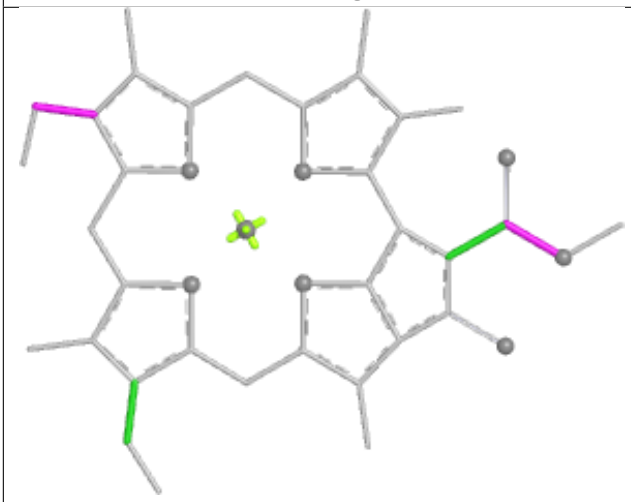
## Ligand CLA 7 408



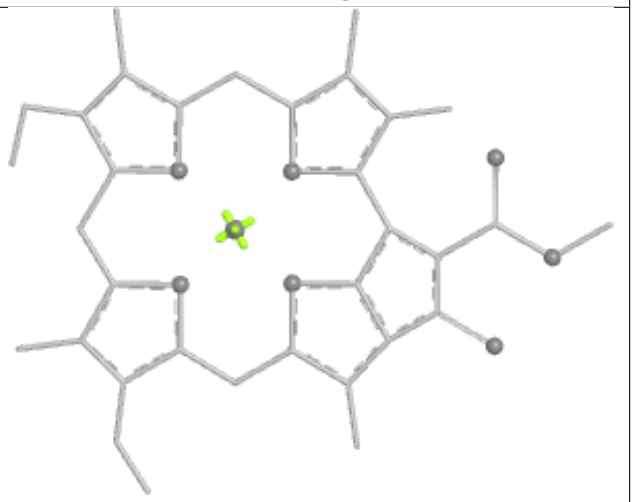
Bond lengths



Bond angles

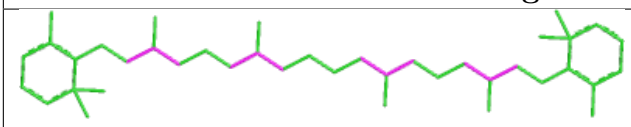


Torsions

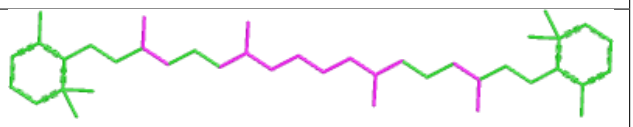


Rings

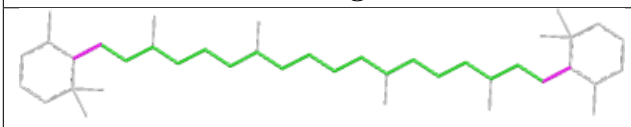
## Ligand BCR A 846



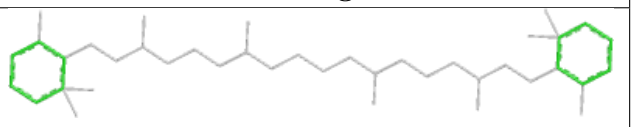
Bond lengths



Bond angles

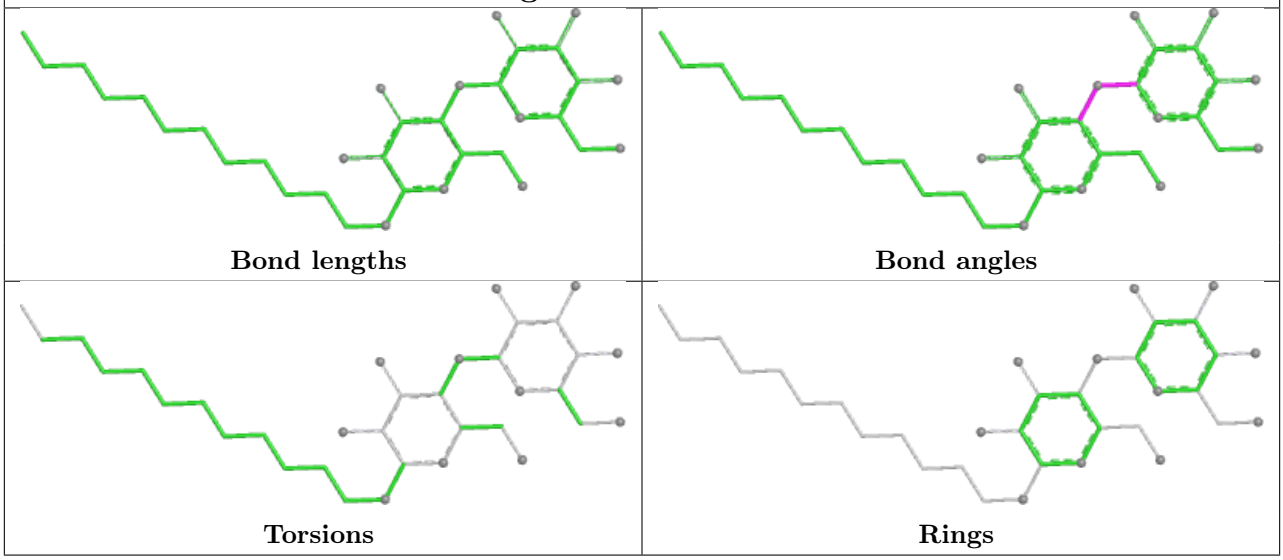


Torsions

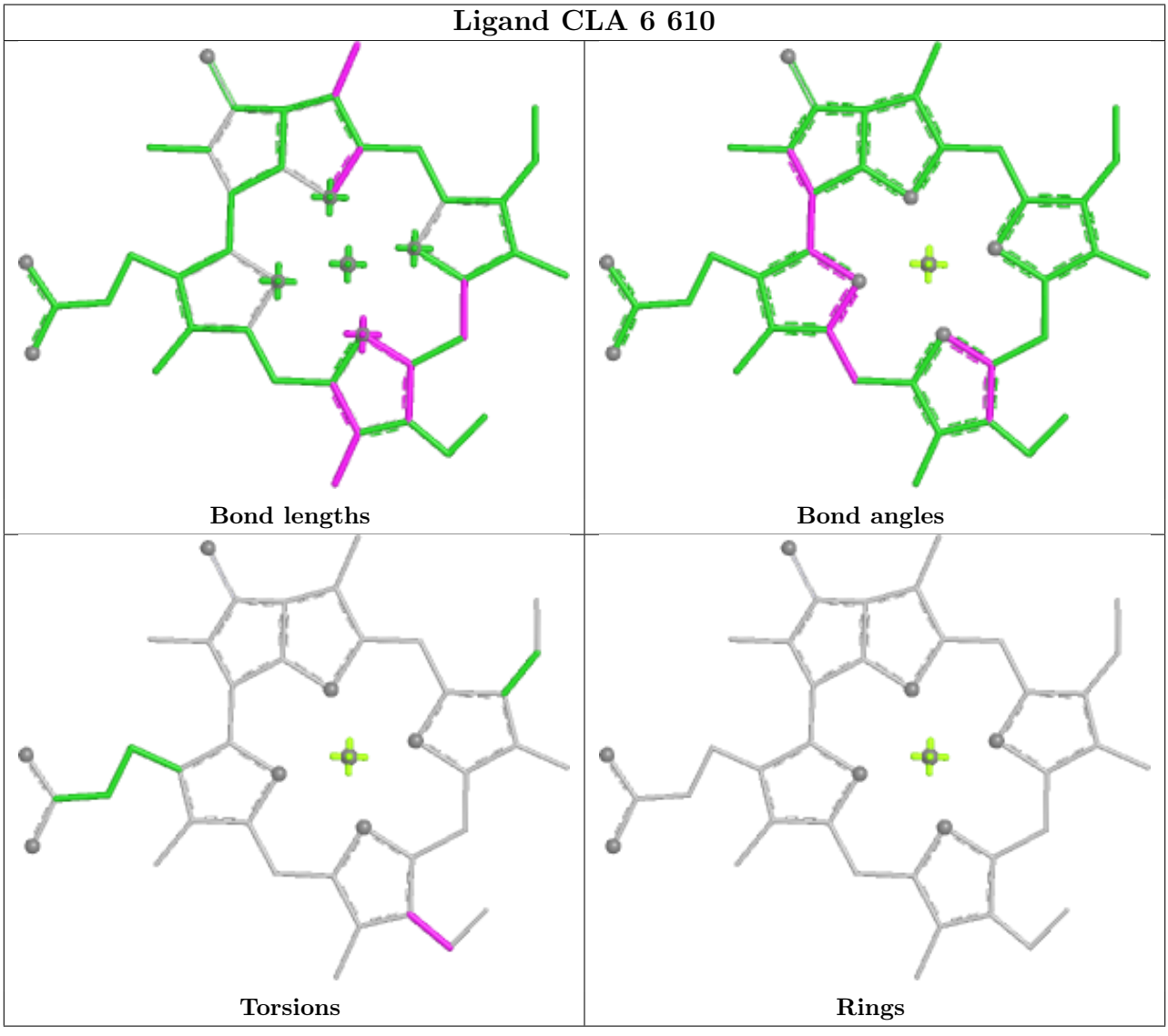


Rings

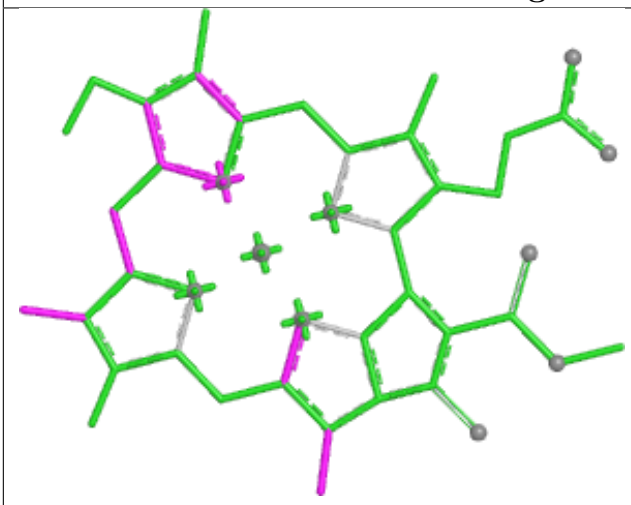
## Ligand LMU A 853



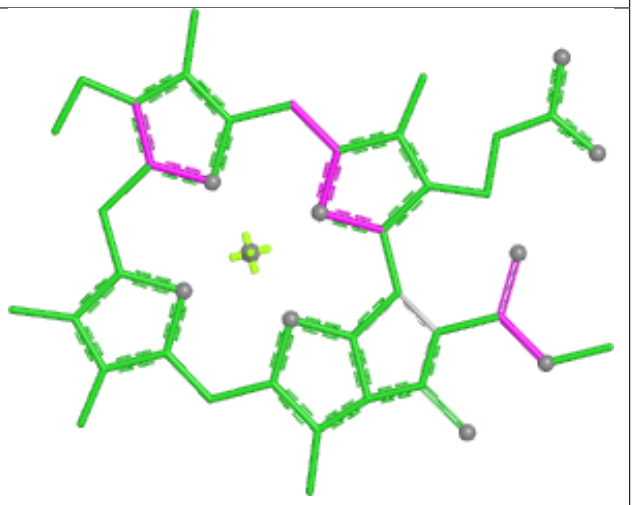

## Ligand CLA 6 610



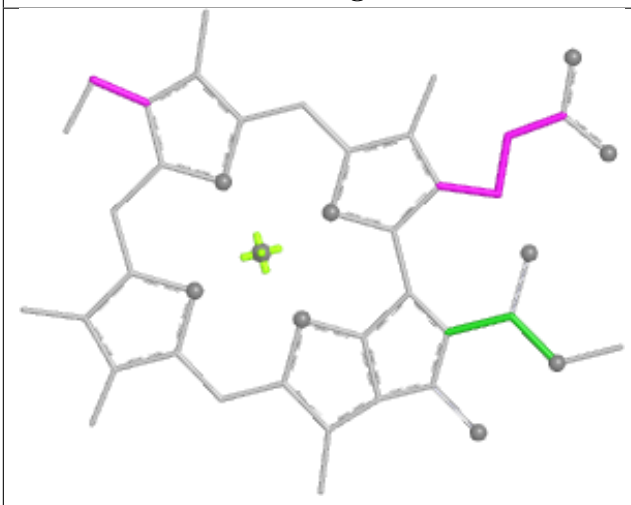
**Ligand CLA 8 610**



**Bond lengths**



**Bond angles**

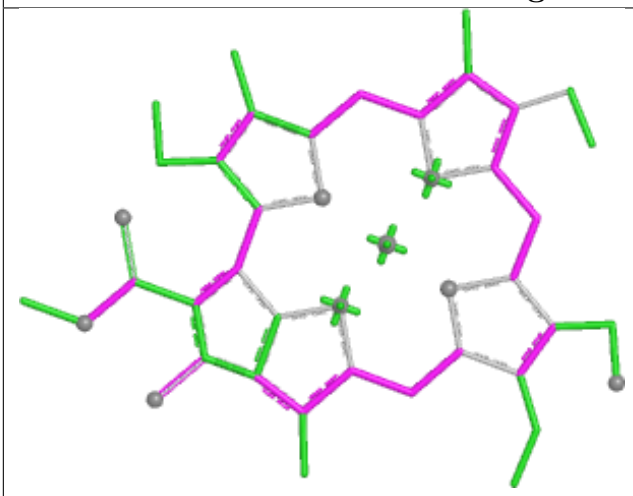


**Torsions**

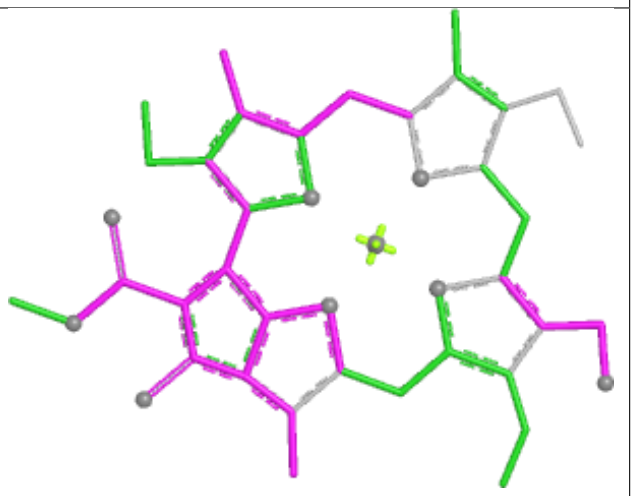


**Rings**

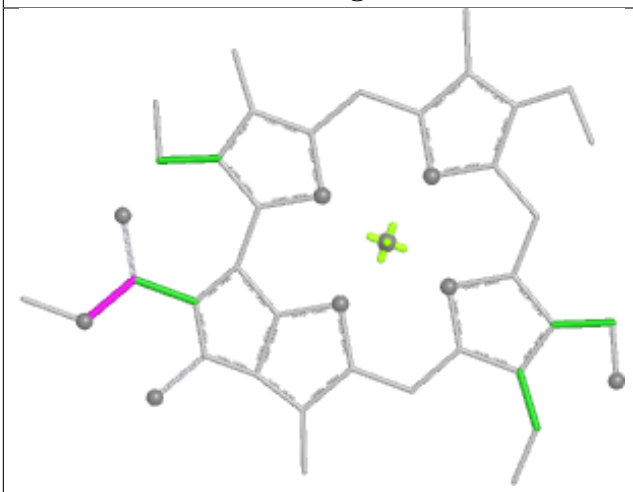
## Ligand CHL 9 601



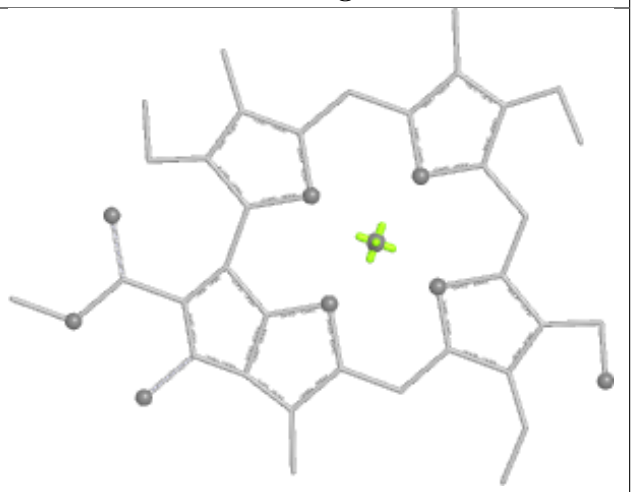
Bond lengths



Bond angles

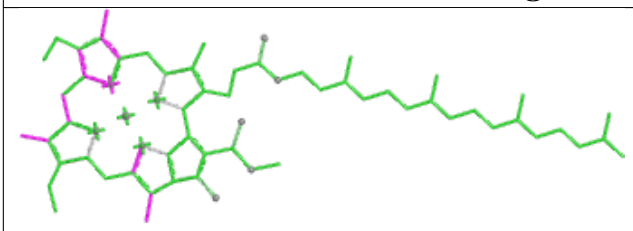


Torsions

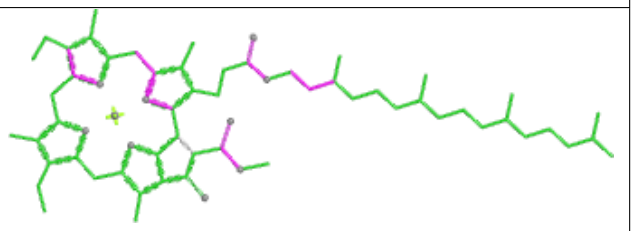


Rings

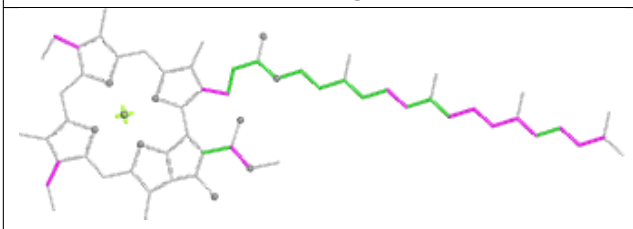
## Ligand CLA B 812



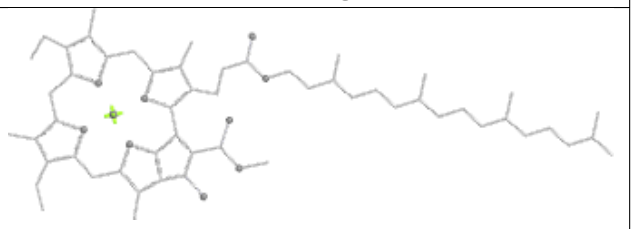
Bond lengths



Bond angles

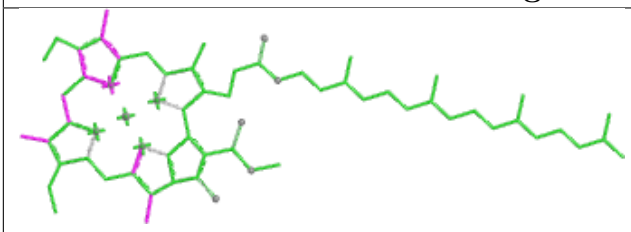


Torsions

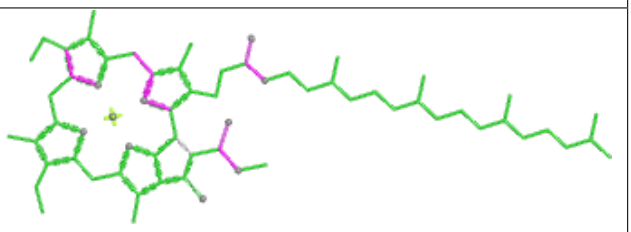


Rings

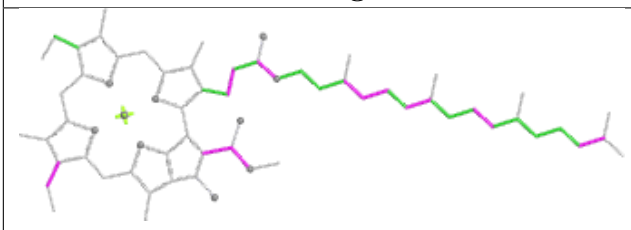
## Ligand CLA A 817



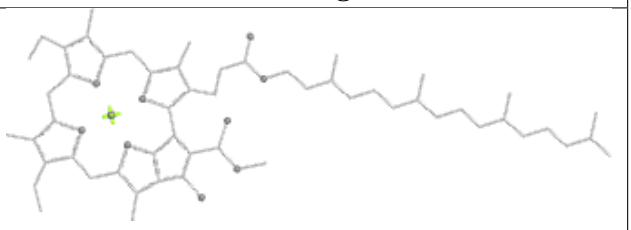
Bond lengths



Bond angles

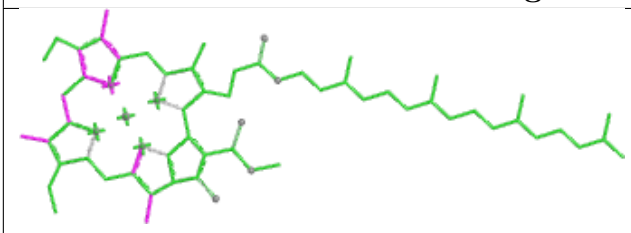


Torsions

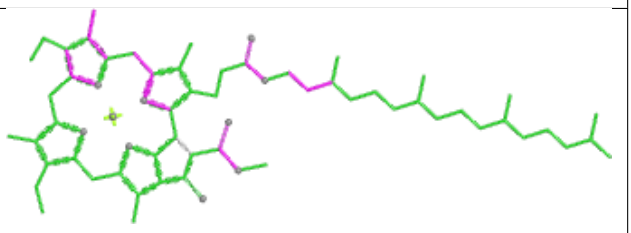


Rings

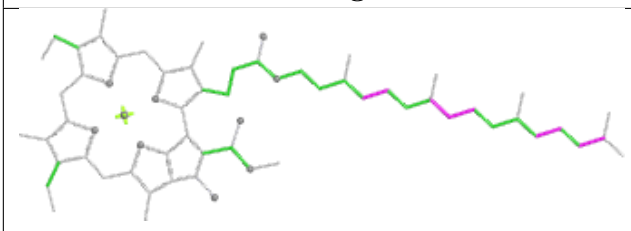
## Ligand CLA B 808



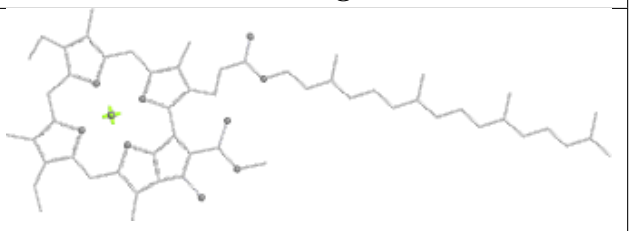
Bond lengths



Bond angles

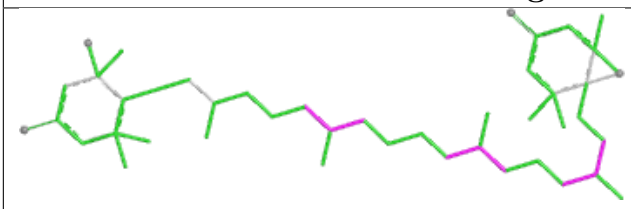


Torsions

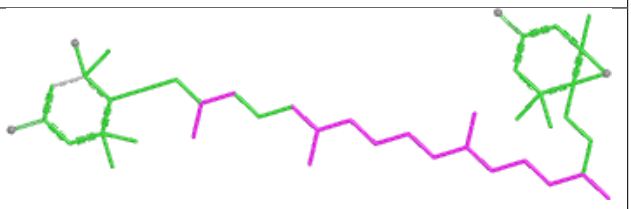


Rings

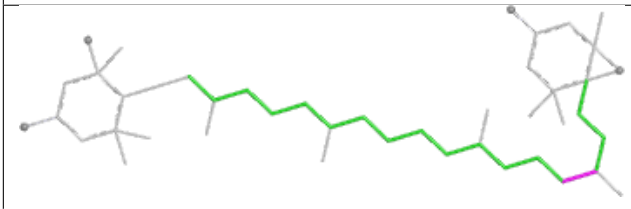
## Ligand NEX c 618



Bond lengths



Bond angles

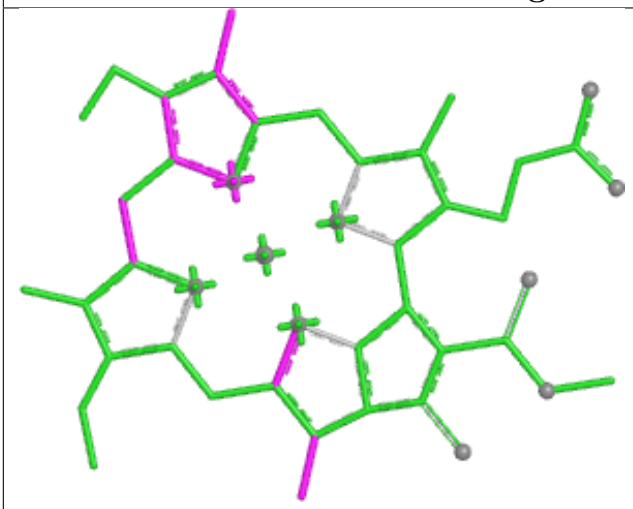


Torsions

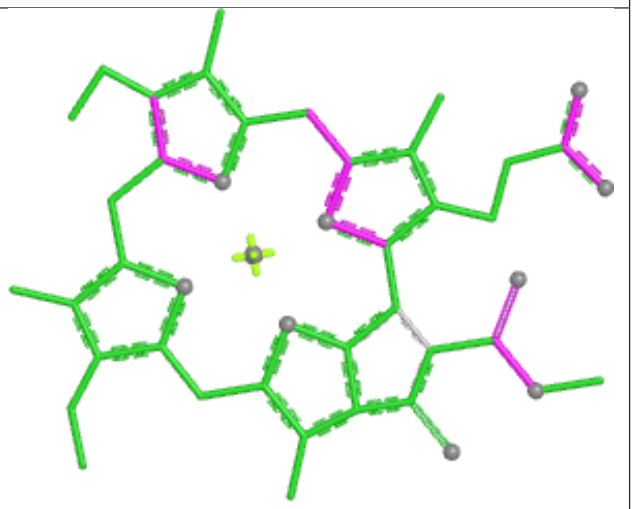


Rings

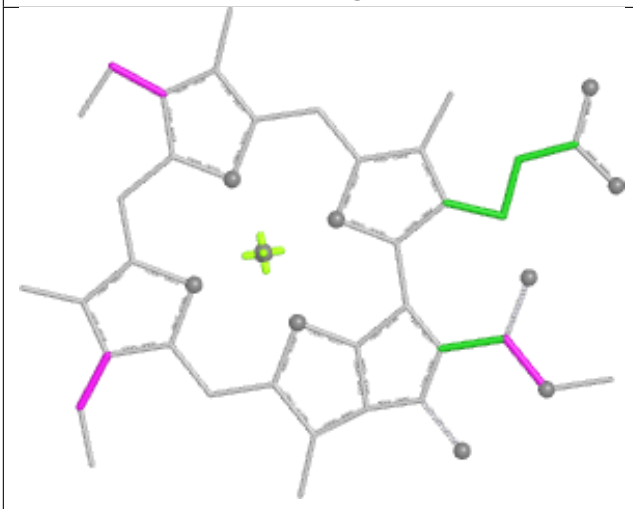
## Ligand CLA 1 315



Bond lengths



Bond angles

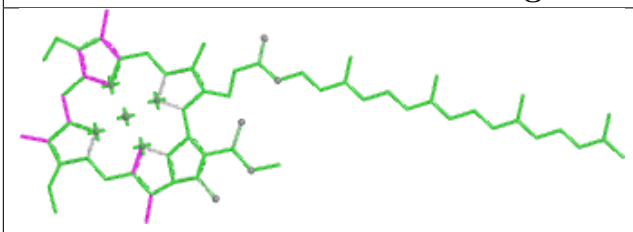


Torsions

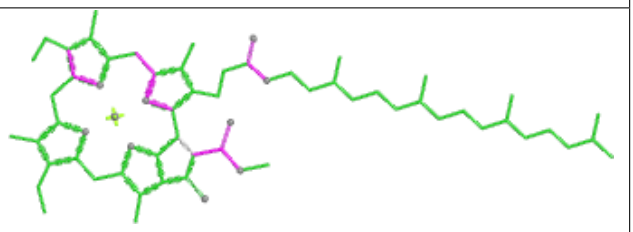


Rings

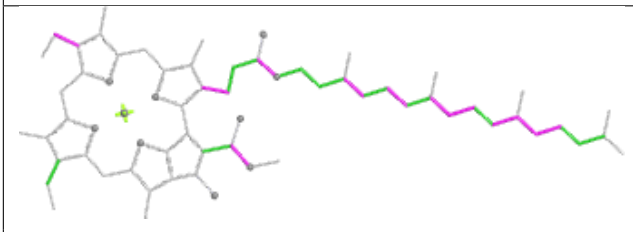
## Ligand CLA B 802



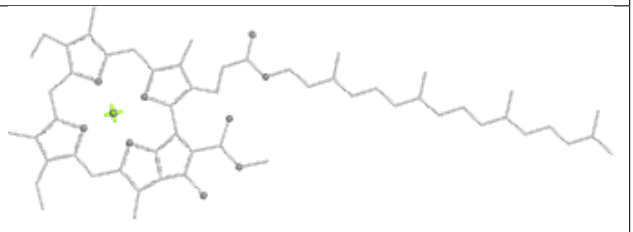
Bond lengths



Bond angles

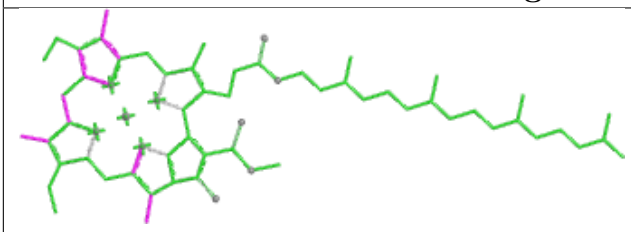


Torsions

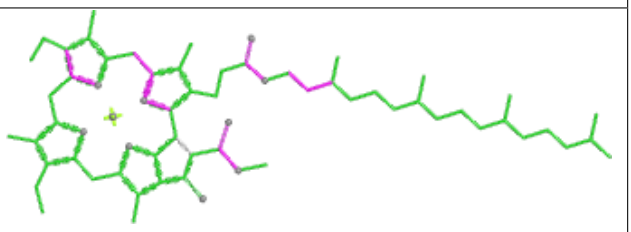


Rings

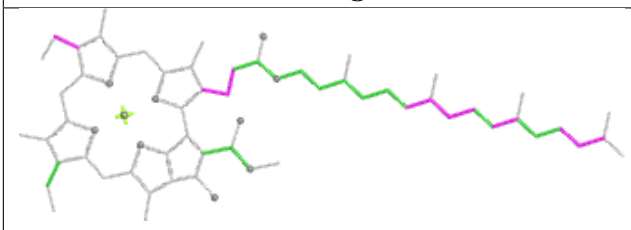
## Ligand CLA B 804



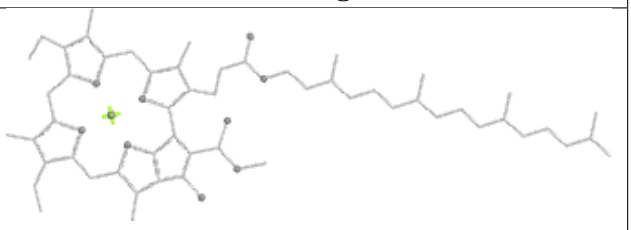
Bond lengths



Bond angles

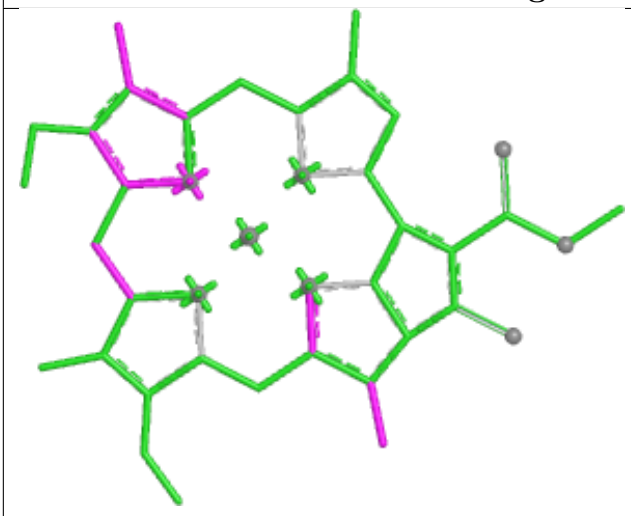


Torsions

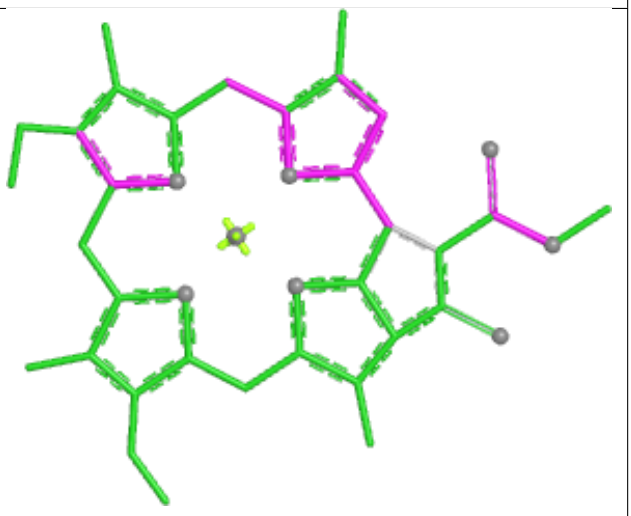


Rings

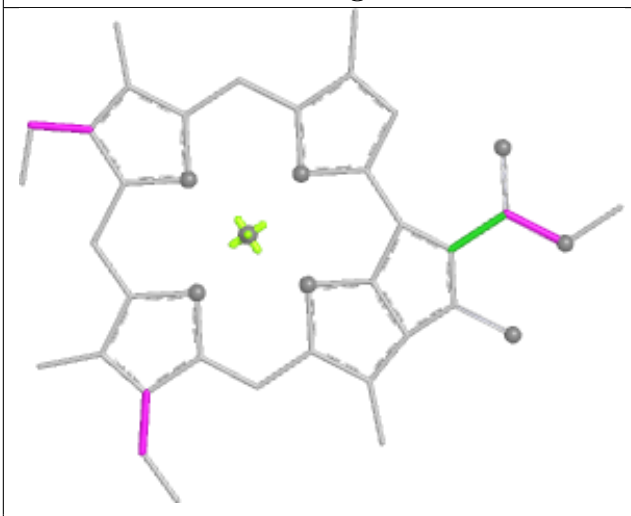
## Ligand CLA 5 605



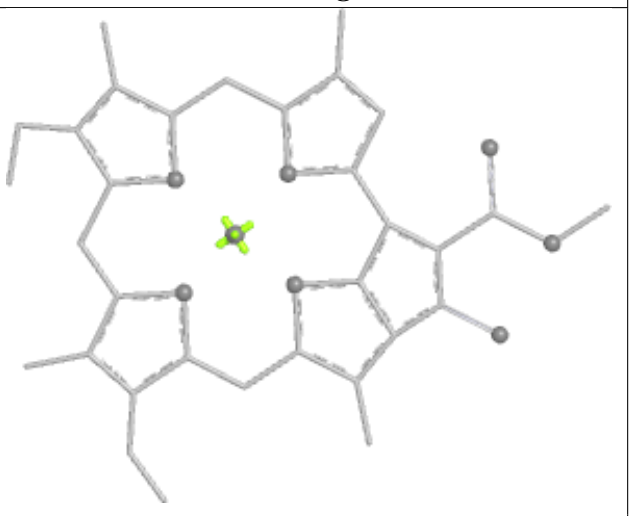
Bond lengths



Bond angles

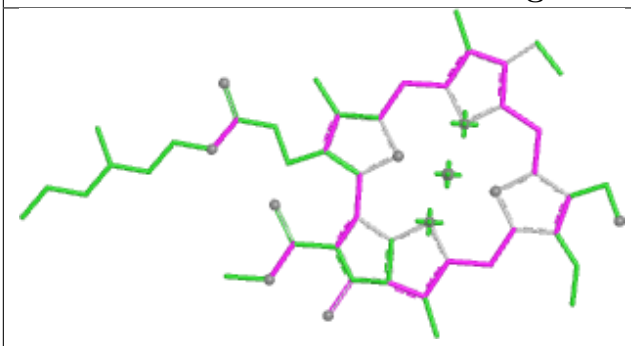


Torsions

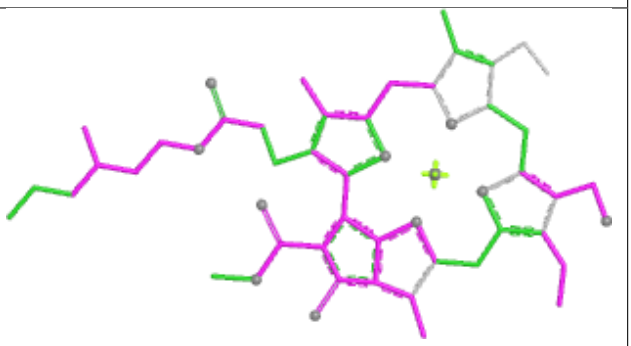


Rings

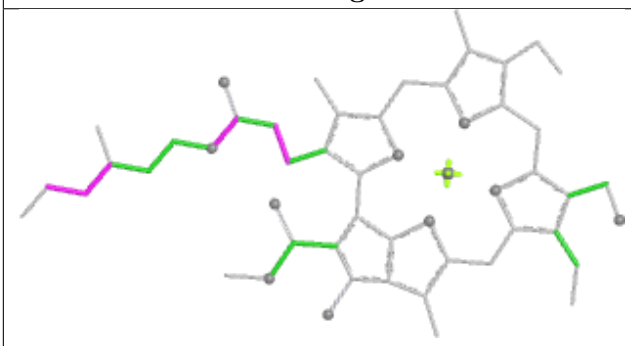
## Ligand CHL b 308



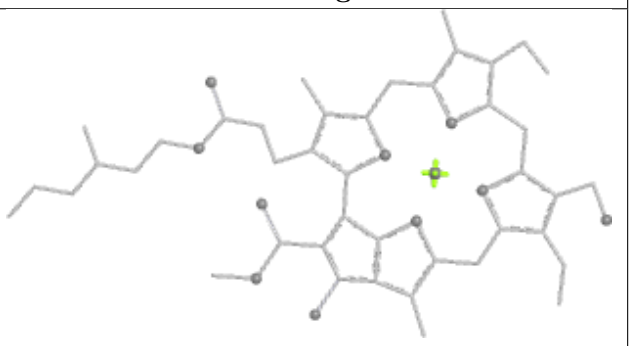
Bond lengths



Bond angles

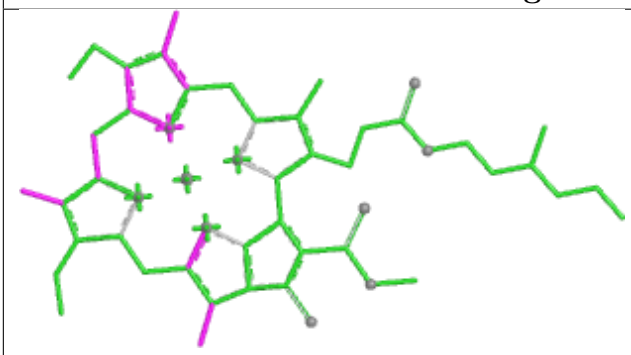


Torsions

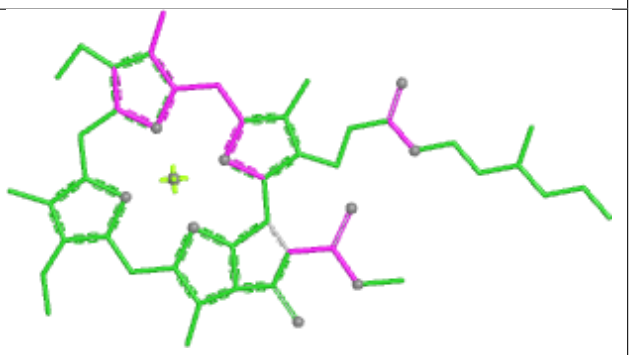


Rings

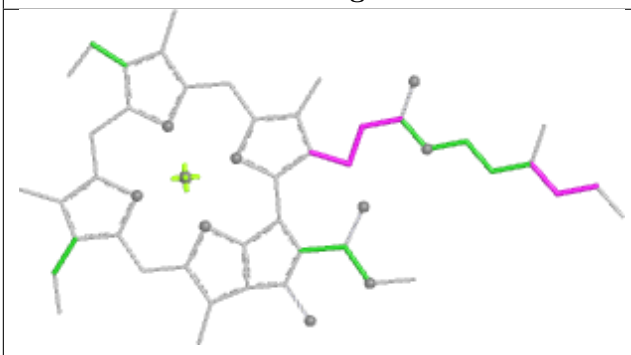
## Ligand CLA A 818



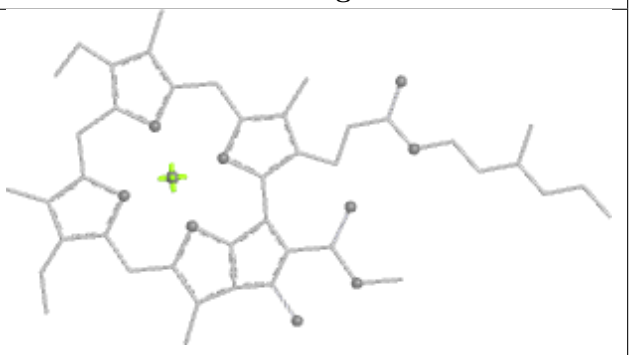
Bond lengths



Bond angles

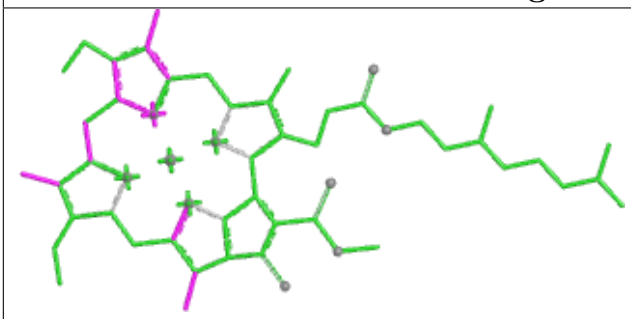


Torsions

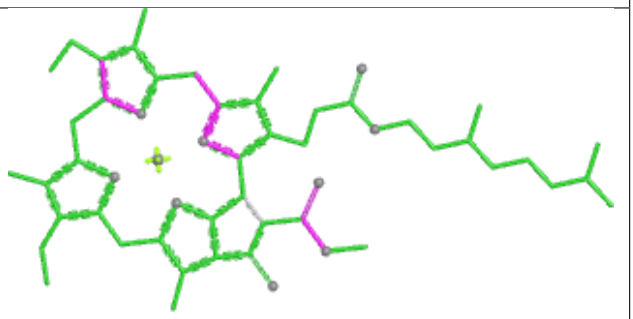


Rings

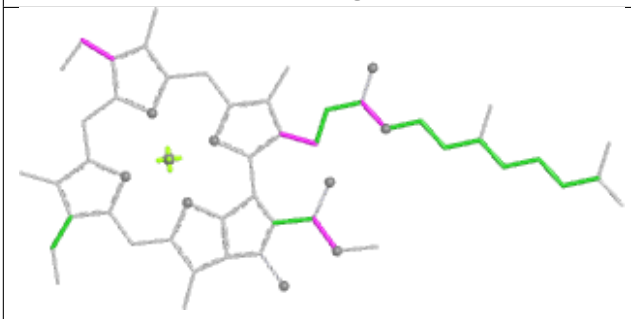
**Ligand CLA 3 403**



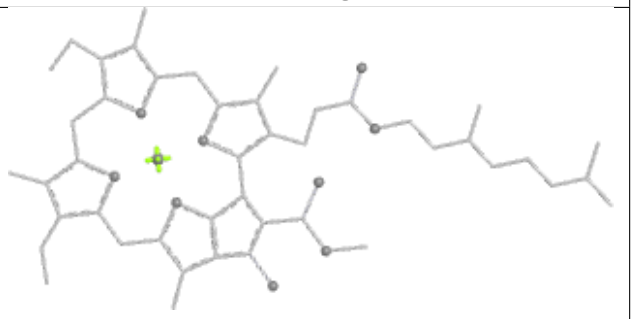
**Bond lengths**



**Bond angles**

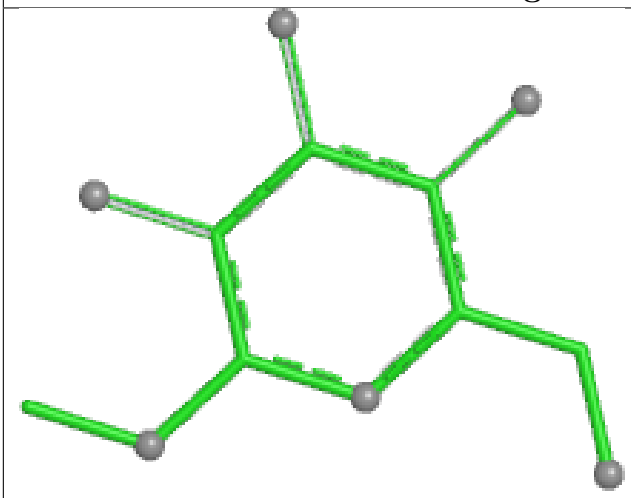


**Torsions**

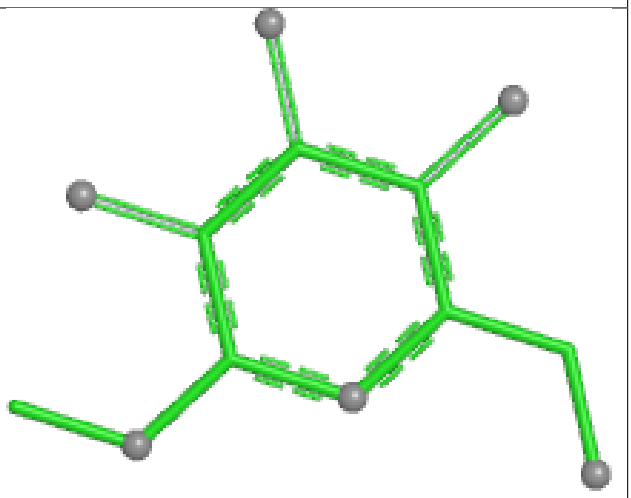


**Rings**

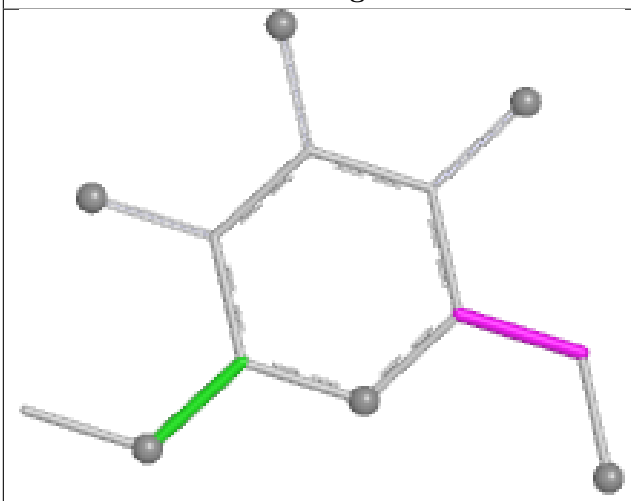
**Ligand LMG 2 615**



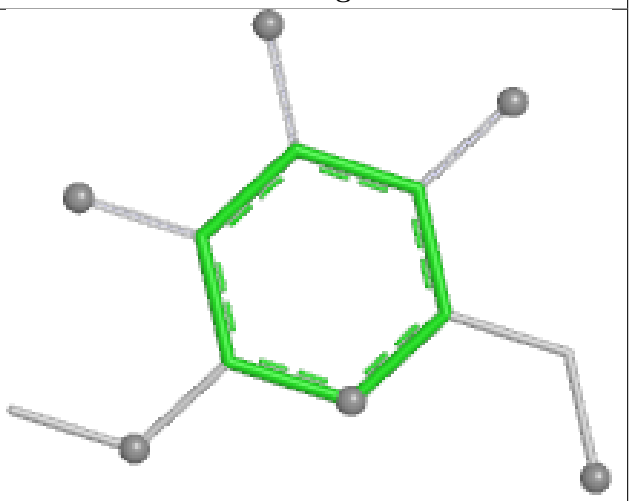
Bond lengths



Bond angles

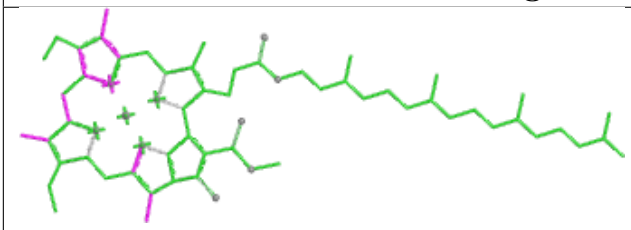


Torsions

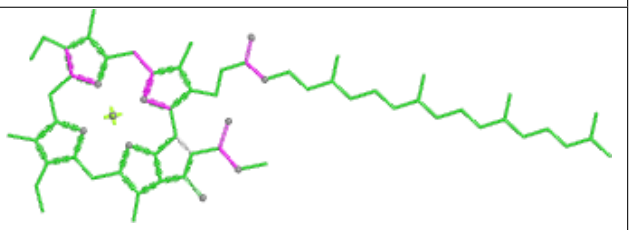


Rings

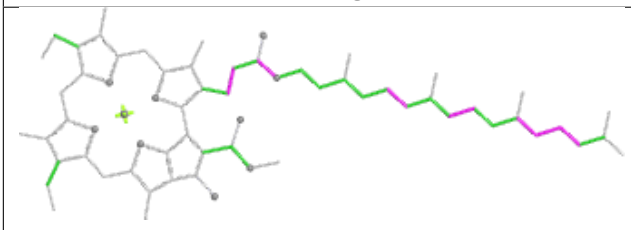
**Ligand CLA A 829**



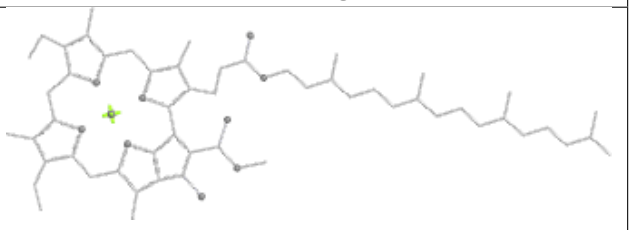
Bond lengths



Bond angles

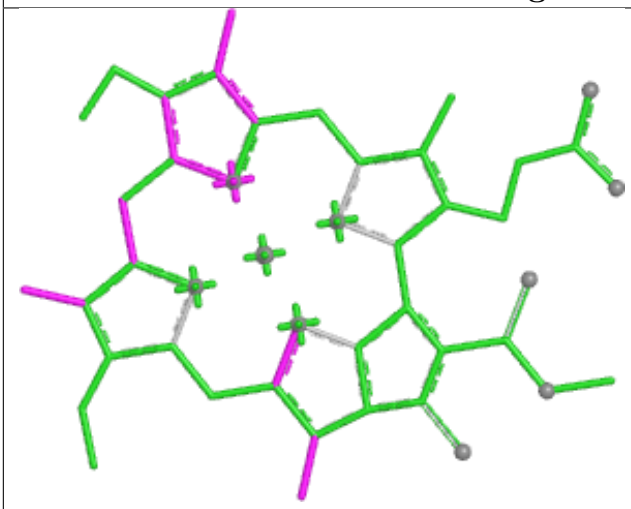


Torsions

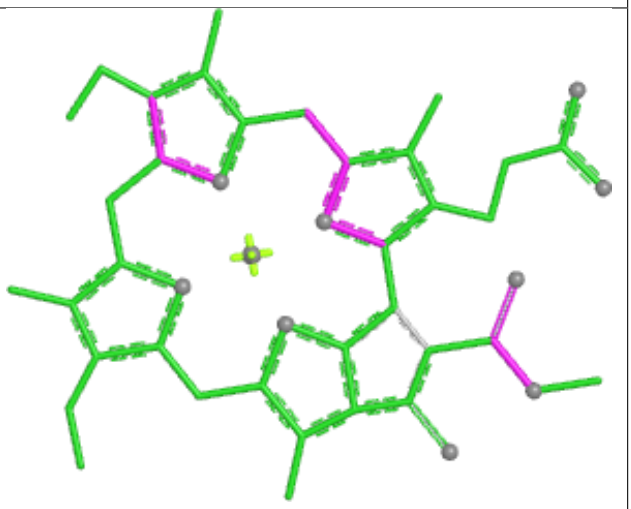


Rings

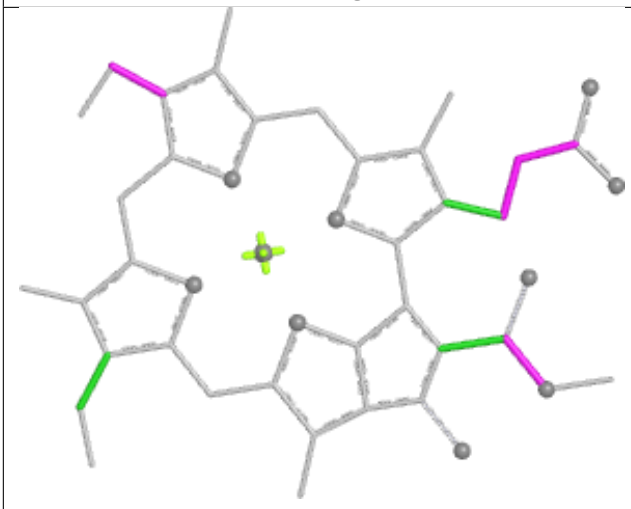
## Ligand CLA 2 603



Bond lengths



Bond angles

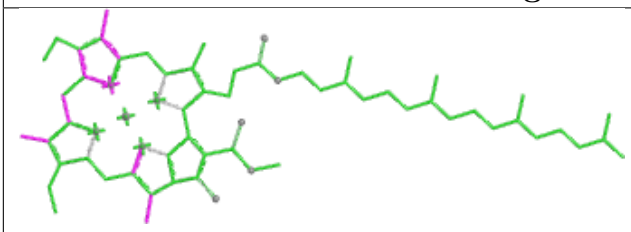


Torsions

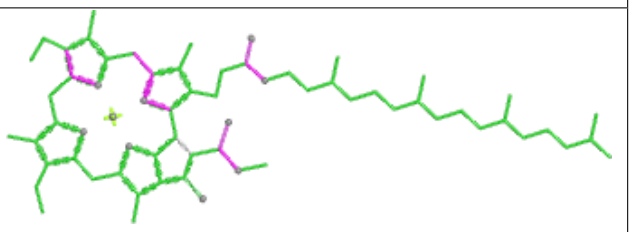


Rings

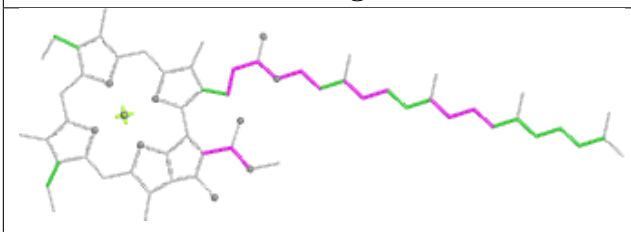
## Ligand CLA A 806



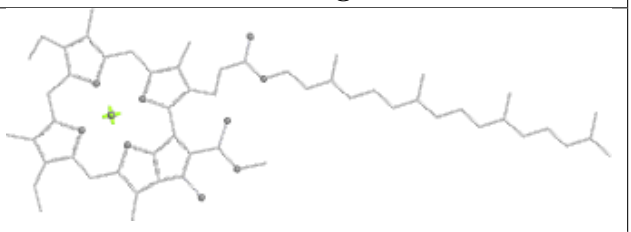
Bond lengths



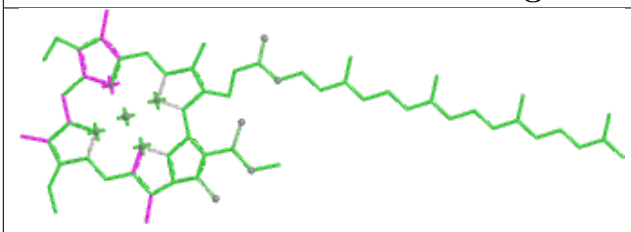
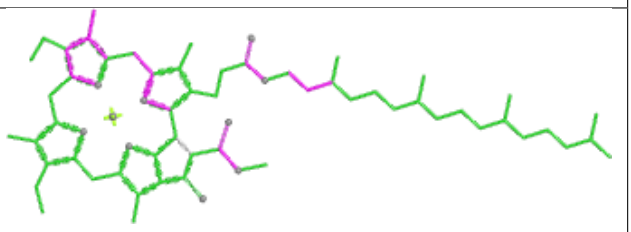
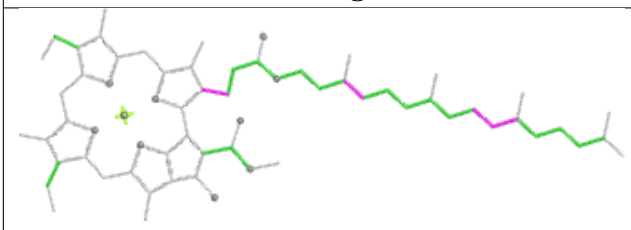
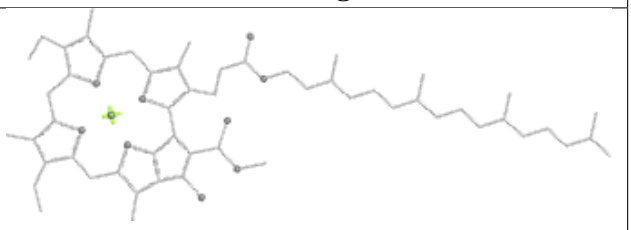
Bond angles

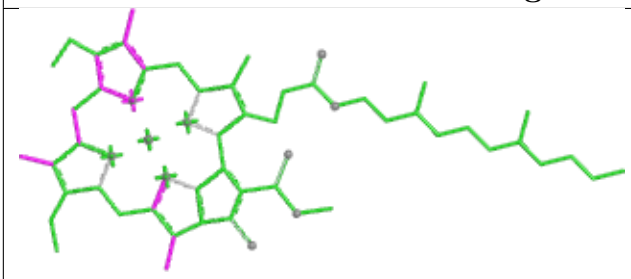
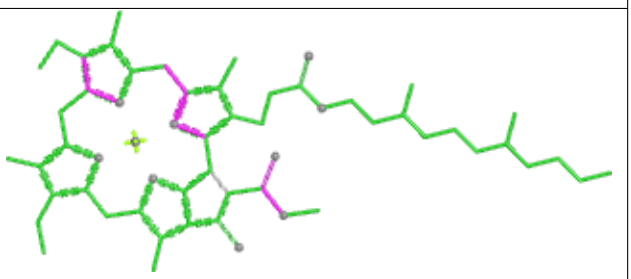
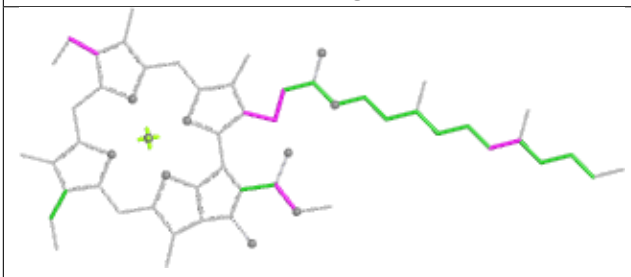
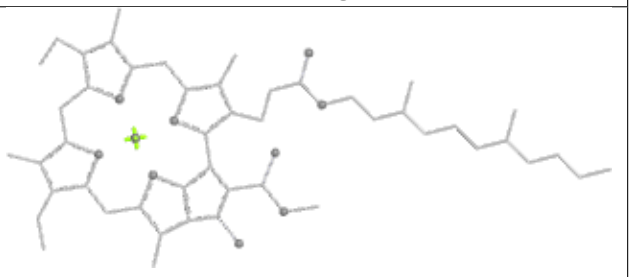


Torsions

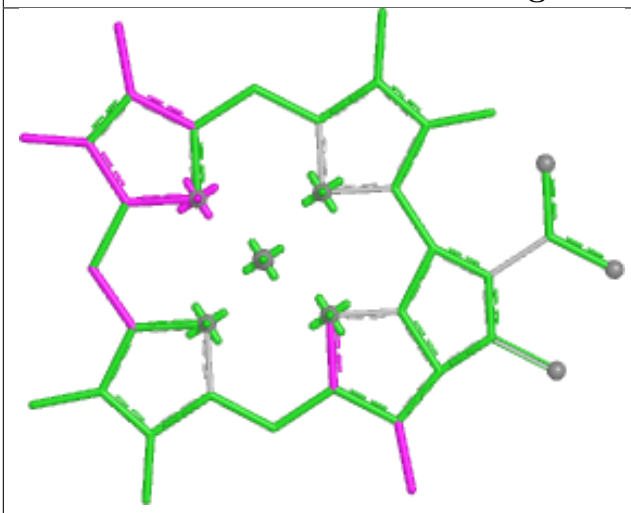


Rings

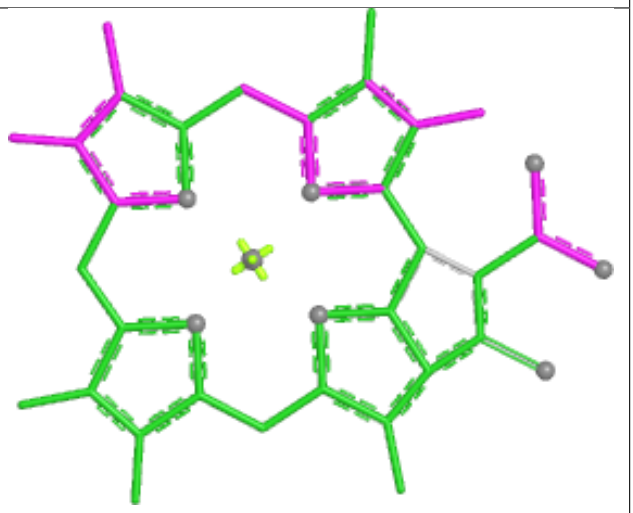
| Ligand CLA B 835 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA B 818 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

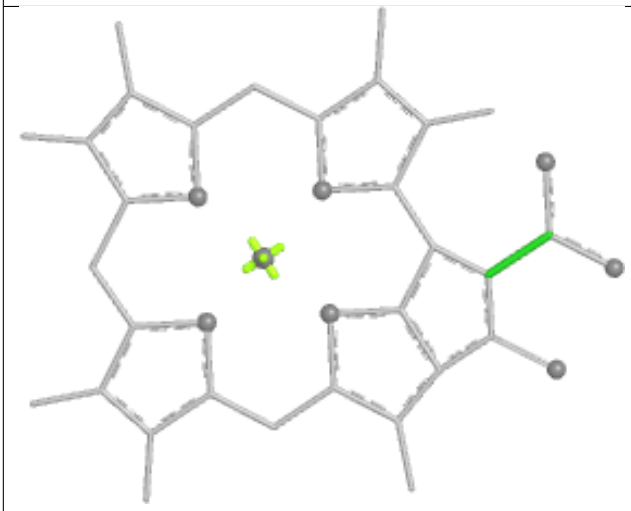
## Ligand CLA 5 610



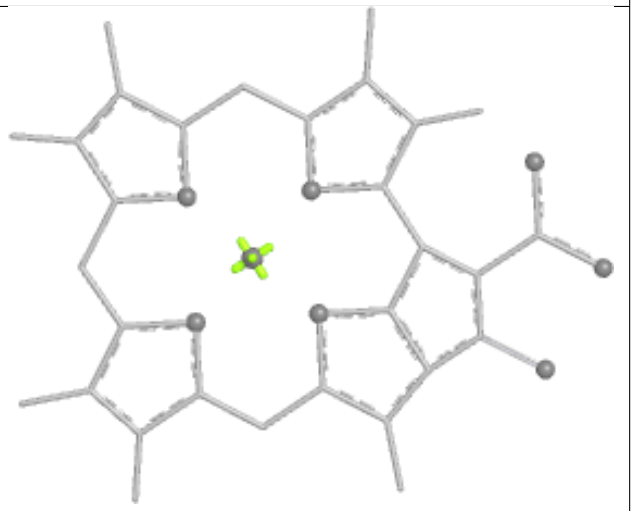
Bond lengths



Bond angles

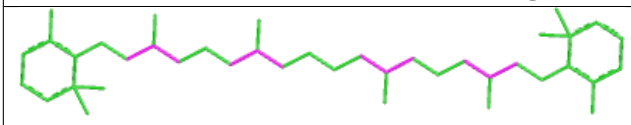


Torsions

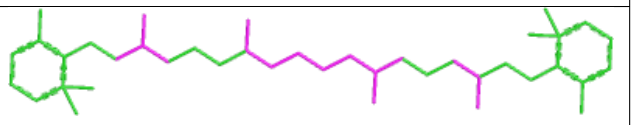


Rings

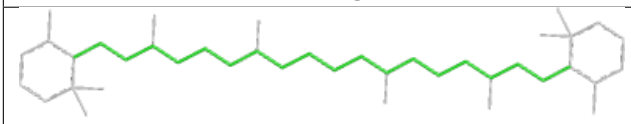
## Ligand BCR F 301



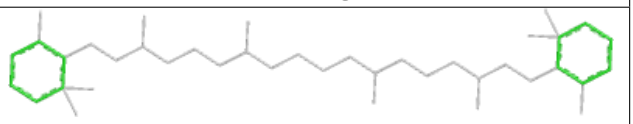
Bond lengths



Bond angles

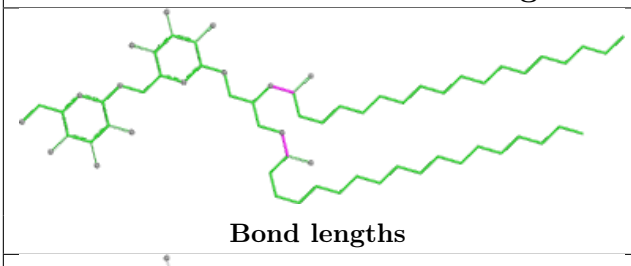


Torsions

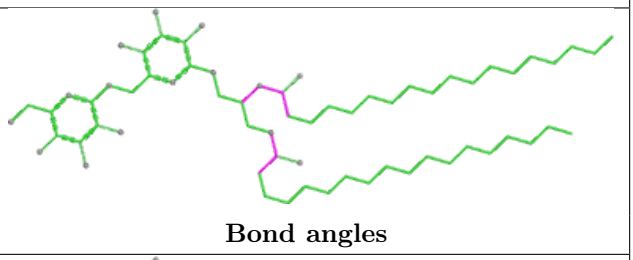


Rings

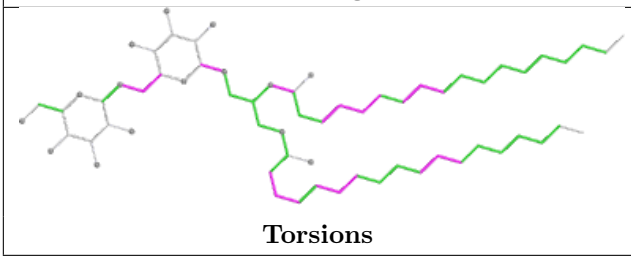
## Ligand DGD B 847



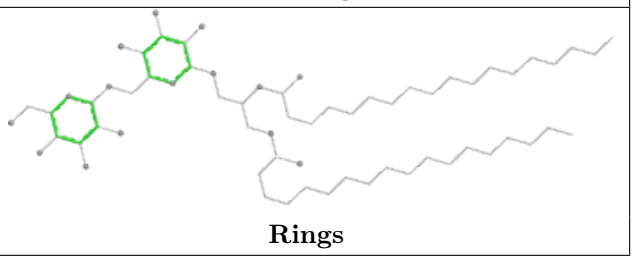
Bond lengths



Bond angles

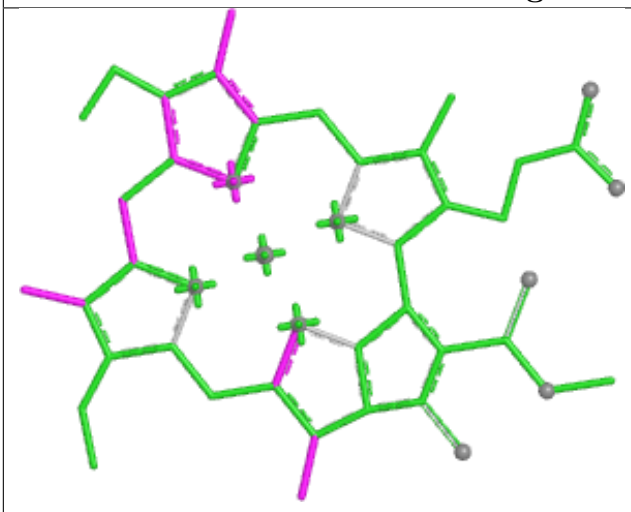


Torsions

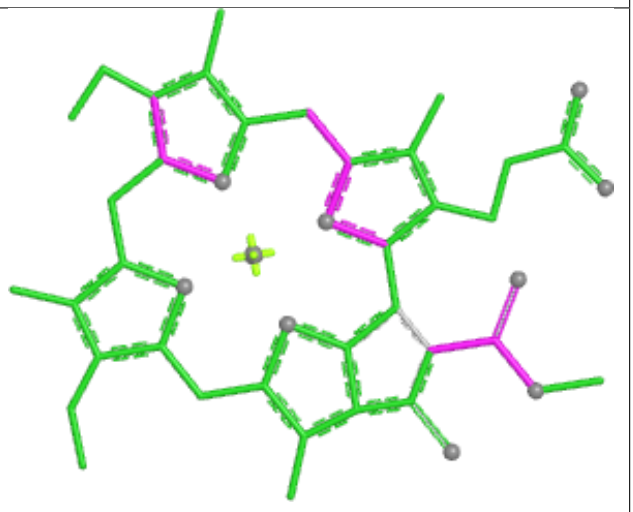


Rings

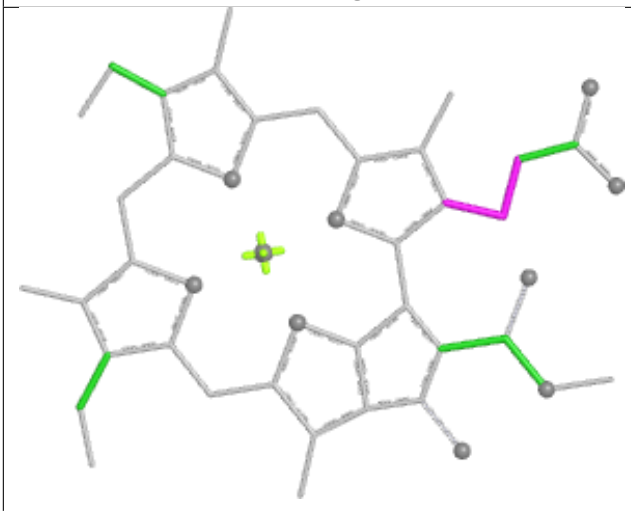
## Ligand CLA L 303



Bond lengths



Bond angles

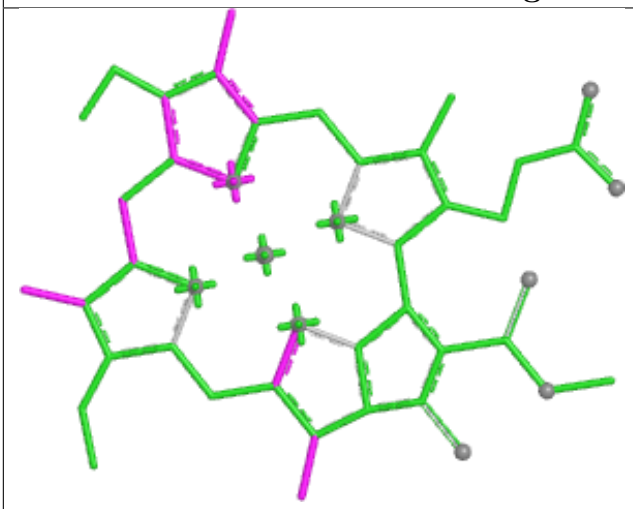


Torsions

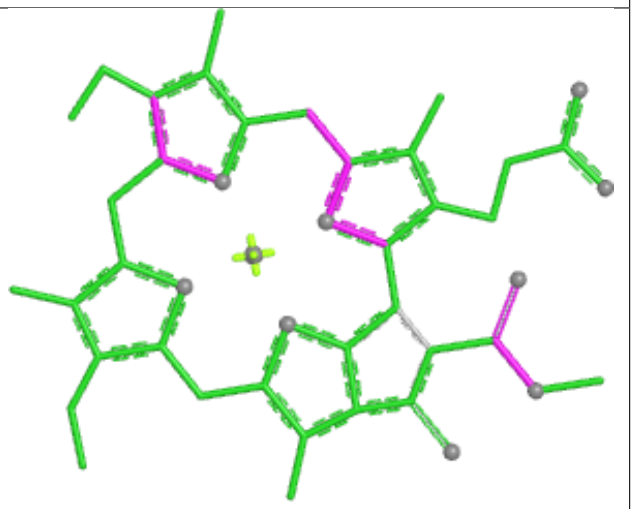


Rings

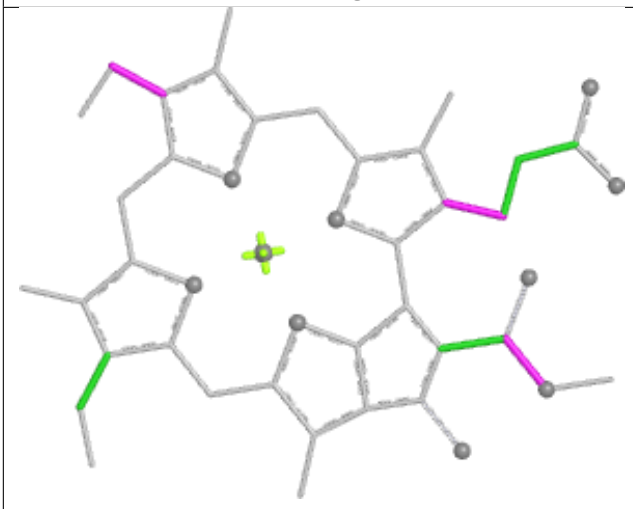
## Ligand CLA H 201



Bond lengths



Bond angles

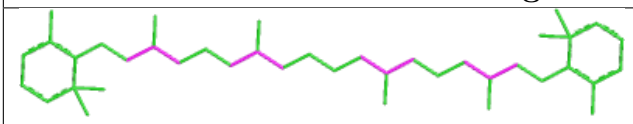


Torsions

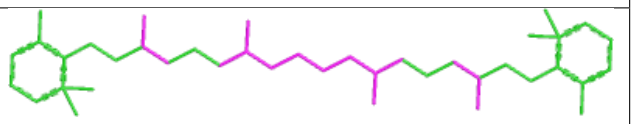


Rings

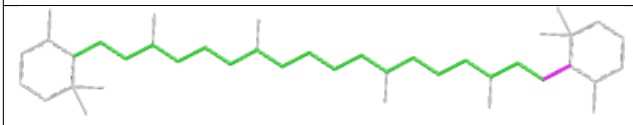
## Ligand BCR B 845



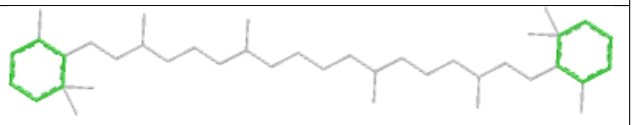
Bond lengths



Bond angles

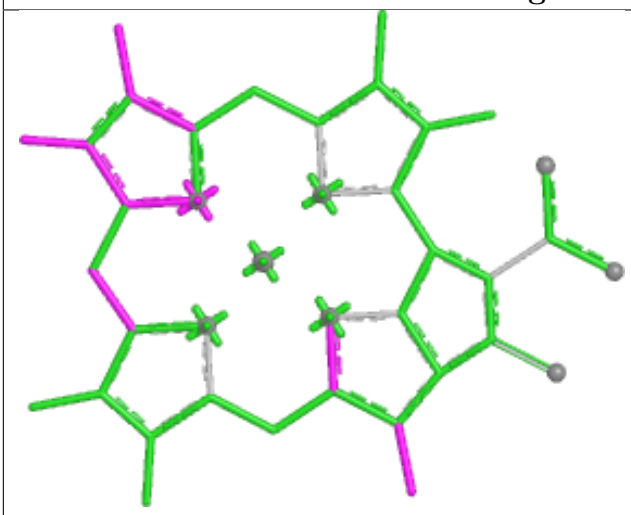


Torsions



Rings

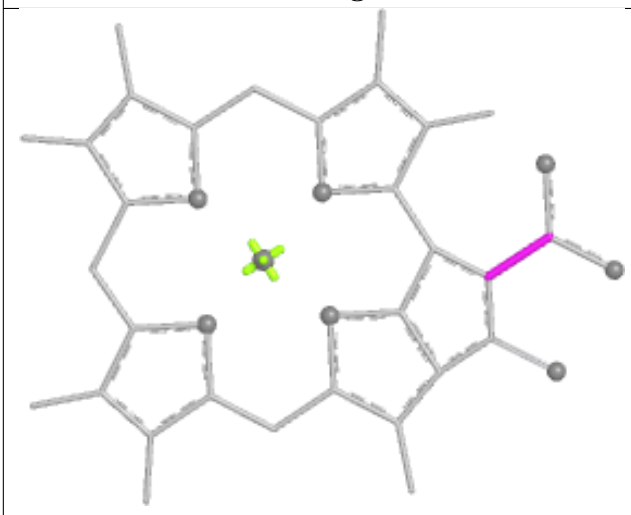
**Ligand CLA 1 314**



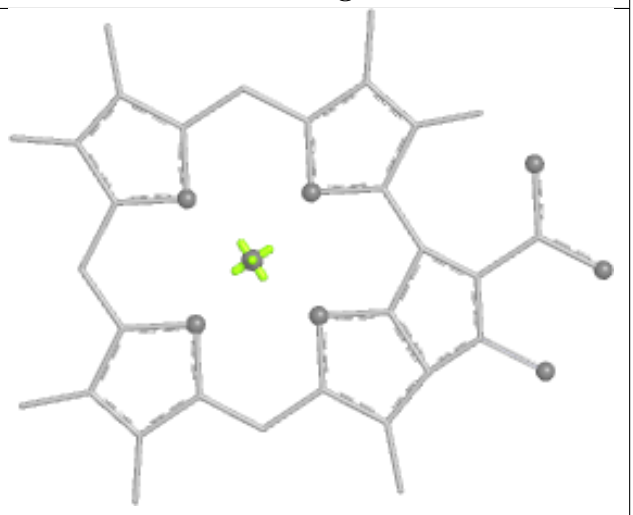
**Bond lengths**



**Bond angles**

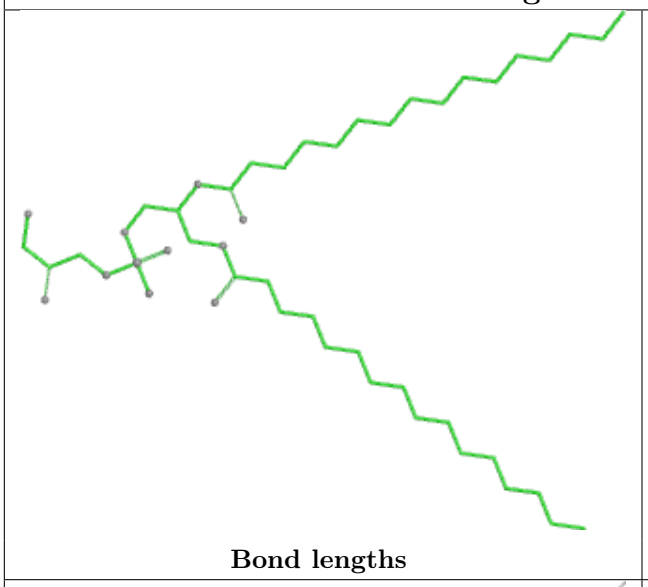


**Torsions**

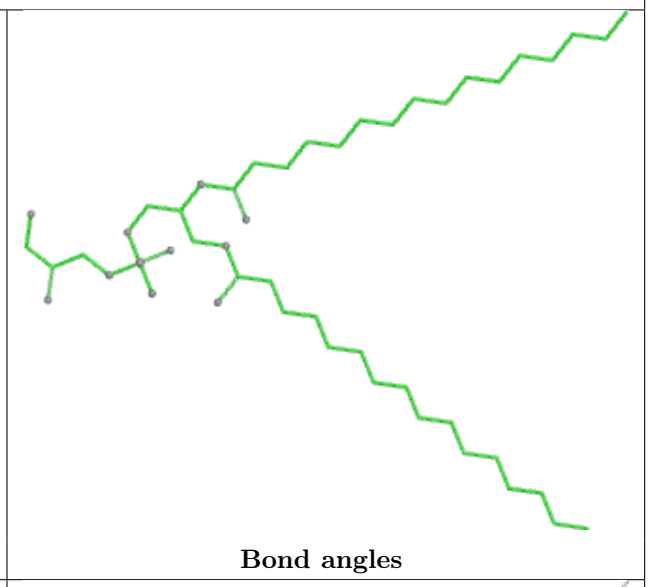


**Rings**

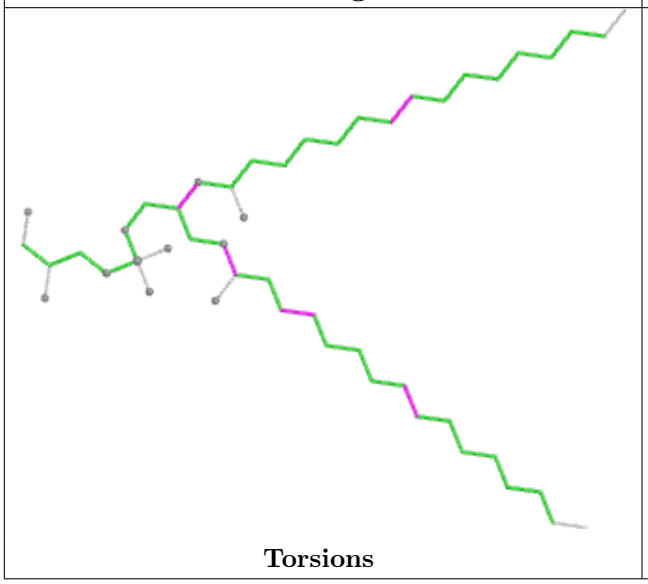
**Ligand LHG A 855**



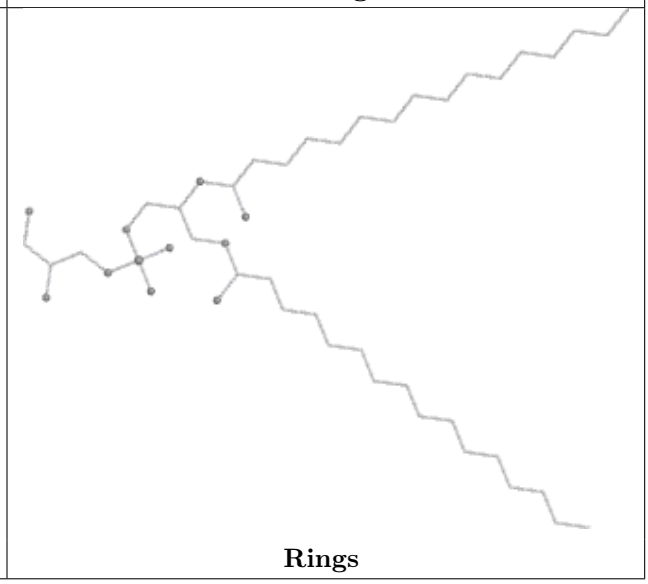
**Bond lengths**



**Bond angles**

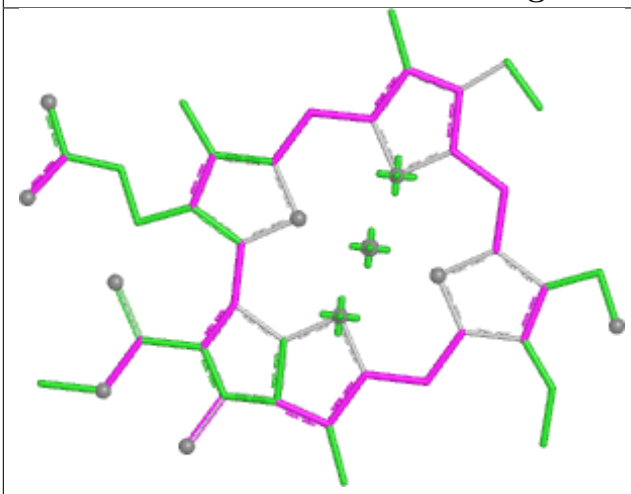


**Torsions**

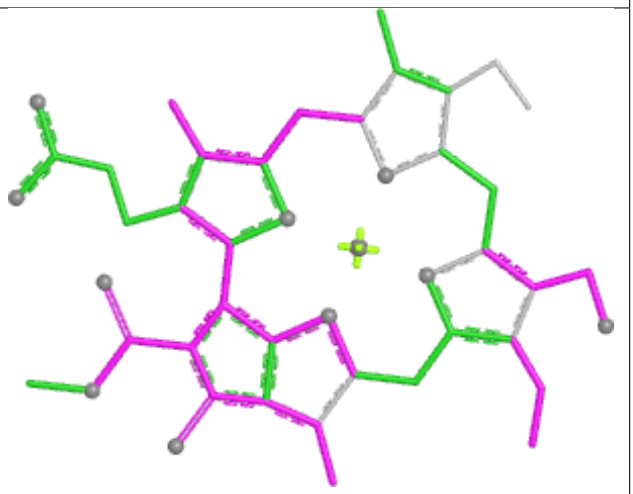


**Rings**

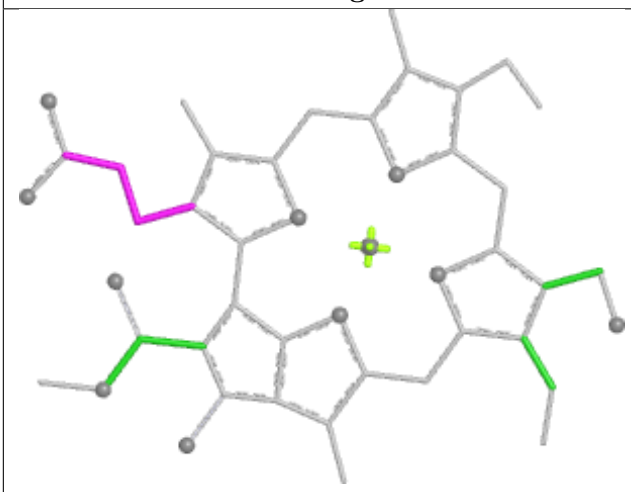
**Ligand CHL 9 606**



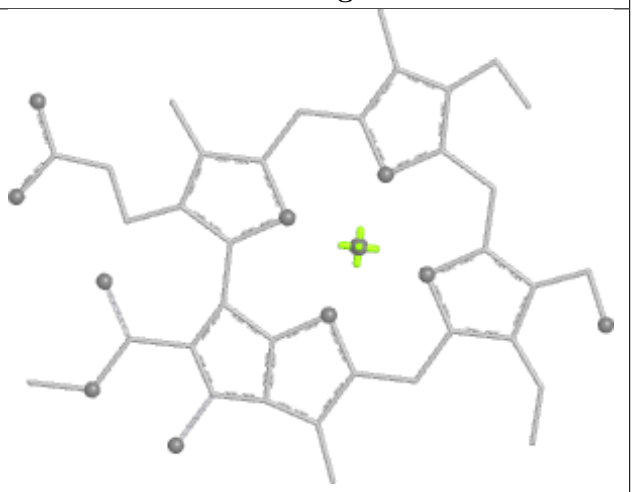
**Bond lengths**



**Bond angles**

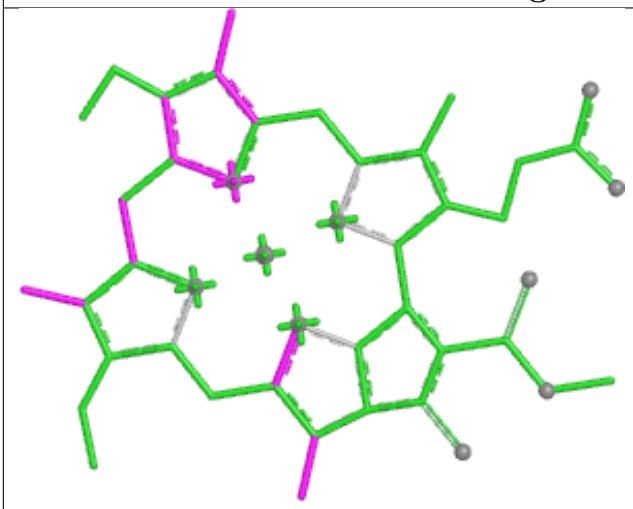


**Torsions**

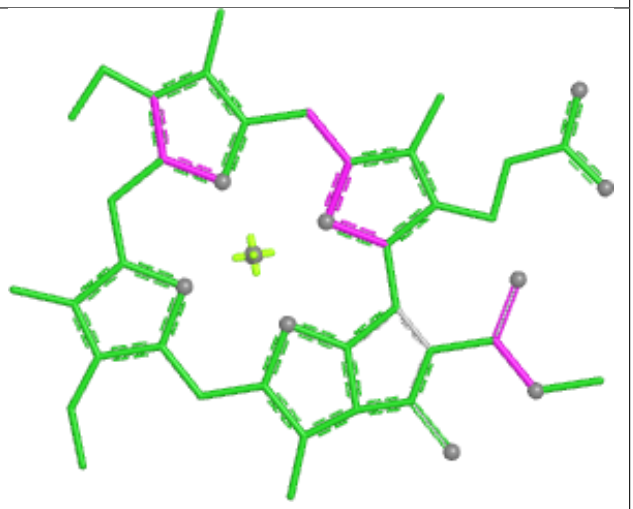


**Rings**

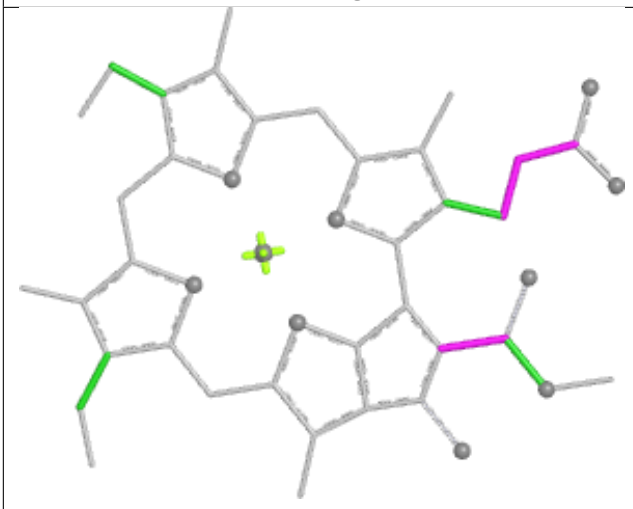
**Ligand CLA c 604**



**Bond lengths**



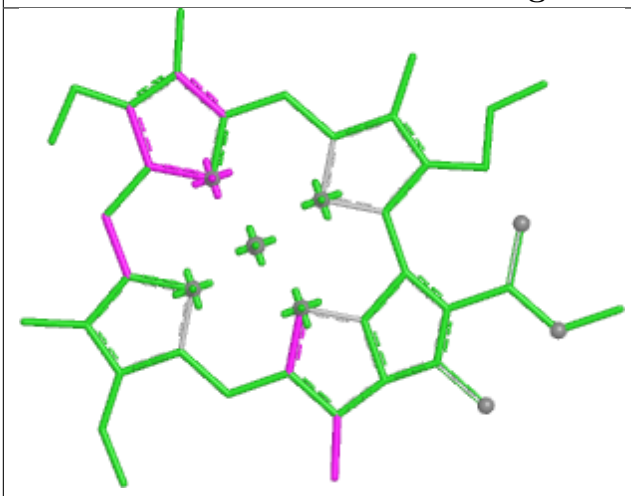
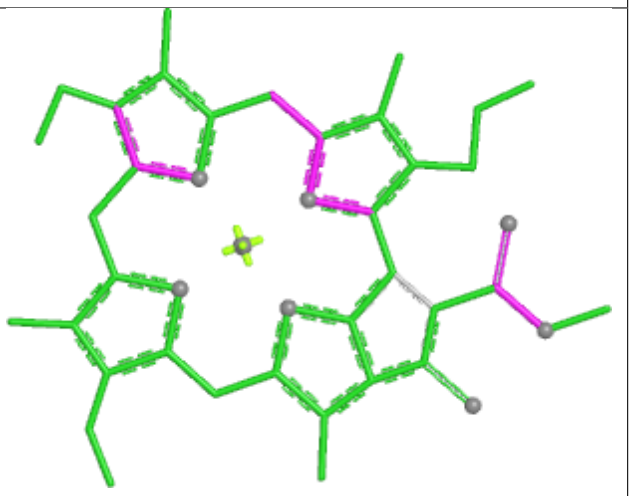
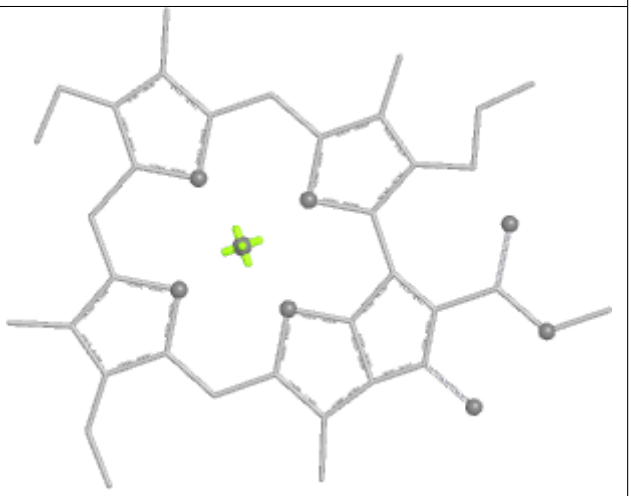
**Bond angles**

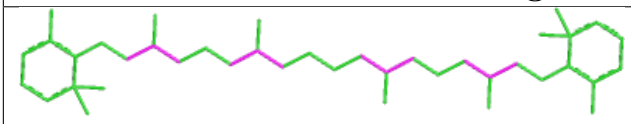
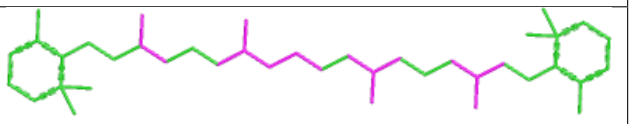
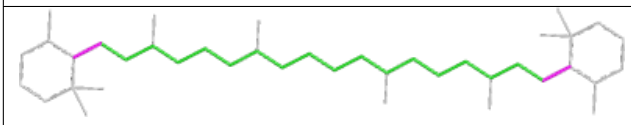
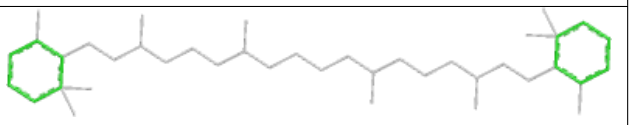


**Torsions**



**Rings**

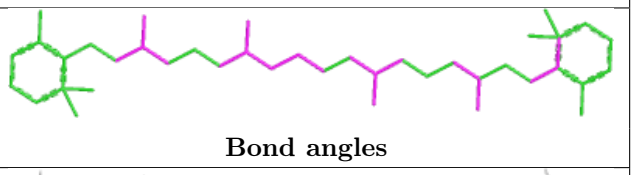
| Ligand CLA 7 410 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand BCR 3 418 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

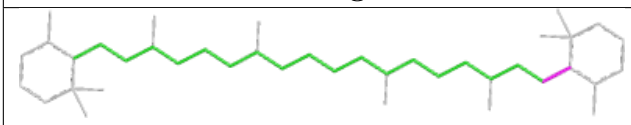
## Ligand BCR L 305



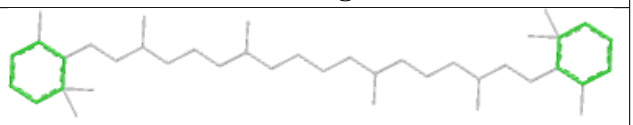
Bond lengths



Bond angles

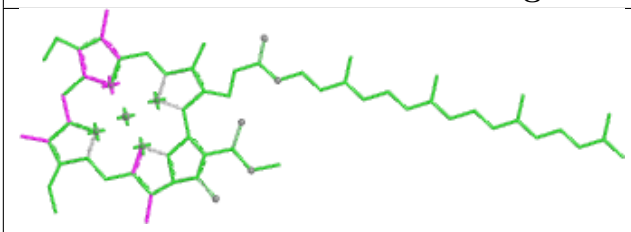


Torsions

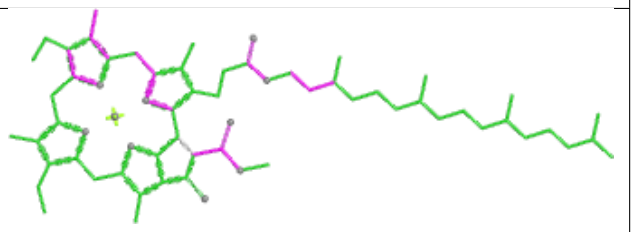


Rings

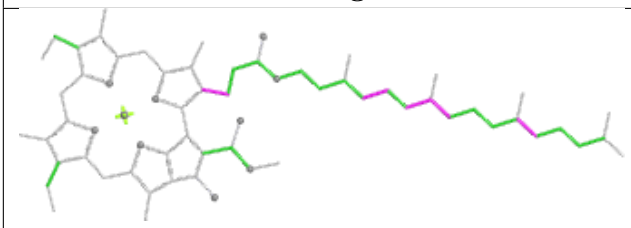
## Ligand CLA A 826



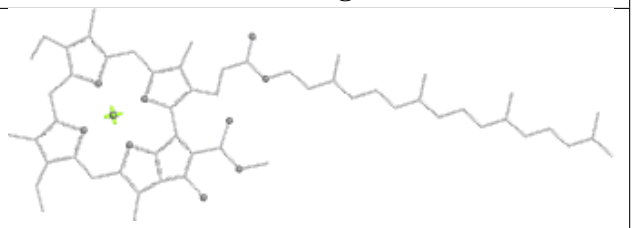
Bond lengths



Bond angles

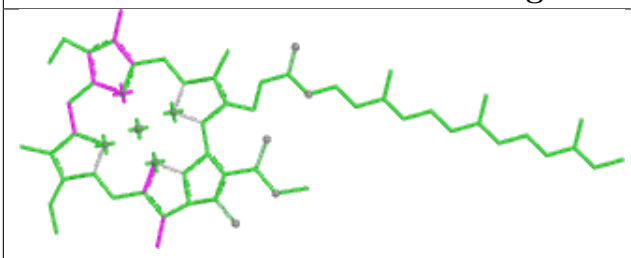


Torsions

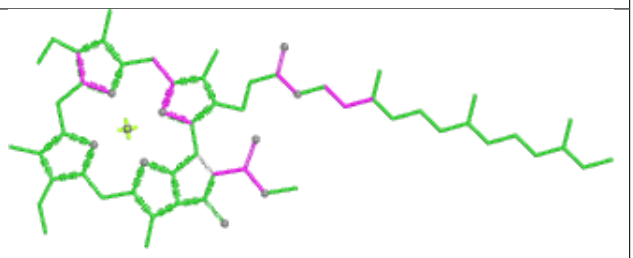


Rings

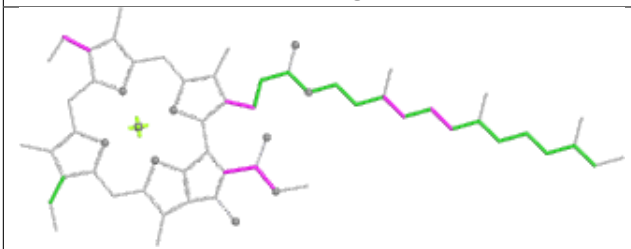
## Ligand CLA F 302



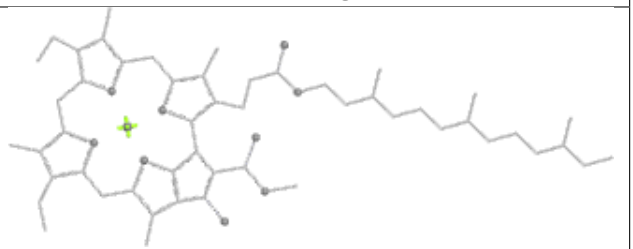
Bond lengths



Bond angles

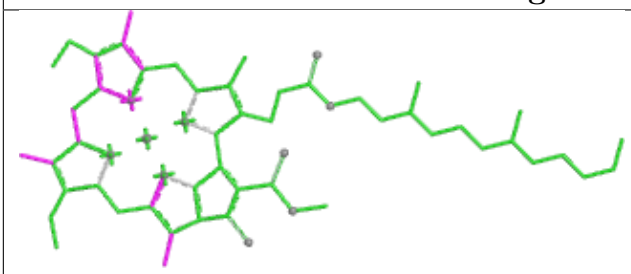


Torsions

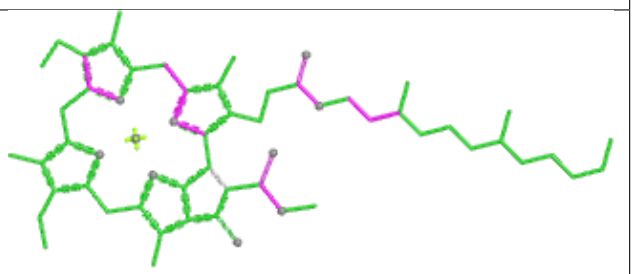


Rings

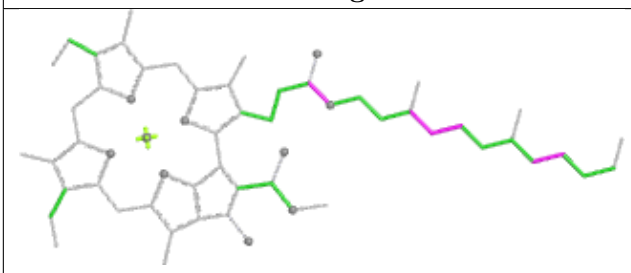
## Ligand CLA 3 408



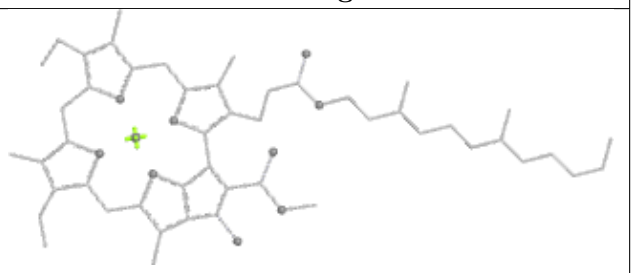
Bond lengths



Bond angles

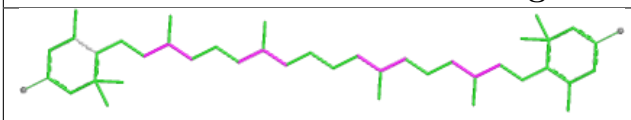


Torsions

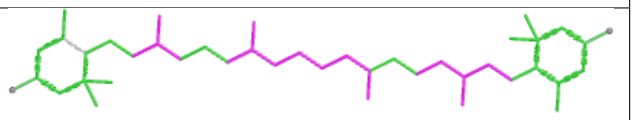


Rings

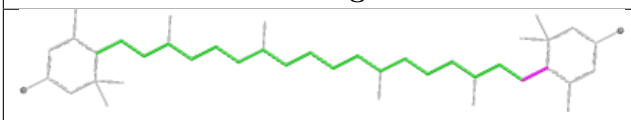
## Ligand LUT 9 614



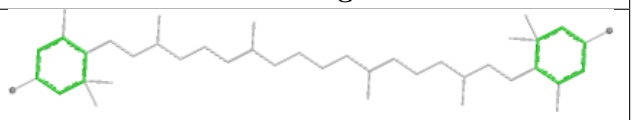
Bond lengths



Bond angles

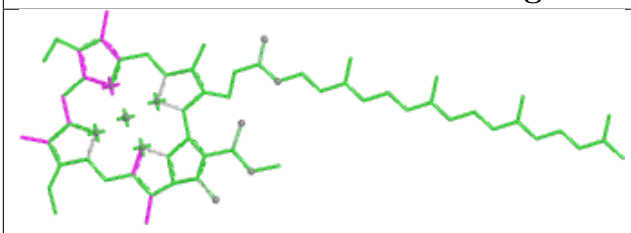


Torsions

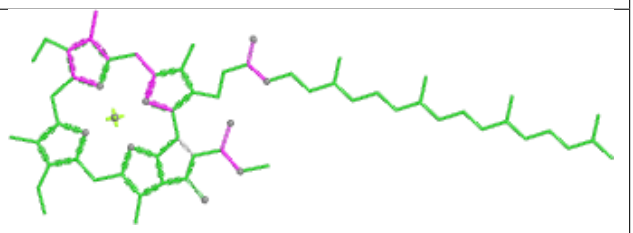


Rings

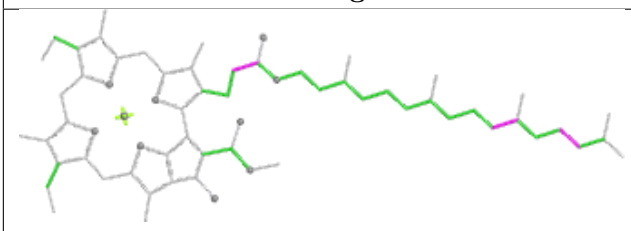
## Ligand CLA B 840



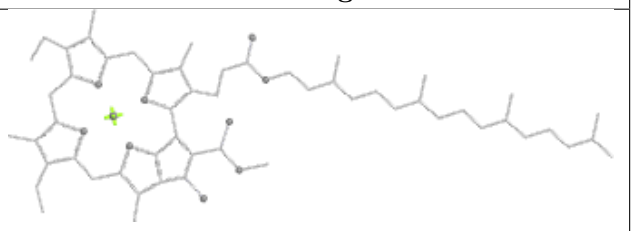
Bond lengths



Bond angles

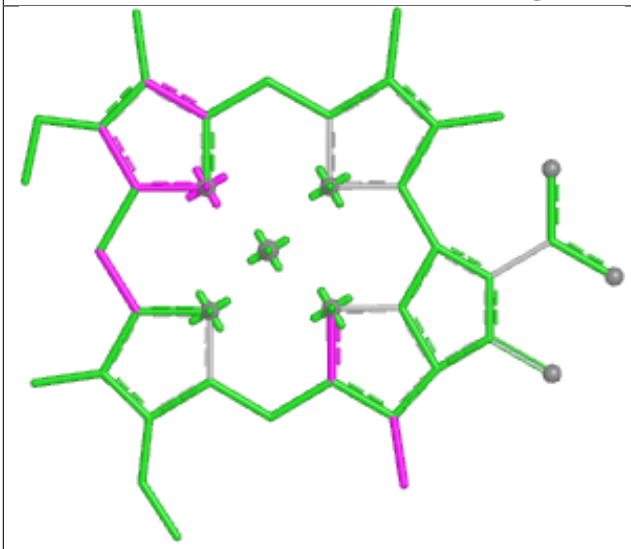


Torsions

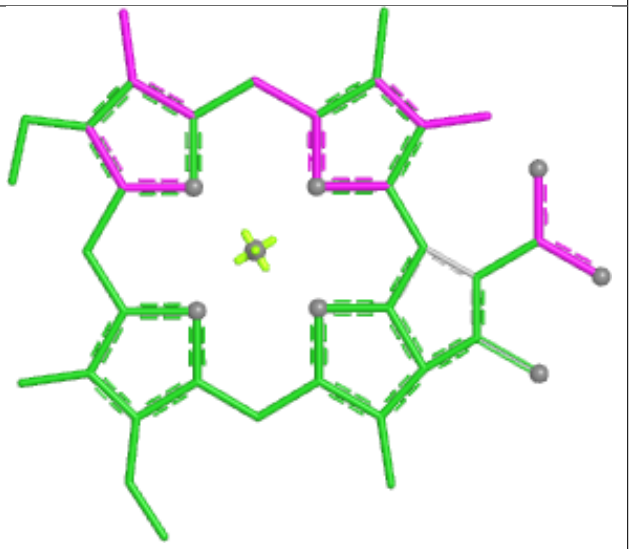


Rings

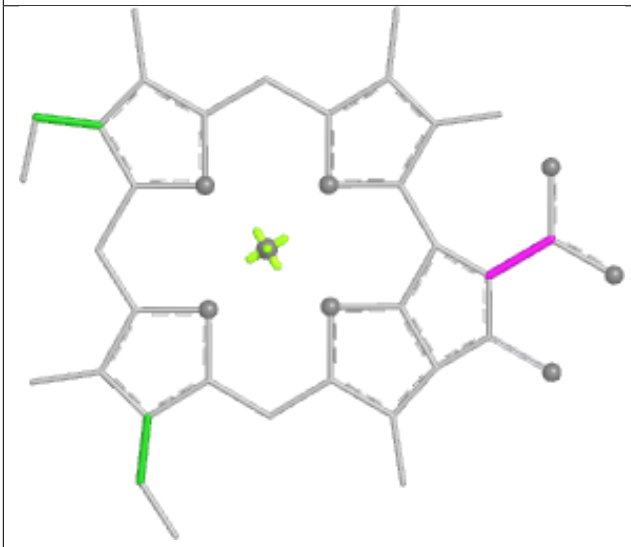
**Ligand CLA 7 414**



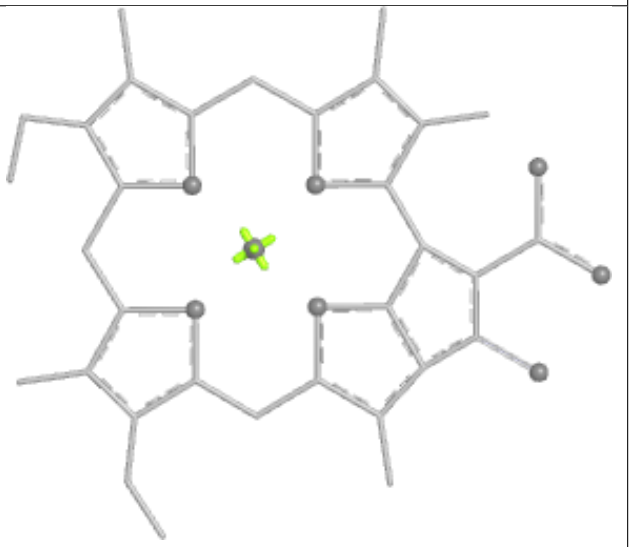
**Bond lengths**



**Bond angles**

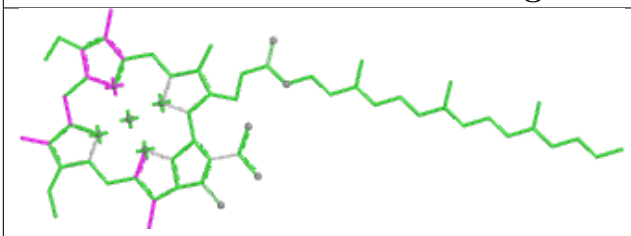


**Torsions**

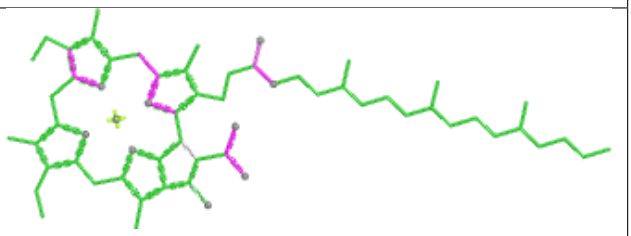


**Rings**

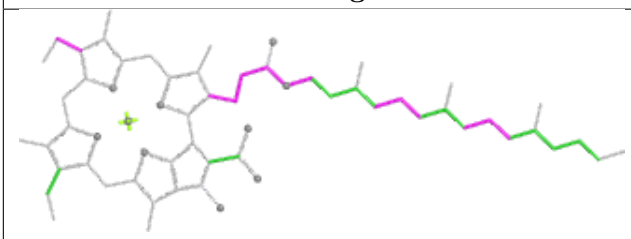
## Ligand CLA B 809



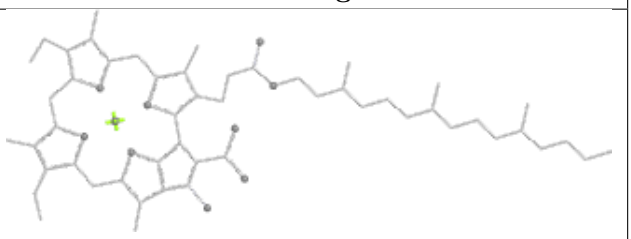
Bond lengths



Bond angles

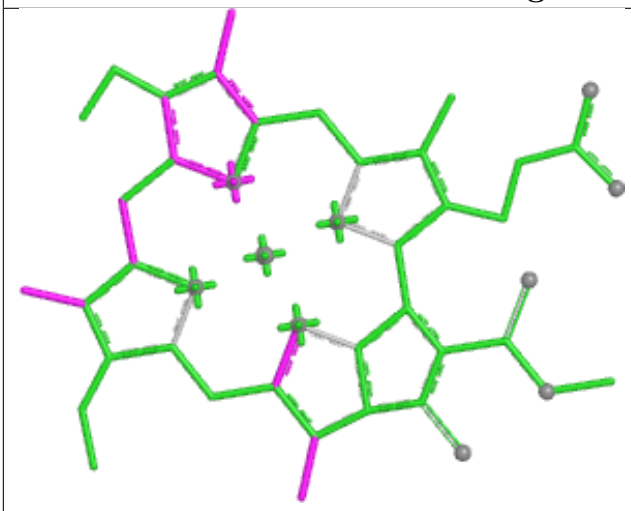


Torsions

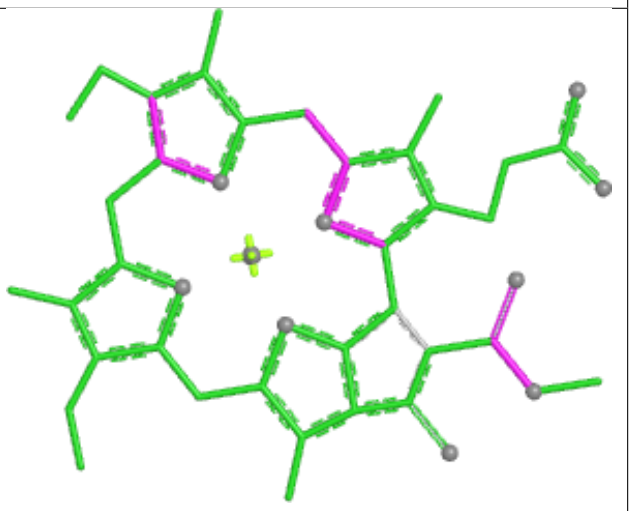


Rings

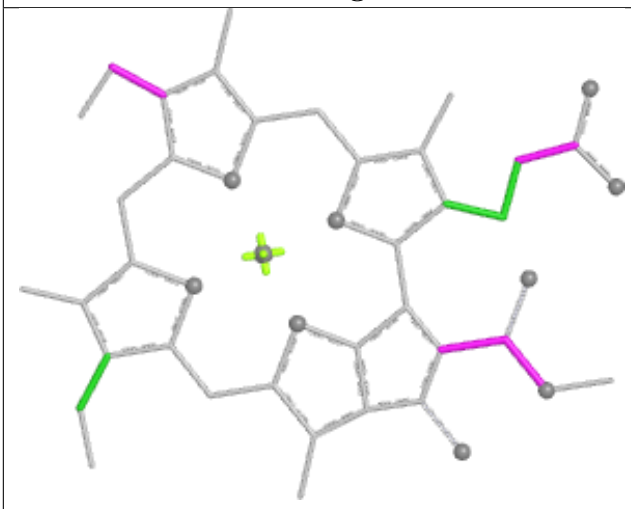
## Ligand CLA b 313



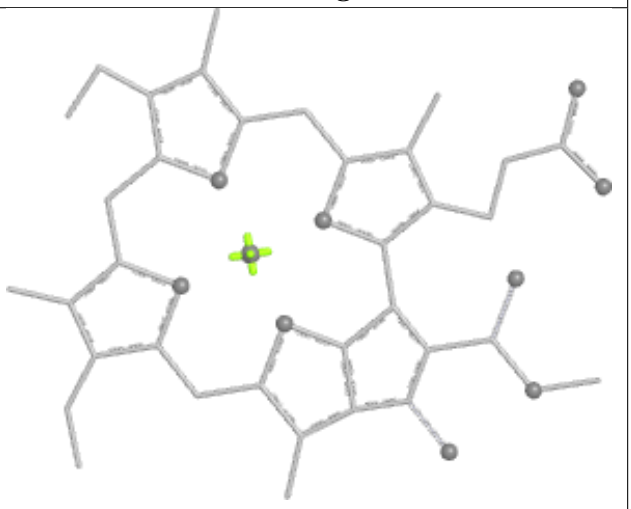
Bond lengths



Bond angles

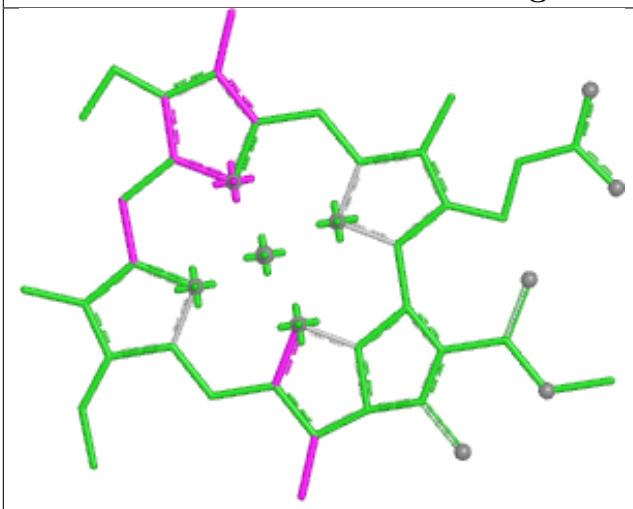


Torsions

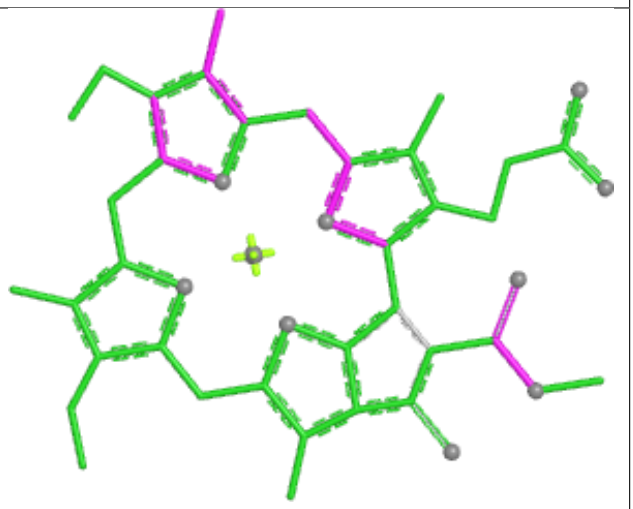


Rings

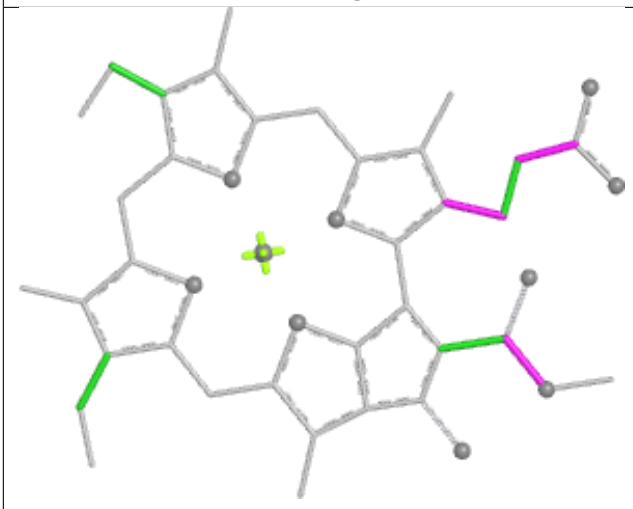
**Ligand CLA c 610**



**Bond lengths**



**Bond angles**

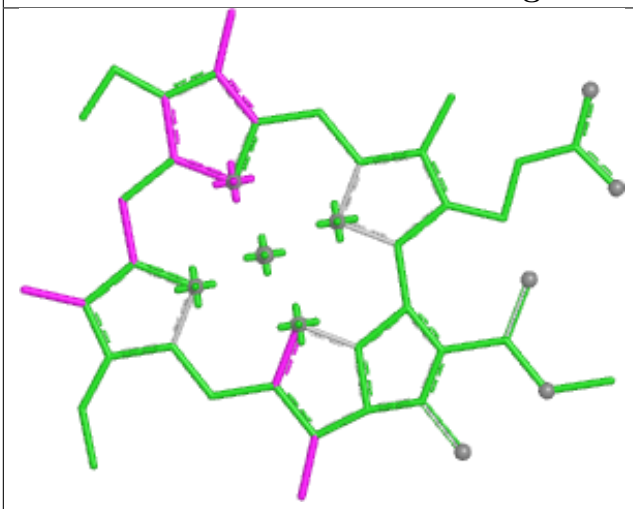


**Torsions**

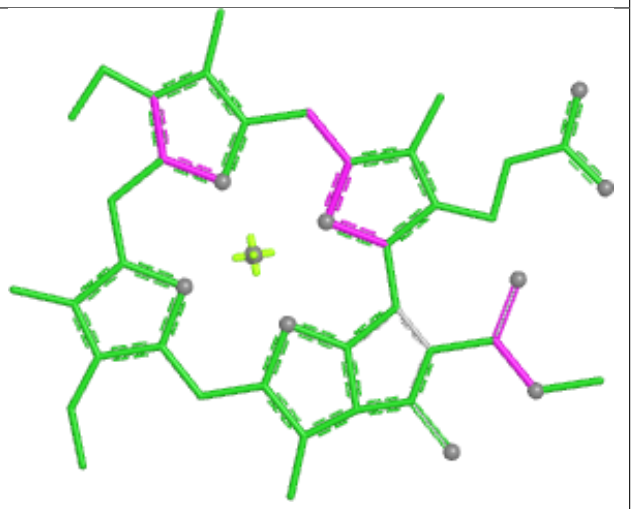


**Rings**

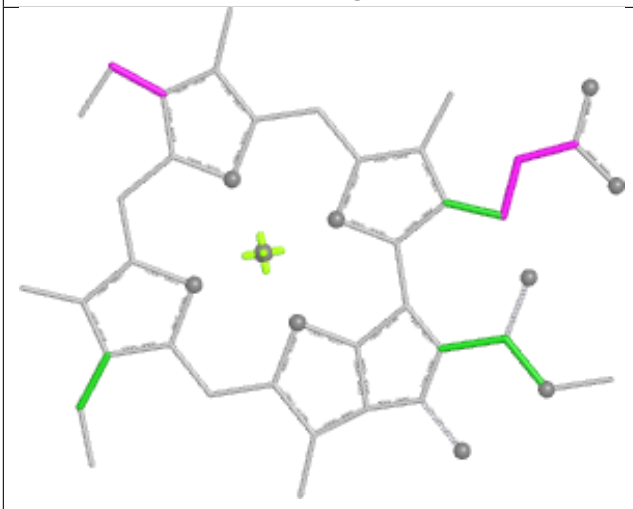
**Ligand CLA K 204**



**Bond lengths**



**Bond angles**

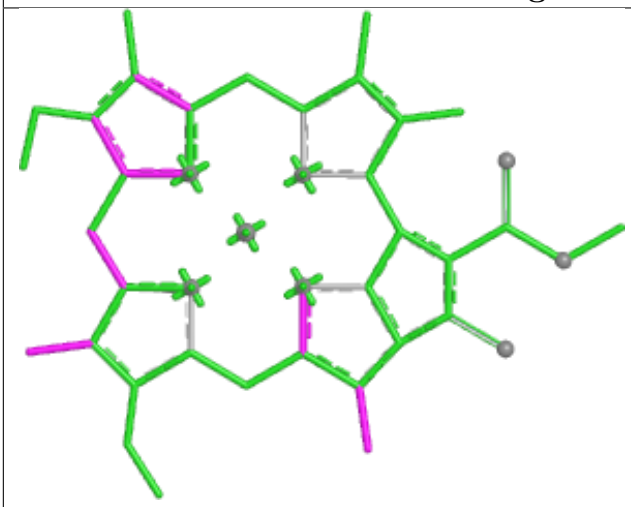


**Torsions**

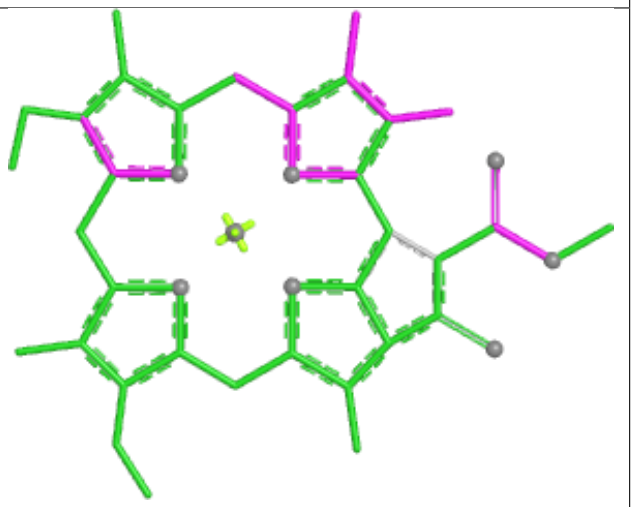


**Rings**

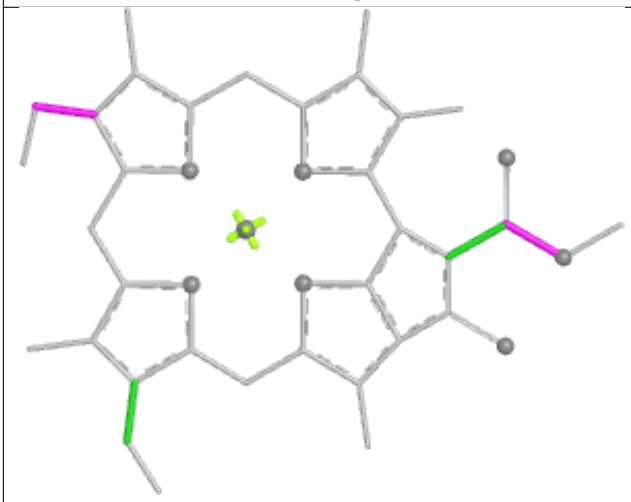
## Ligand CLA 8 618



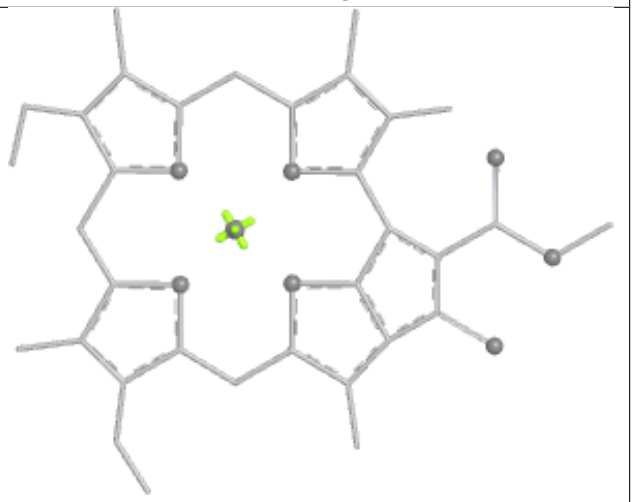
Bond lengths



Bond angles

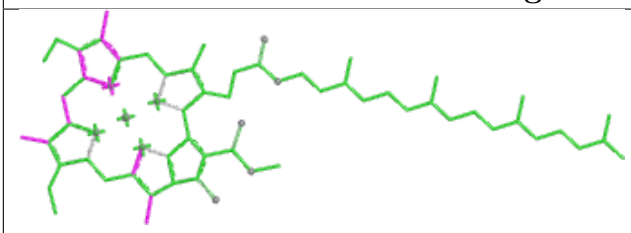


Torsions

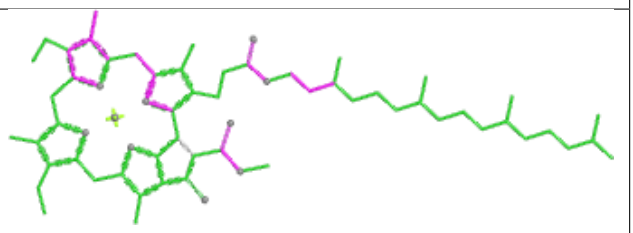


Rings

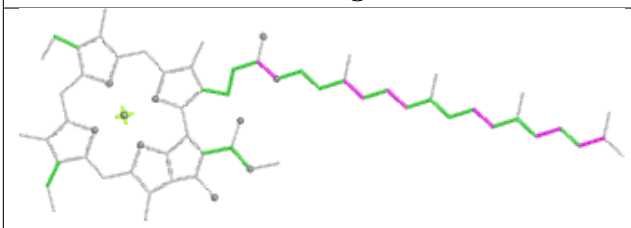
## Ligand CLA B 825



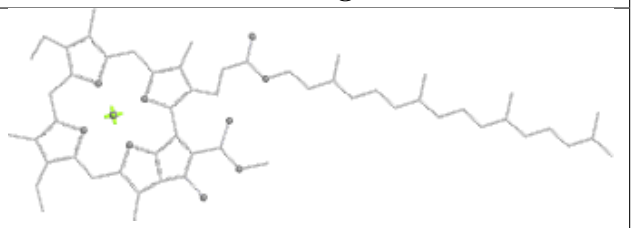
Bond lengths



Bond angles

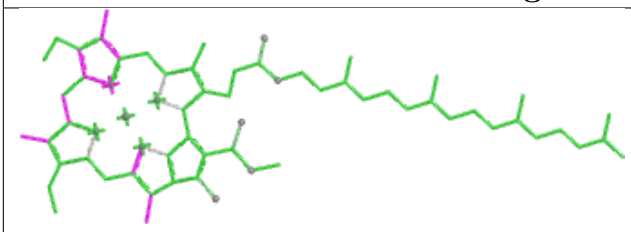


Torsions

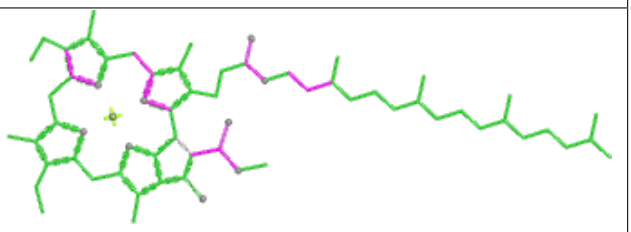


Rings

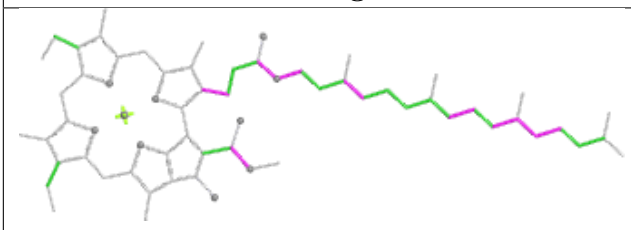
## Ligand CLA A 819



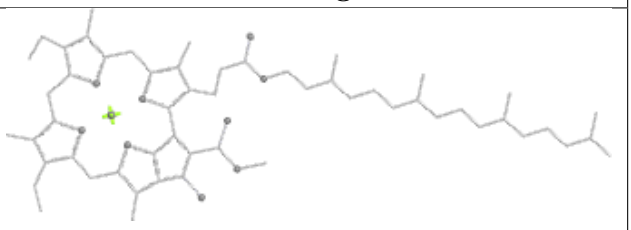
Bond lengths



Bond angles

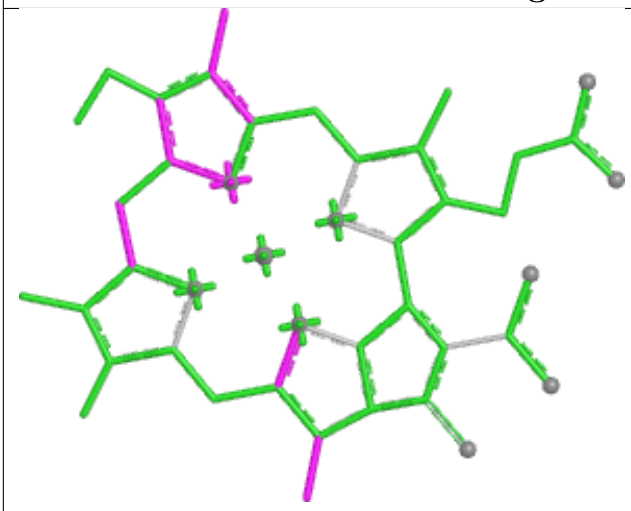


Torsions

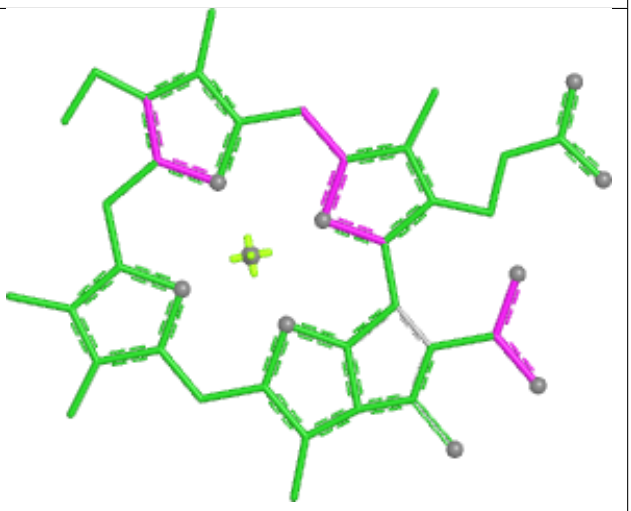


Rings

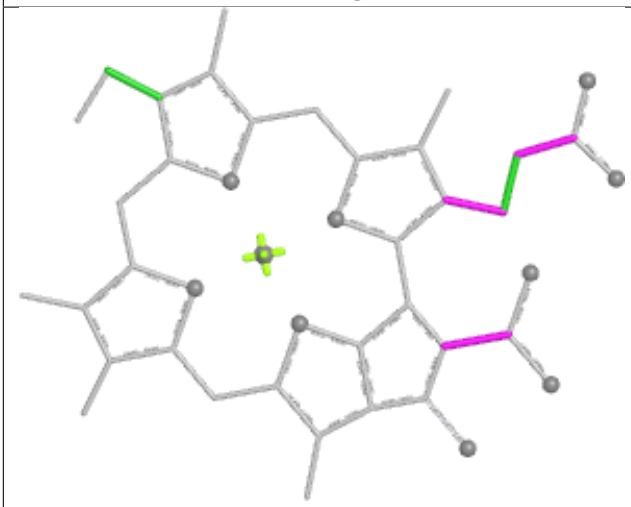
## Ligand CLA 5 609



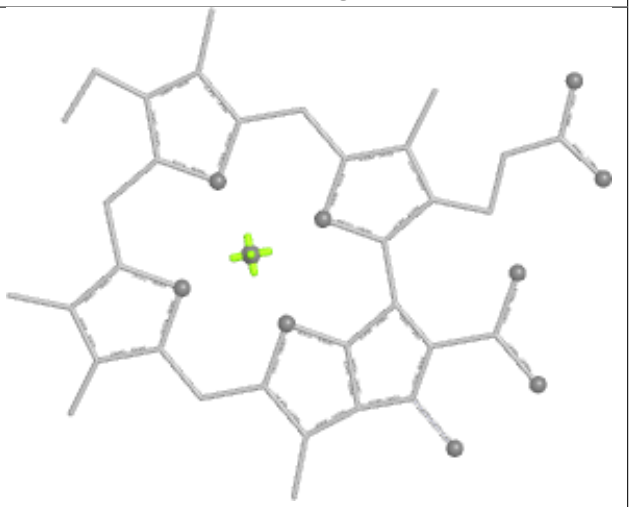
Bond lengths



Bond angles

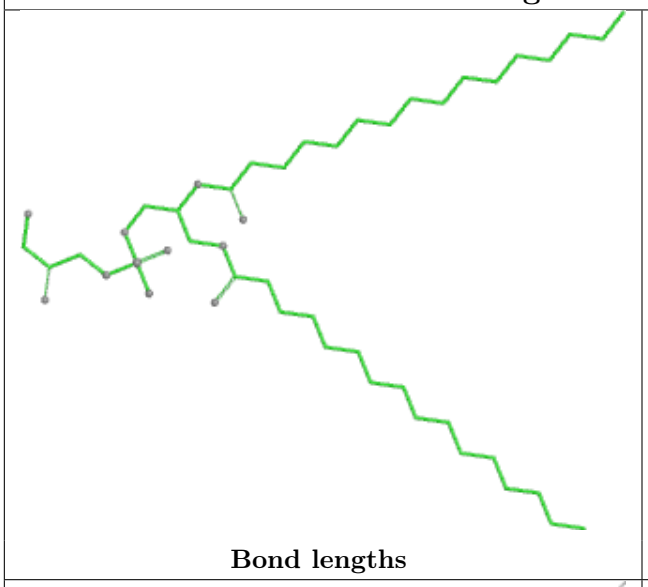


Torsions

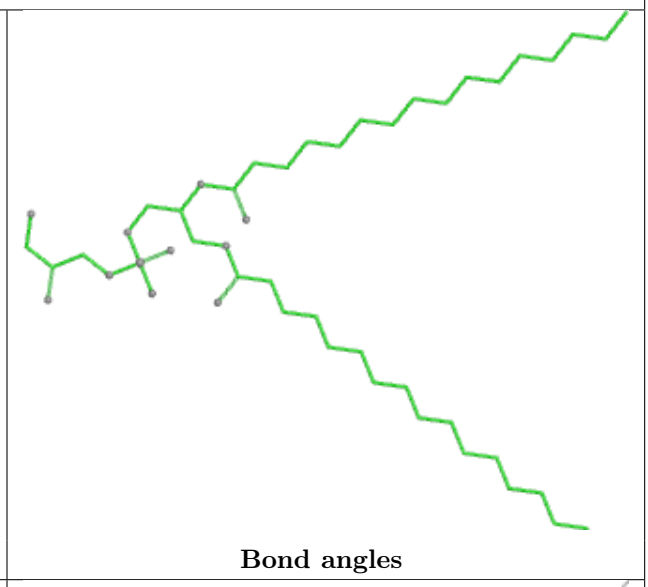


Rings

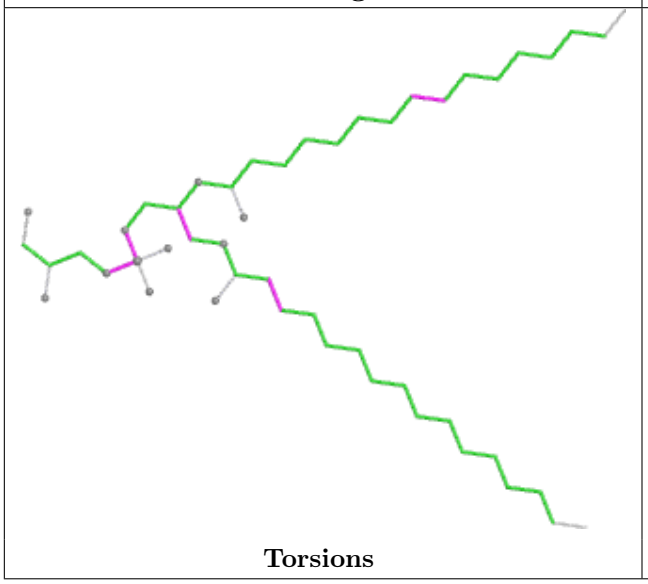
**Ligand LHG A 844**



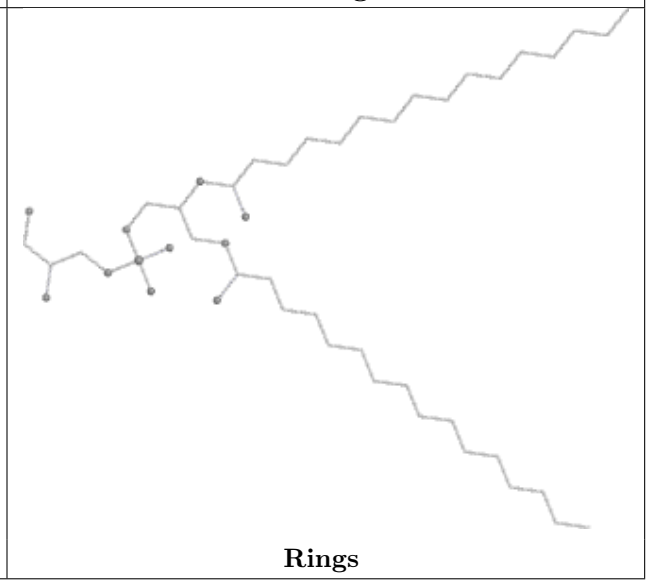
**Bond lengths**



**Bond angles**

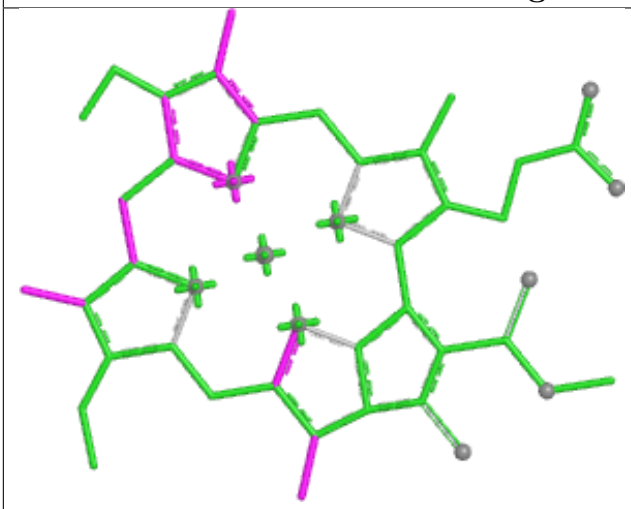


**Torsions**

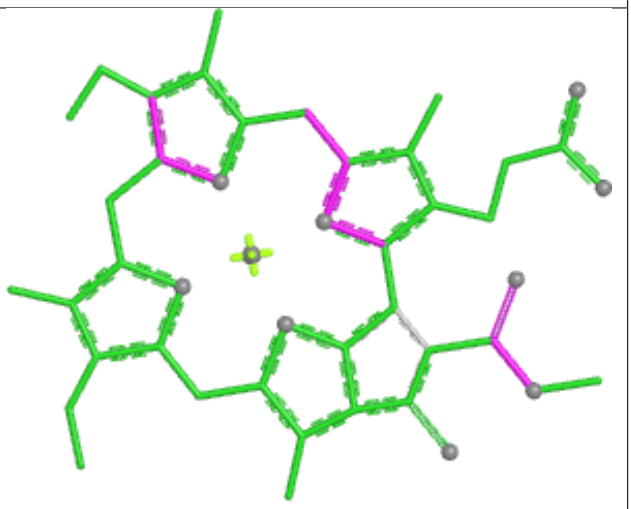


**Rings**

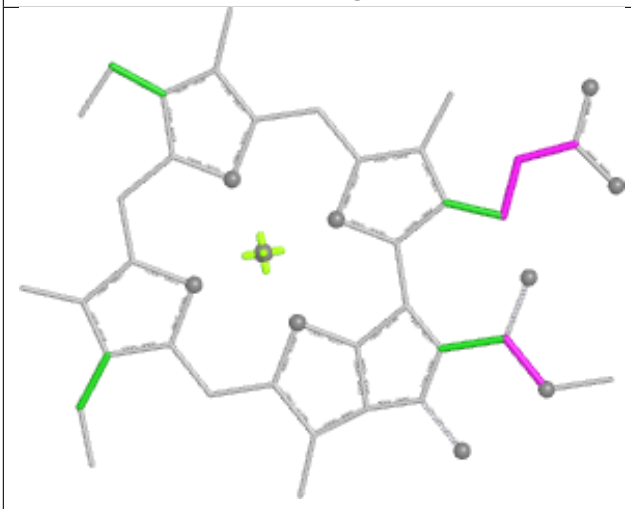
**Ligand CLA 1 312**



**Bond lengths**



**Bond angles**

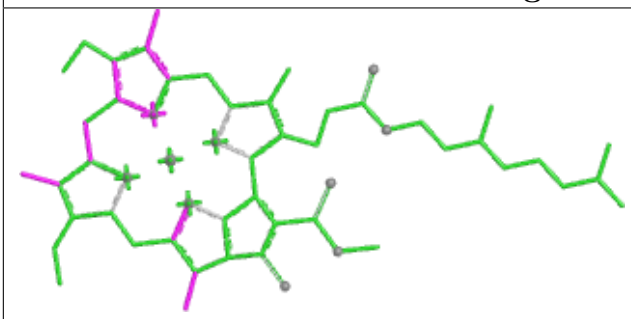


**Torsions**

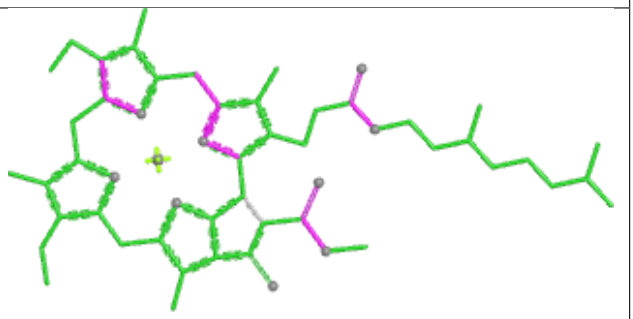


**Rings**

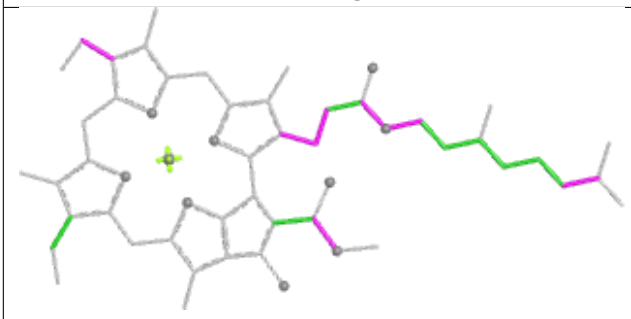
## Ligand CLA A 824



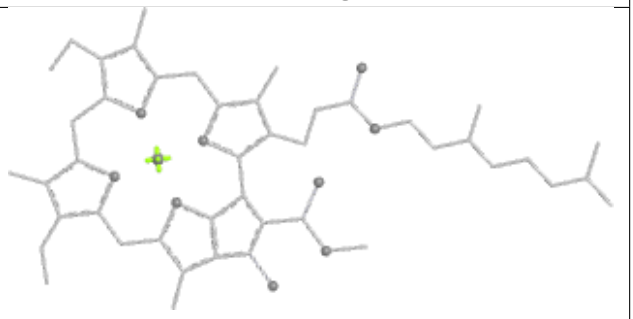
Bond lengths



Bond angles

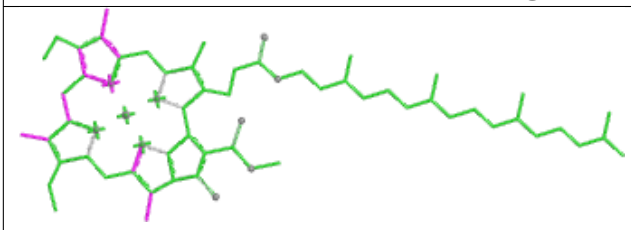


Torsions

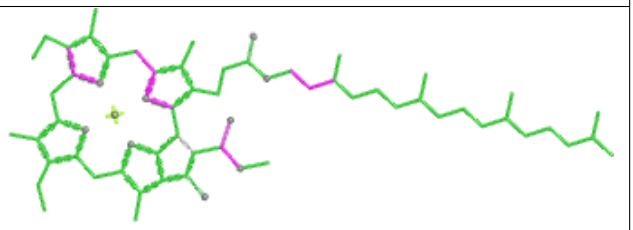


Rings

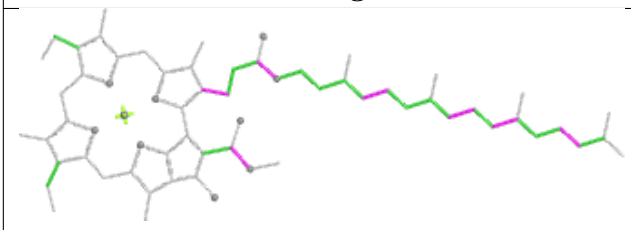
## Ligand CLA A 807



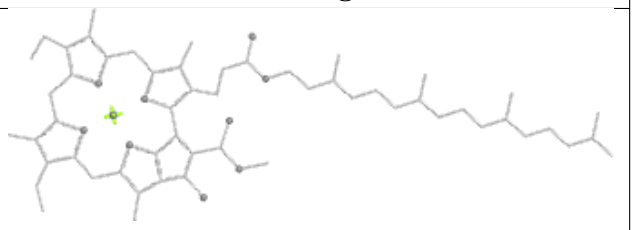
Bond lengths



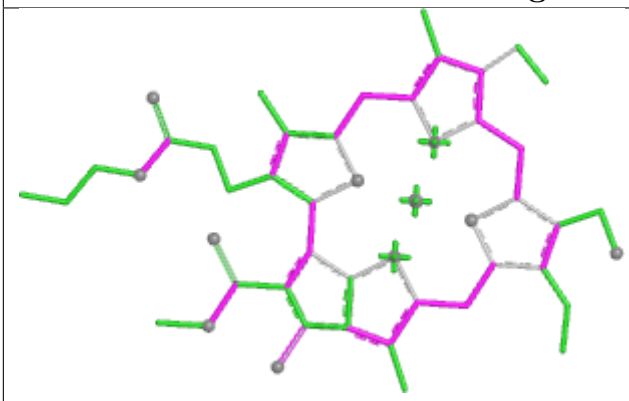
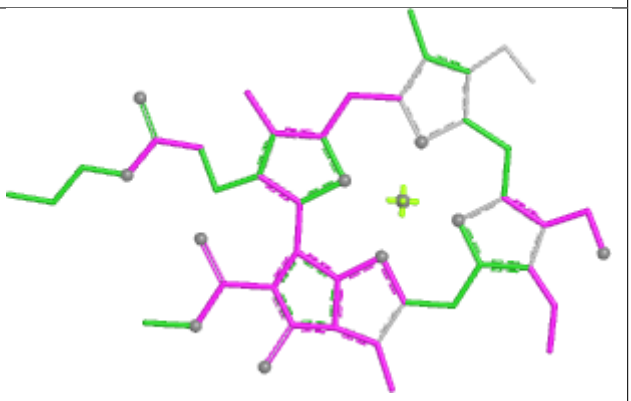
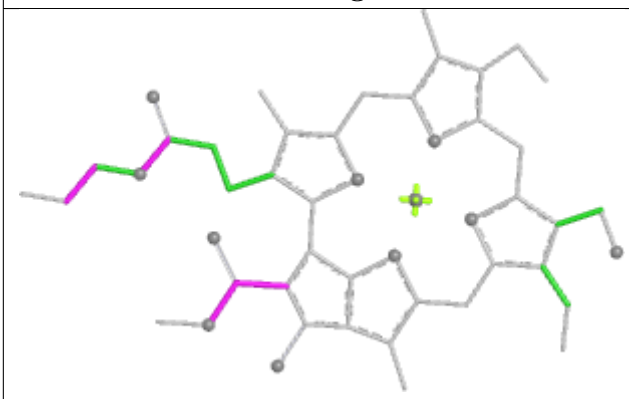
Bond angles

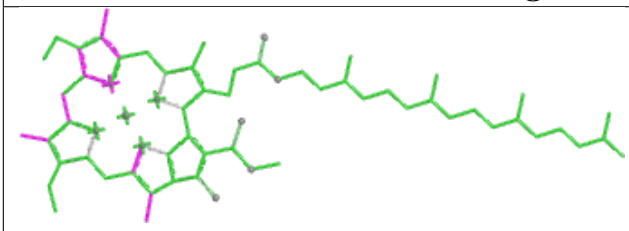
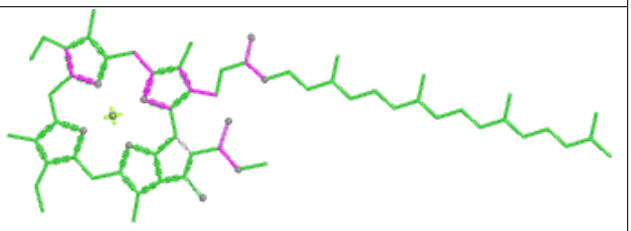
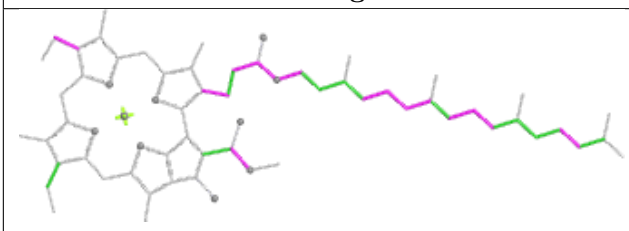
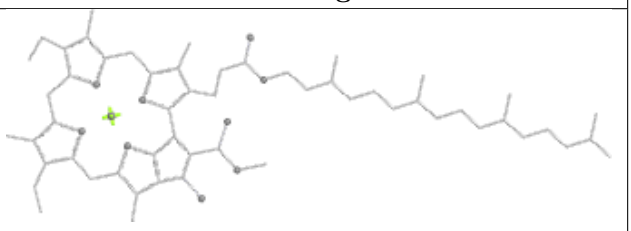


Torsions

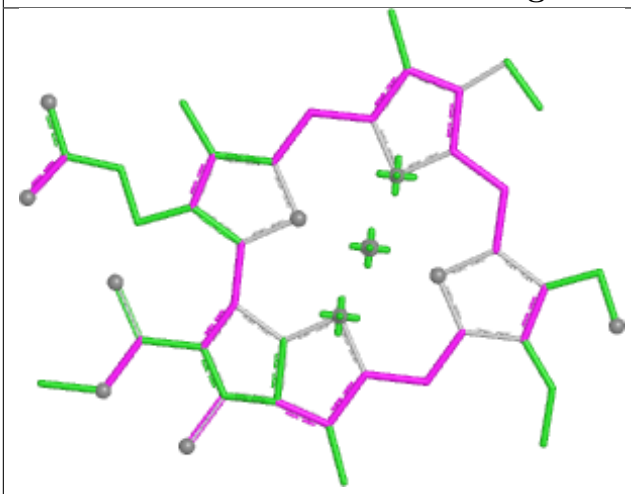


Rings

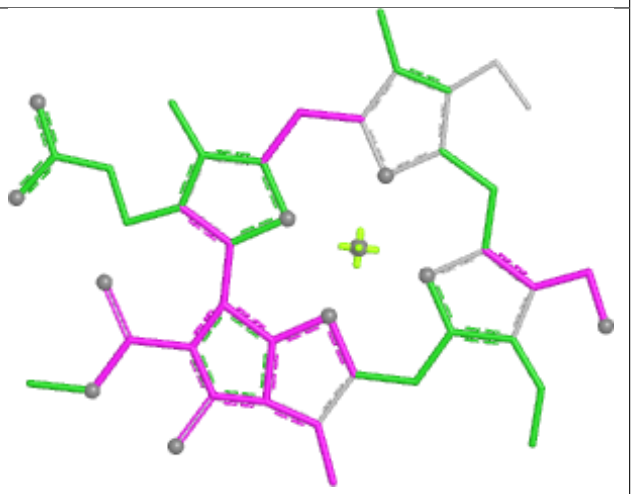
| Ligand CHL c 601 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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

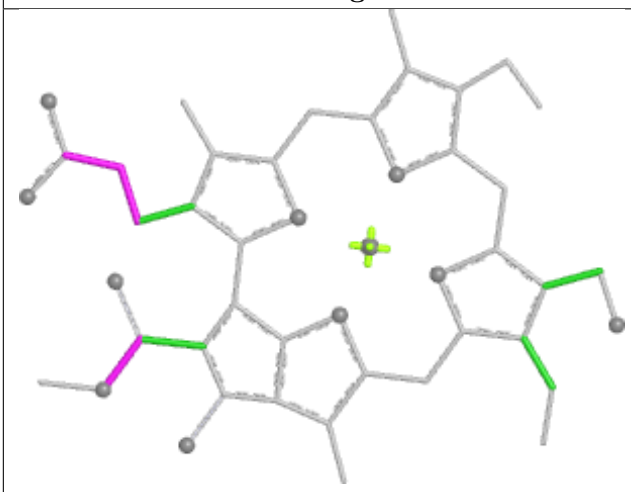
**Ligand CHL 5 606**



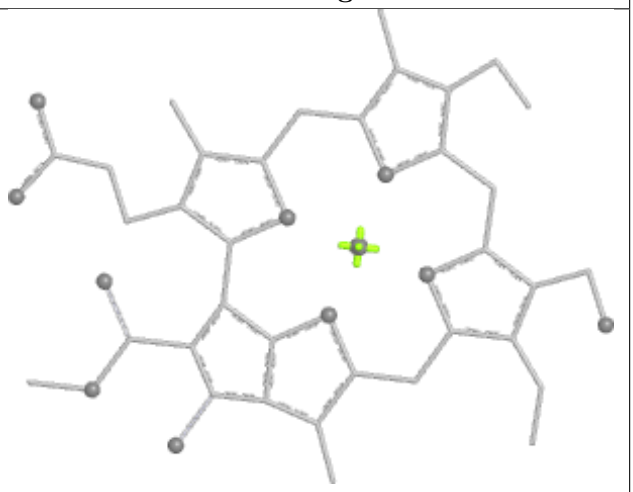
**Bond lengths**



**Bond angles**

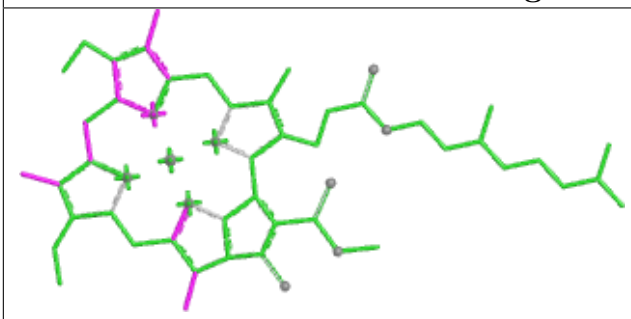


**Torsions**

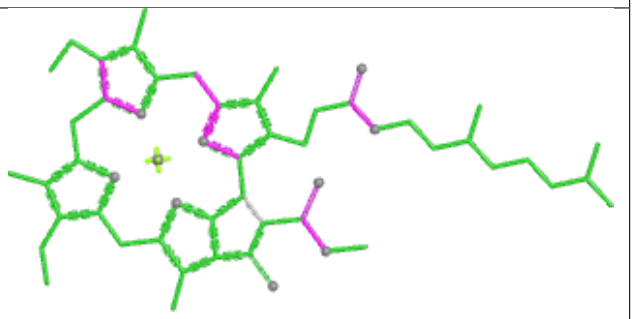


**Rings**

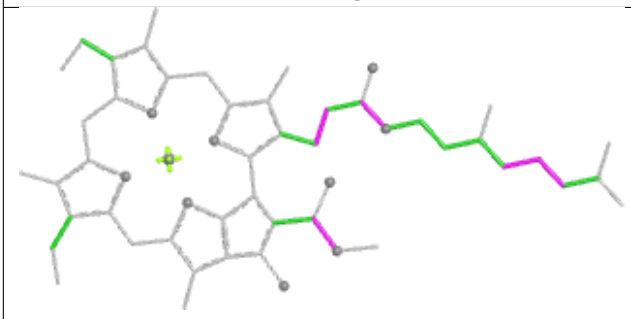
## Ligand CLA B 803



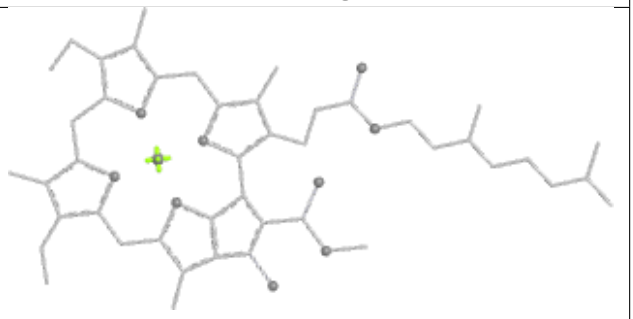
Bond lengths



Bond angles

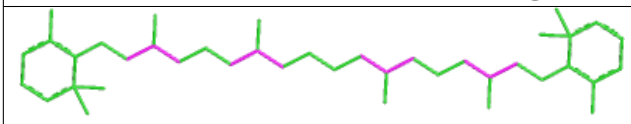


Torsions



Rings

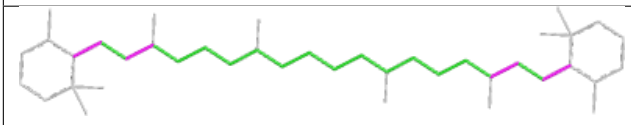
## Ligand BCR 3 419



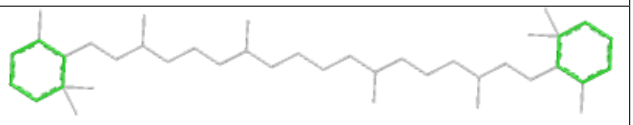
Bond lengths



Bond angles

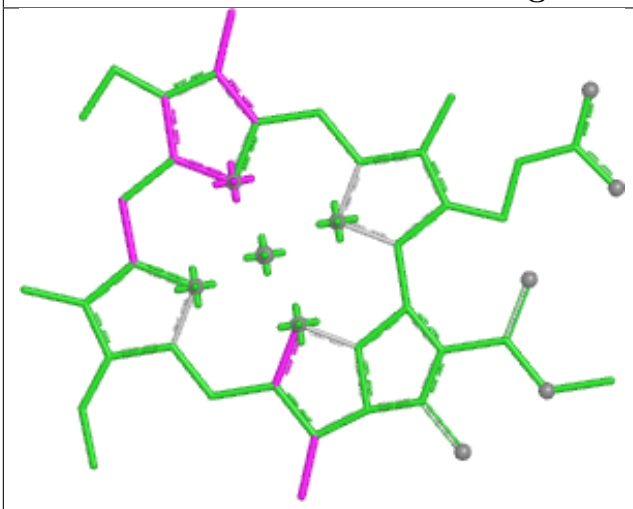


Torsions

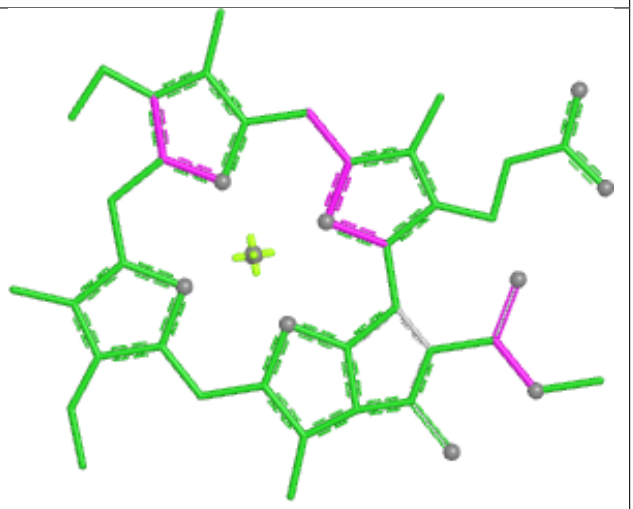


Rings

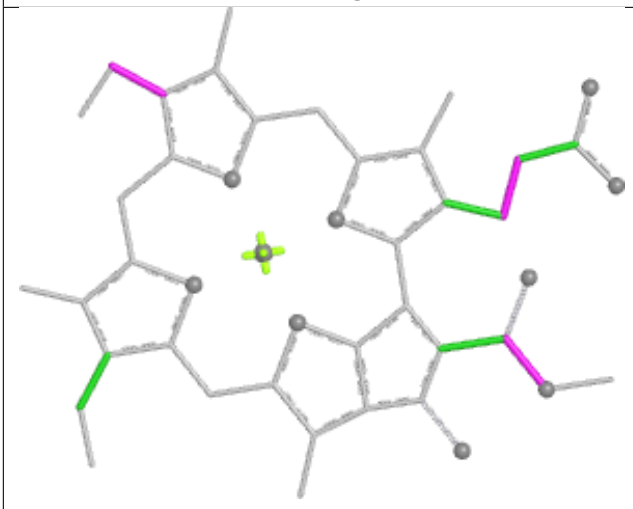
## Ligand CLA 1 313



Bond lengths



Bond angles

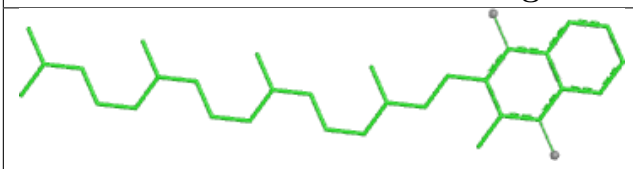


Torsions

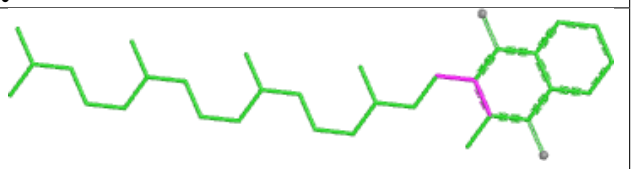


Rings

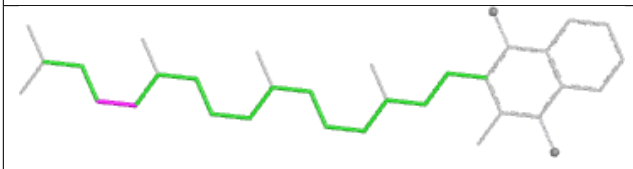
## Ligand PQN B 841



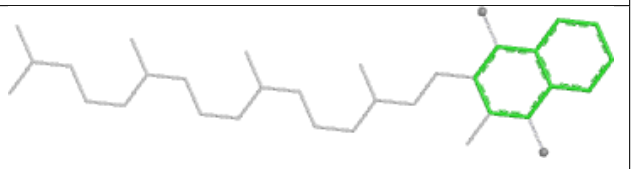
Bond lengths



Bond angles

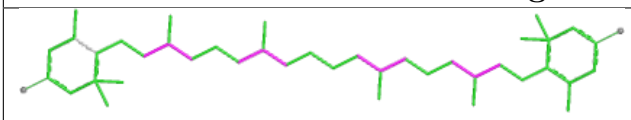


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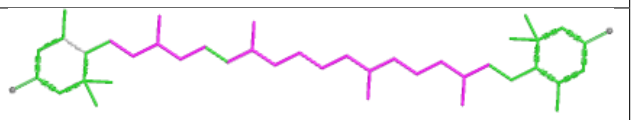


Rings

## Ligand LUT 6 616



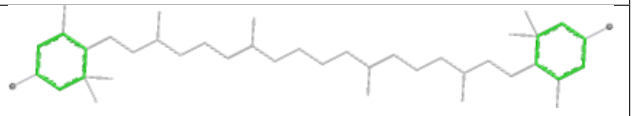
Bond lengths



Bond angles

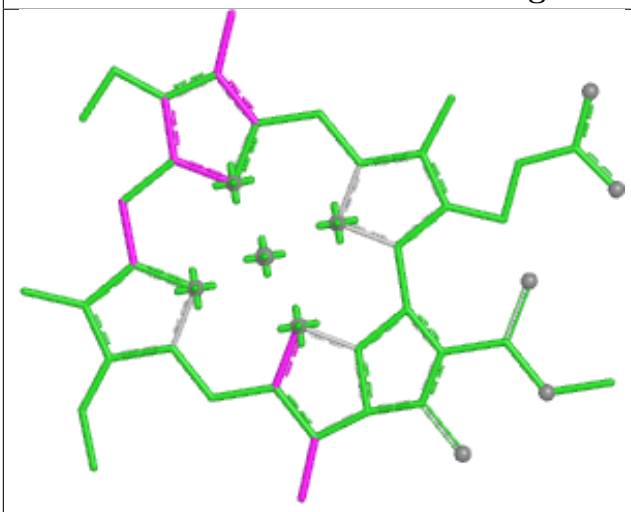


Torsions

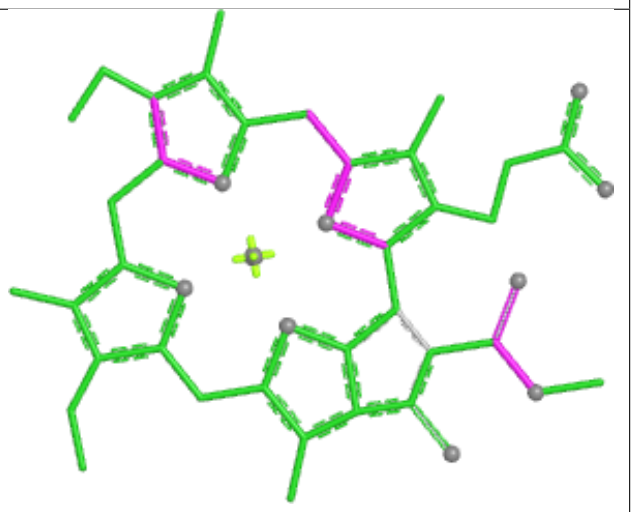


Rings

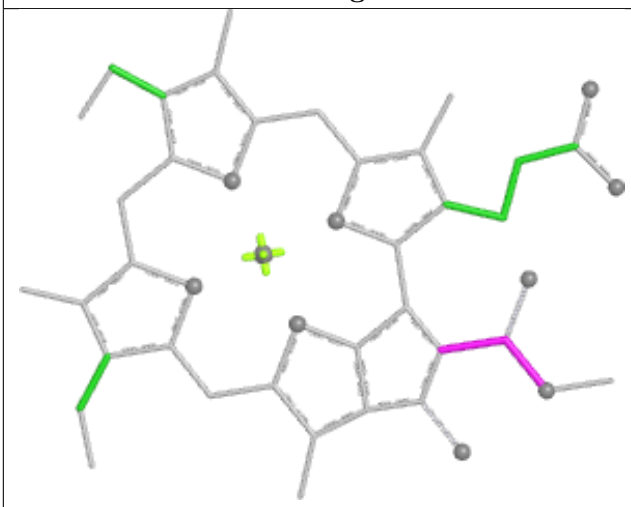
## Ligand CLA 9 612



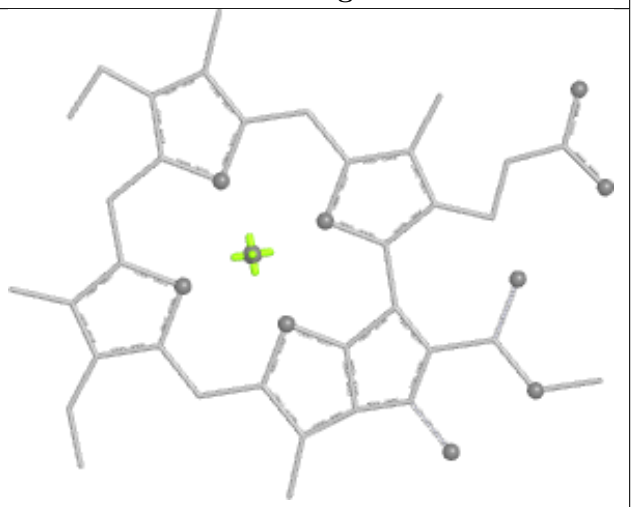
Bond lengths



Bond angles

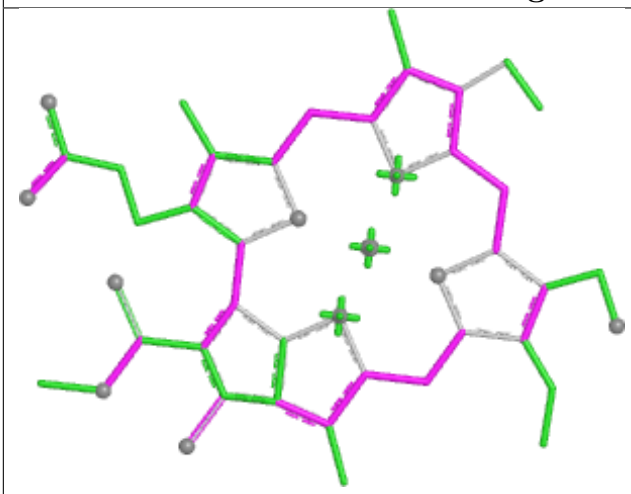


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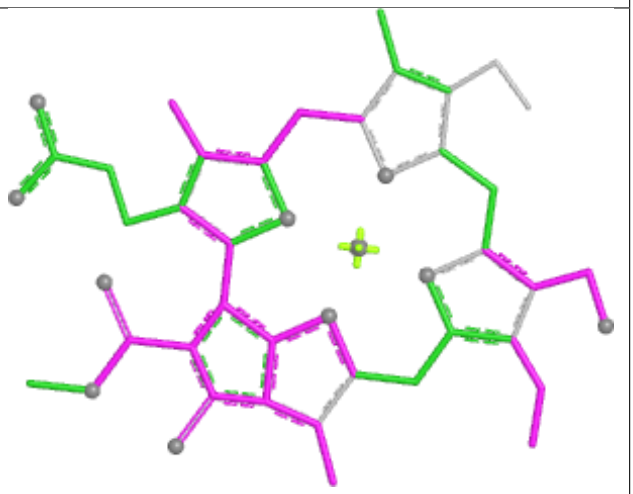


Rings

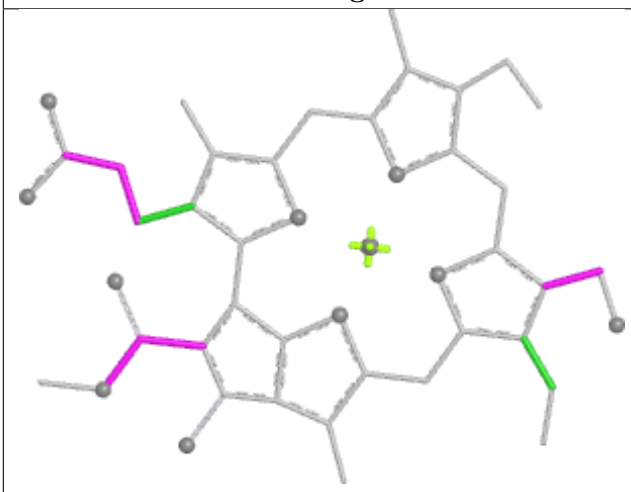
**Ligand CHL 9 607**



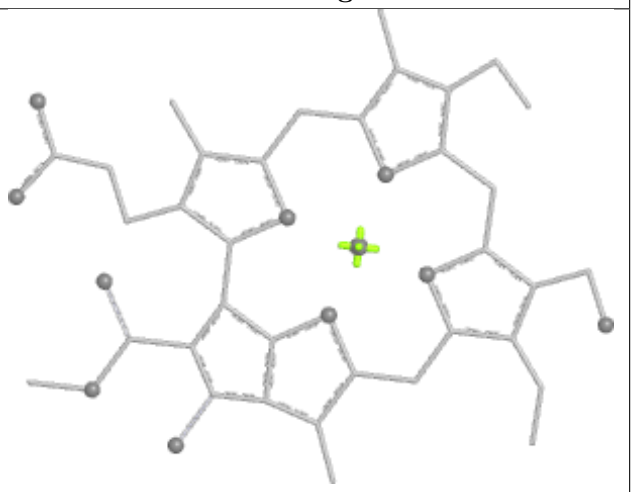
**Bond lengths**



**Bond angles**

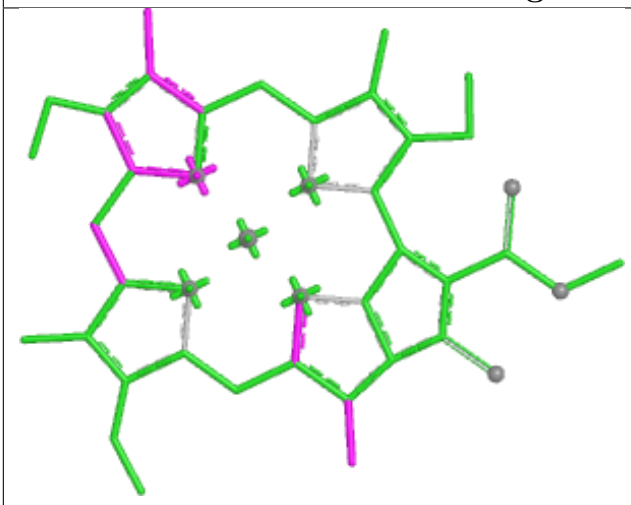


**Torsions**

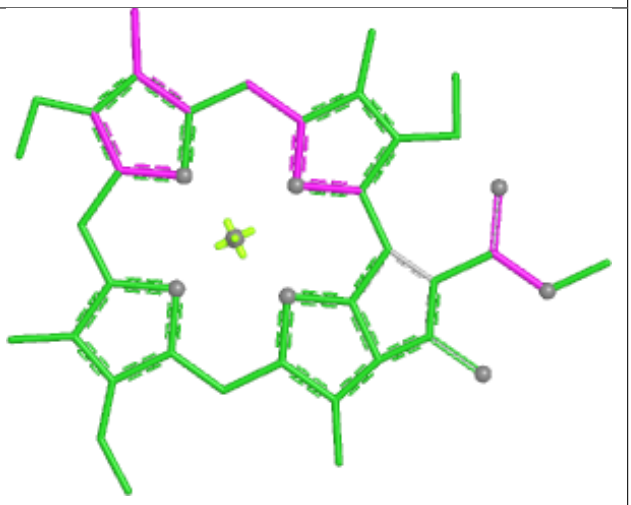


**Rings**

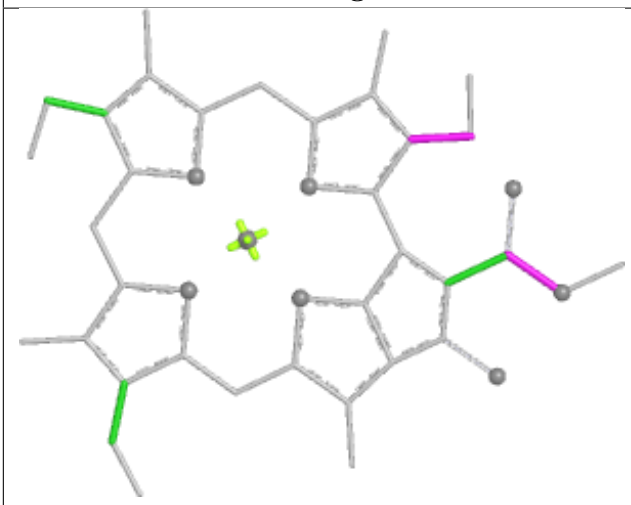
## Ligand CLA L 304



Bond lengths



Bond angles

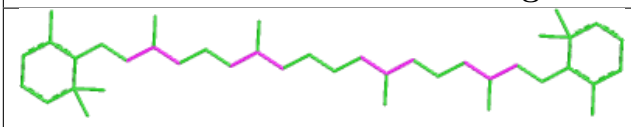


Torsions

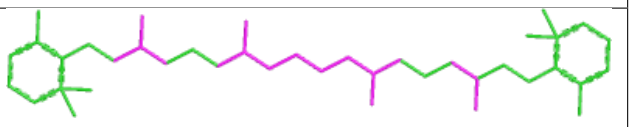


Rings

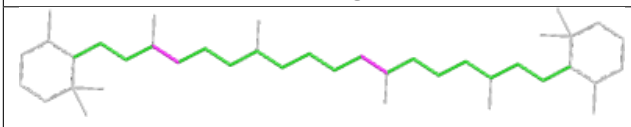
## Ligand BCR A 850



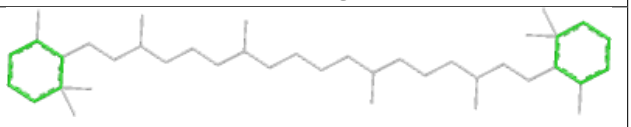
Bond lengths



Bond angles

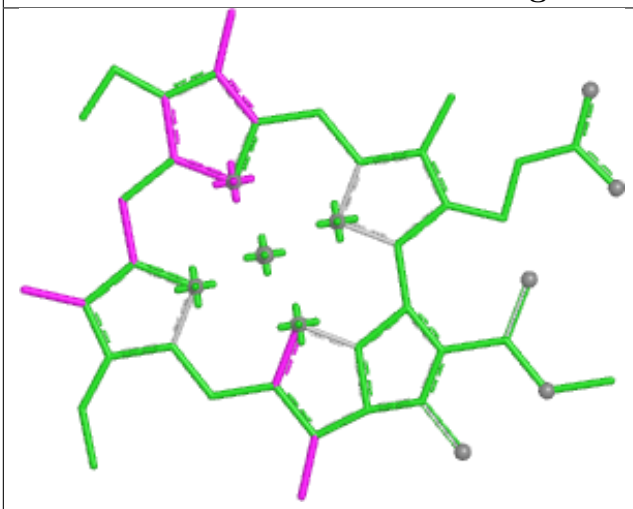


Torsions

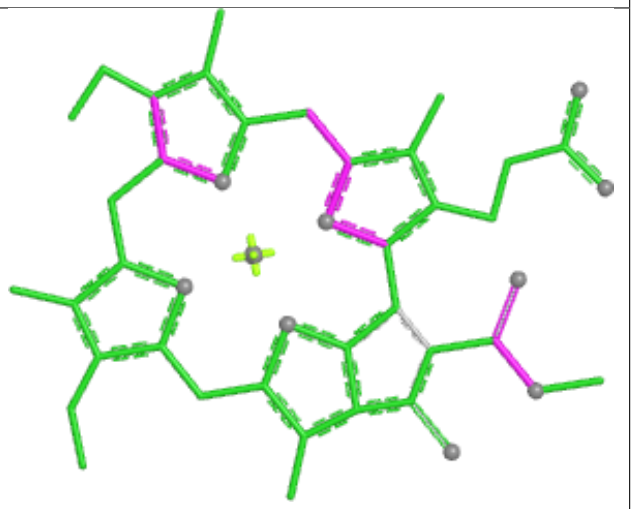


Rings

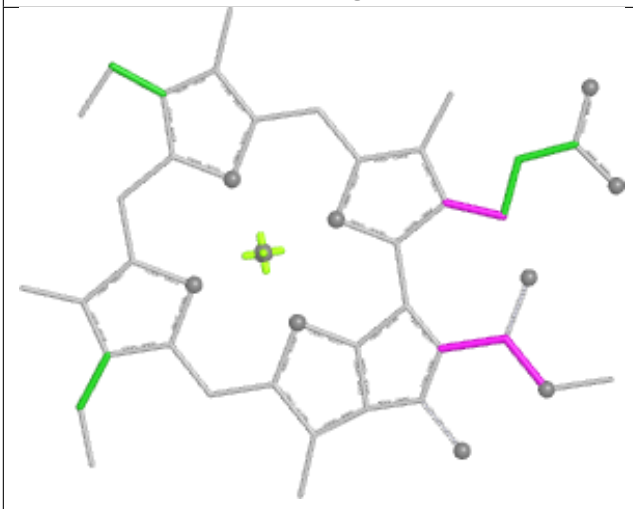
**Ligand CLA c 614**



**Bond lengths**



**Bond angles**

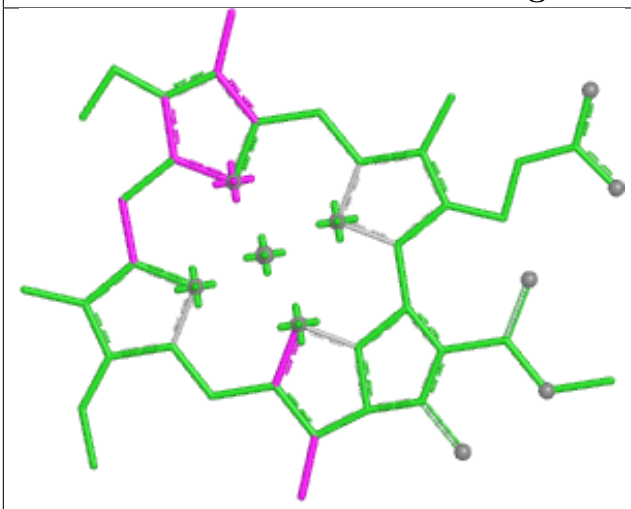


**Torsions**

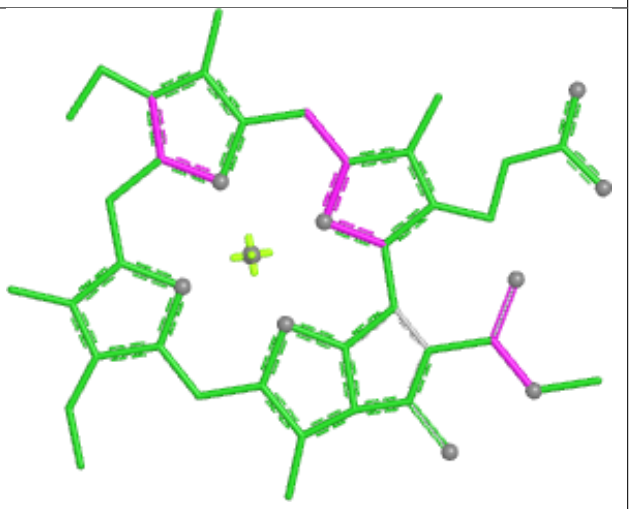


**Rings**

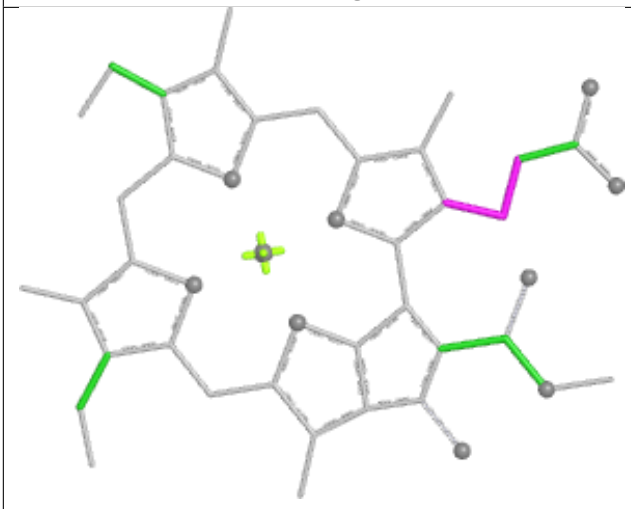
**Ligand CLA 4 610**



**Bond lengths**



**Bond angles**

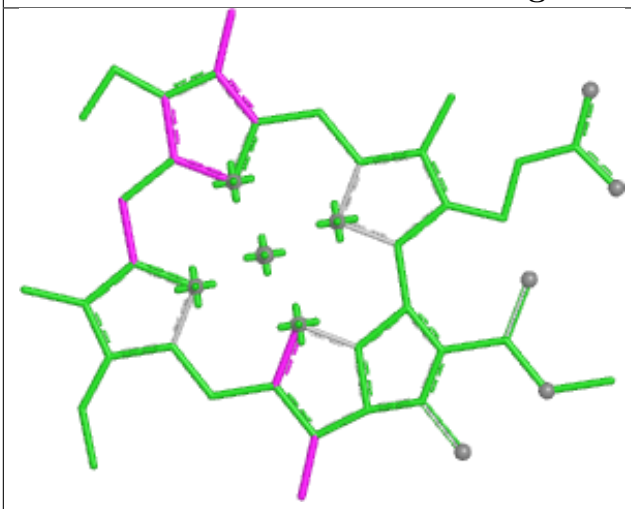


**Torsions**

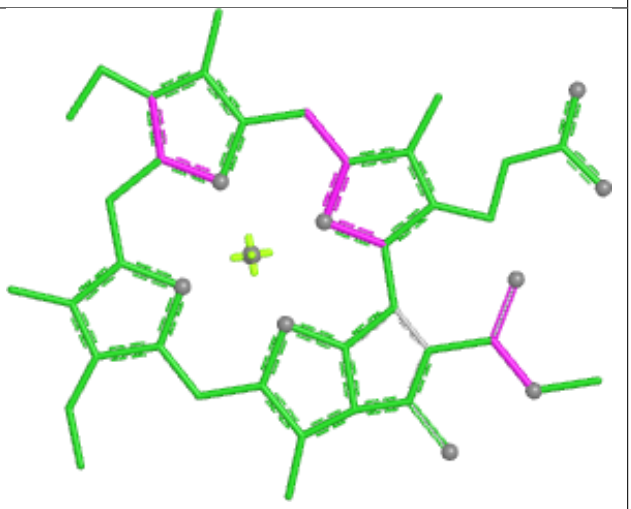


**Rings**

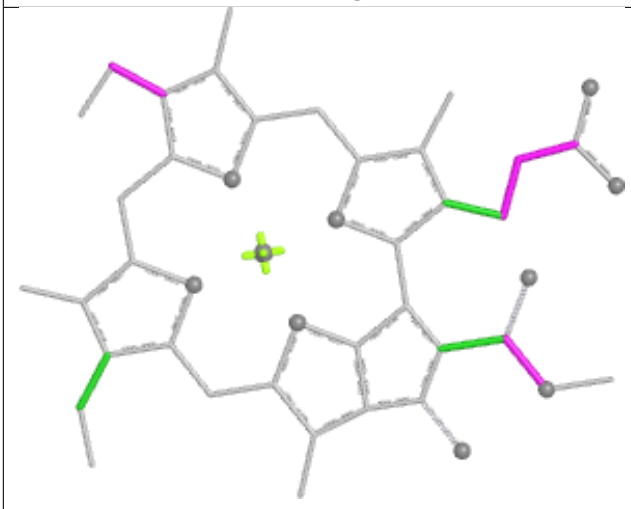
**Ligand CLA 6 612**



**Bond lengths**



**Bond angles**

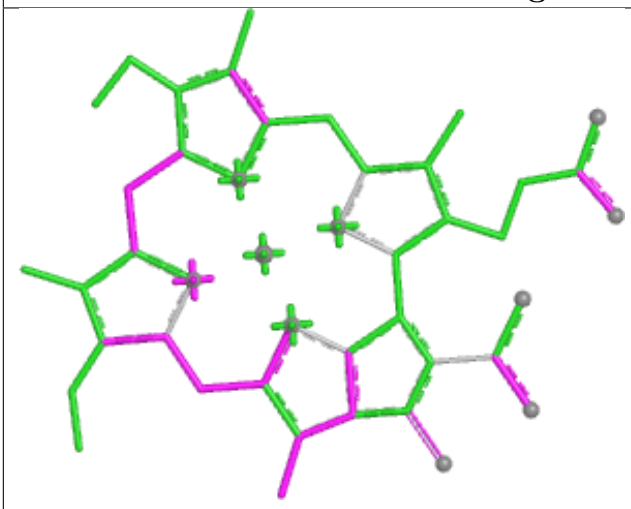


**Torsions**

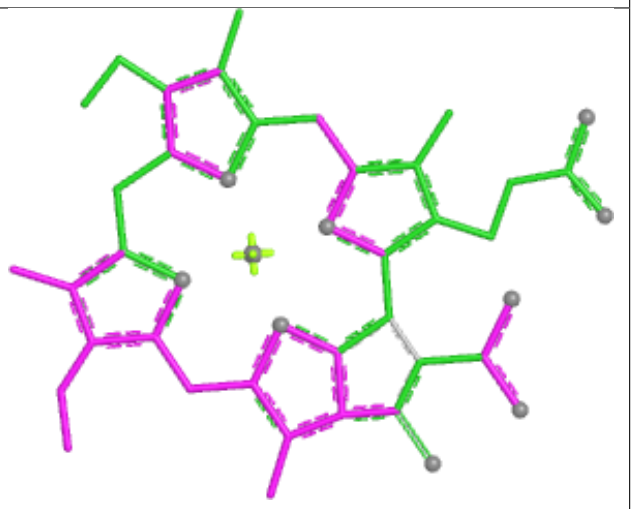


**Rings**

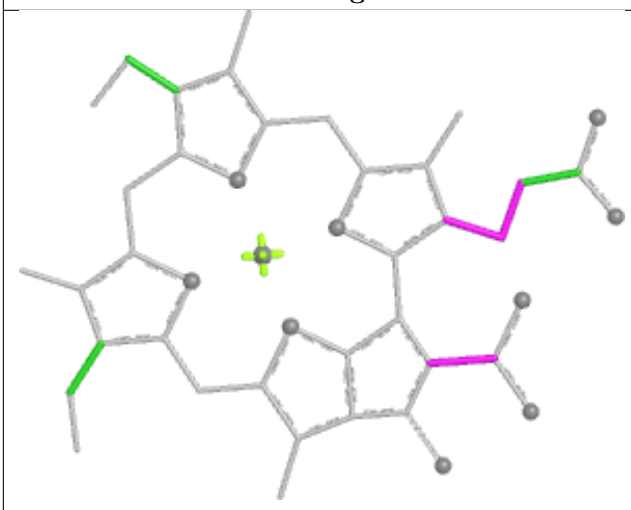
**Ligand CLA 7 407**



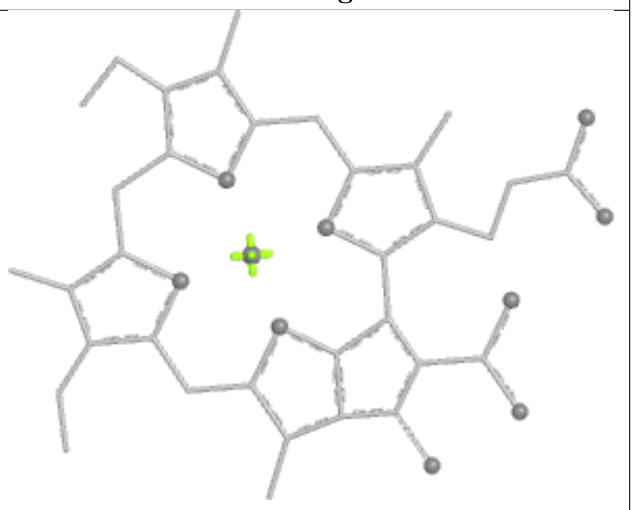
**Bond lengths**



**Bond angles**

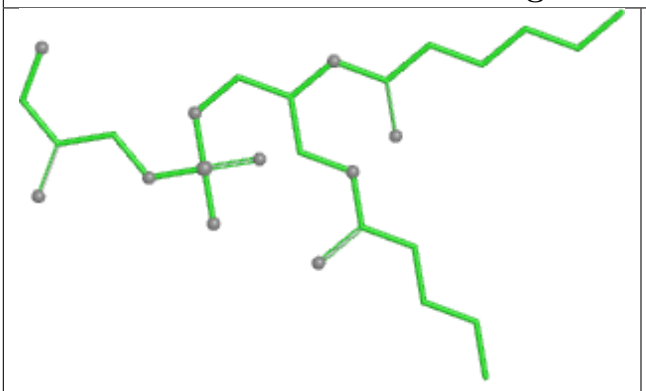


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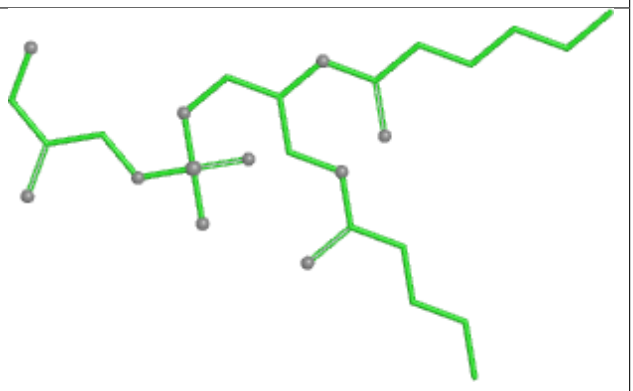


**Rings**

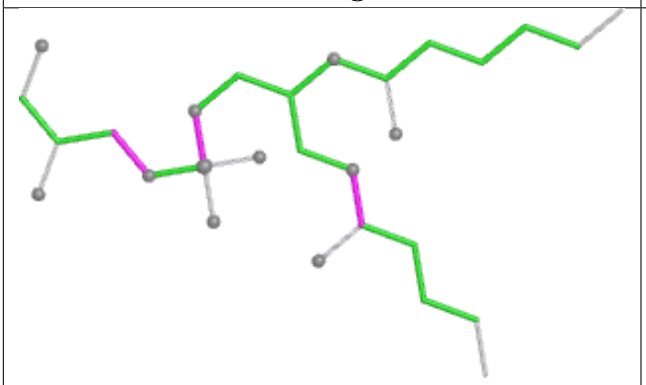
## Ligand LHG 5 617



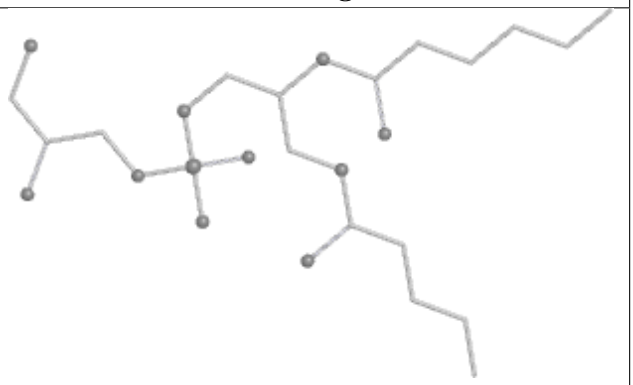
Bond lengths



Bond angles

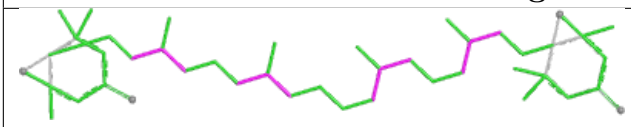


Torsions

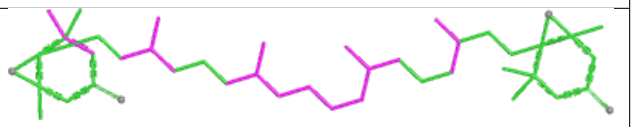


Rings

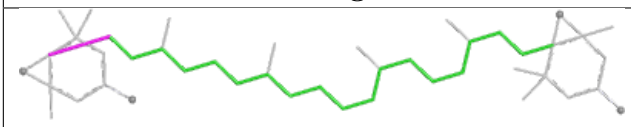
## Ligand XAT c 617



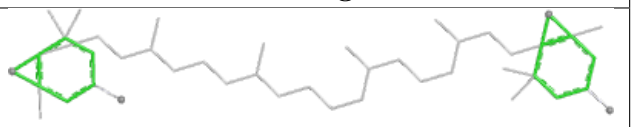
Bond lengths



Bond angles

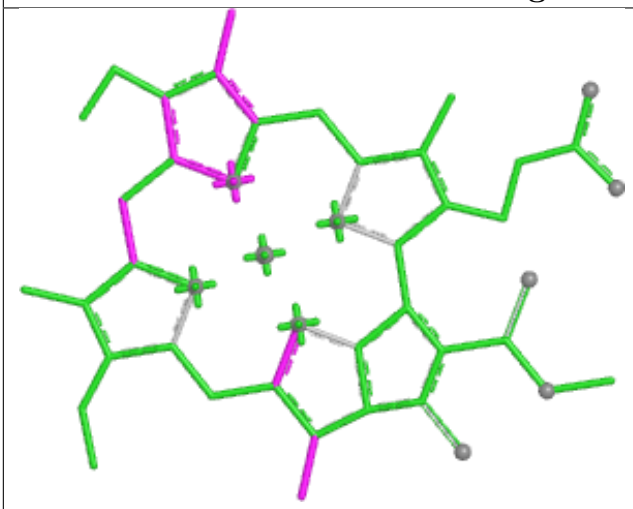


Torsions

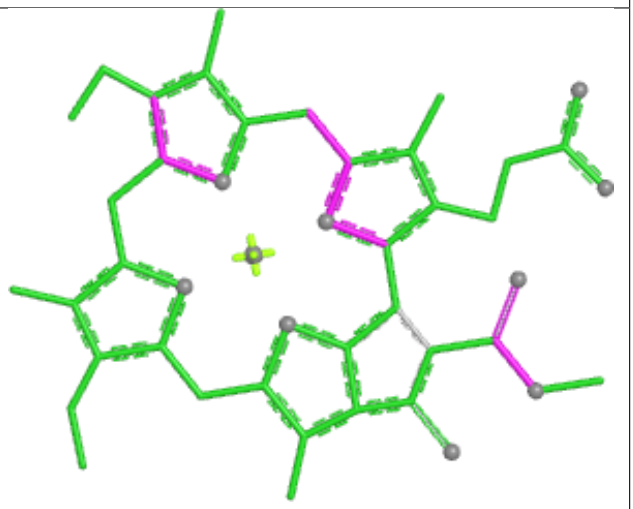


Rings

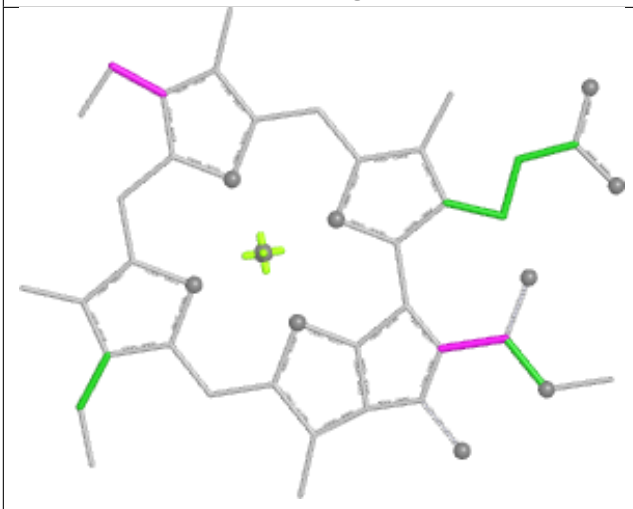
**Ligand CLA 4 601**



**Bond lengths**



**Bond angles**

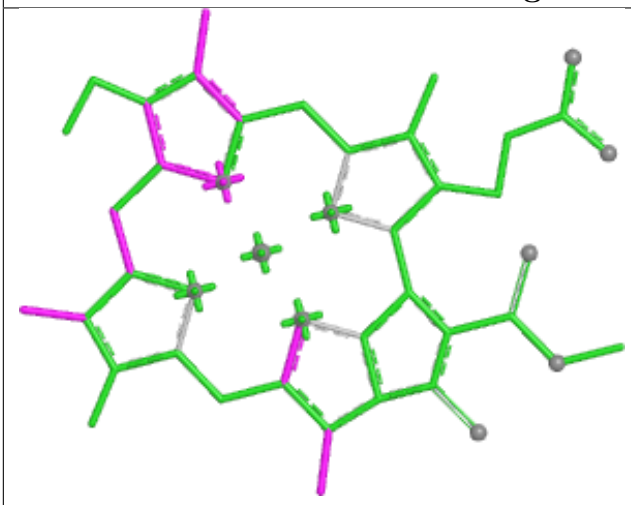


**Torsions**

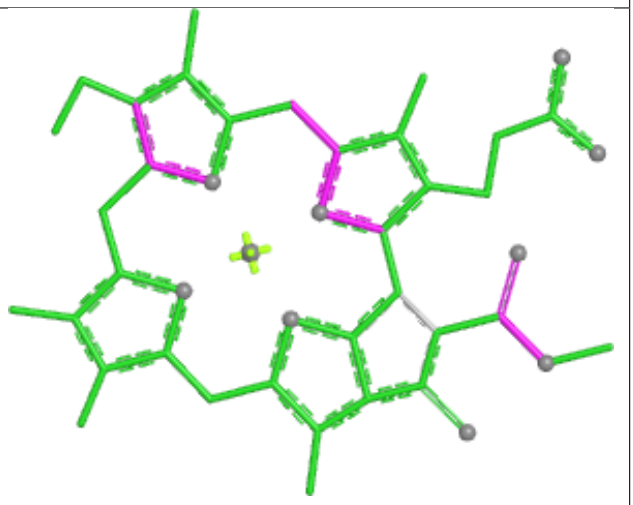


**Rings**

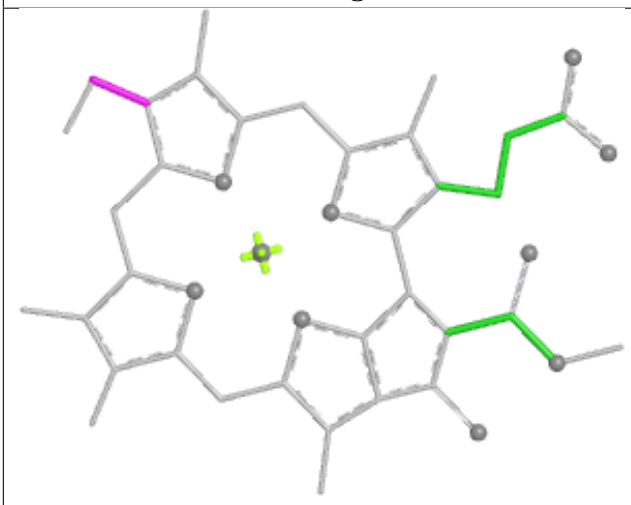
**Ligand CLA A 820**



**Bond lengths**



**Bond angles**

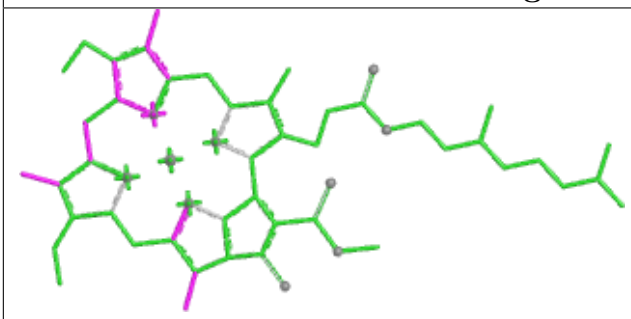


**Torsions**

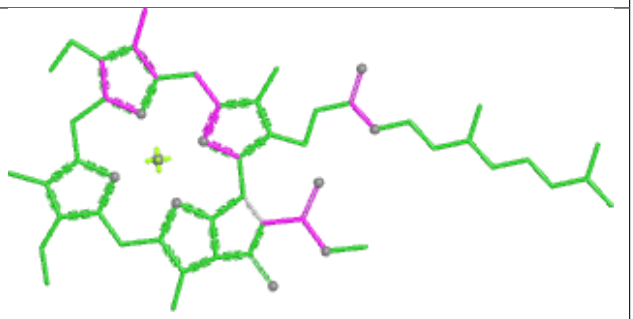


**Rings**

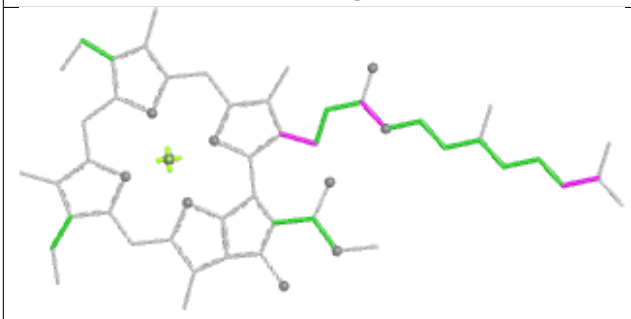
## Ligand CLA A 805



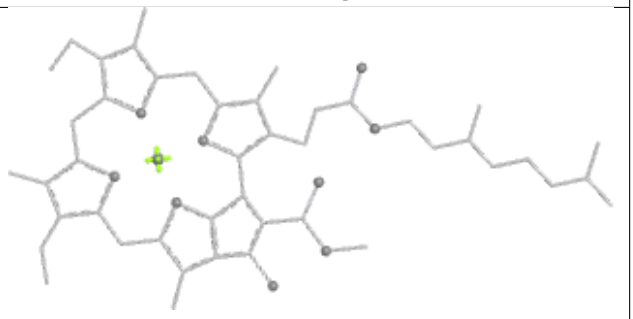
Bond lengths



Bond angles

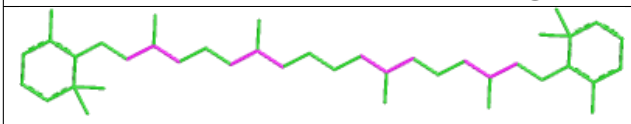


Torsions



Rings

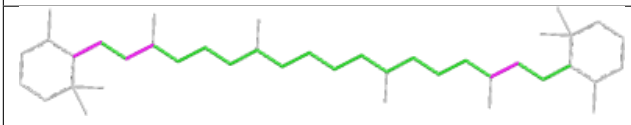
## Ligand BCR 7 418



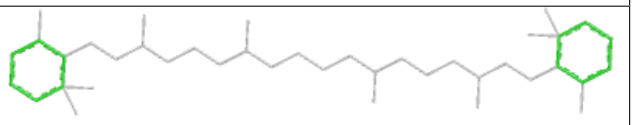
Bond lengths



Bond angles

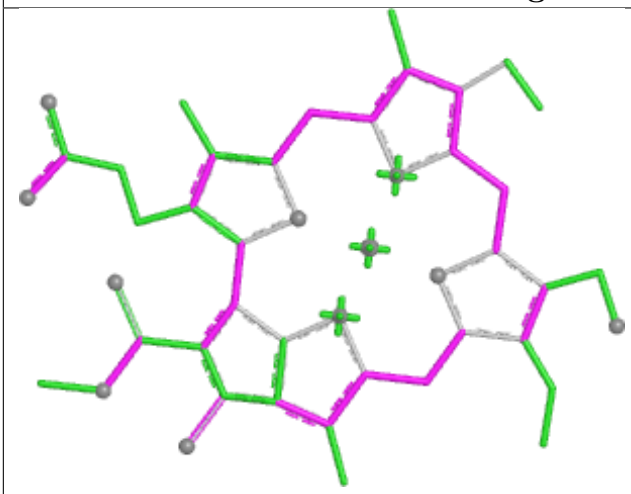


Torsions

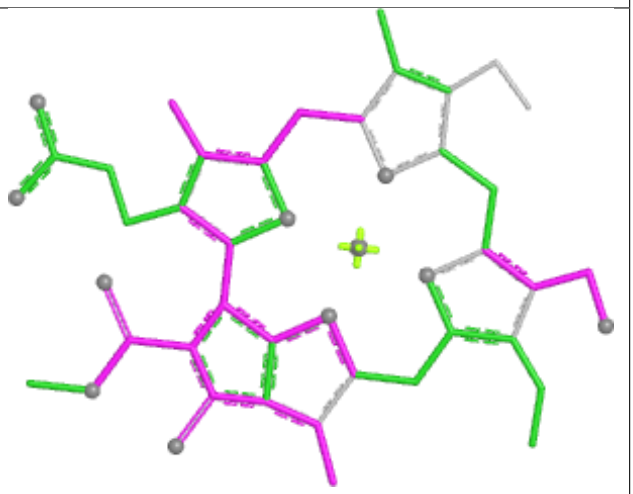


Rings

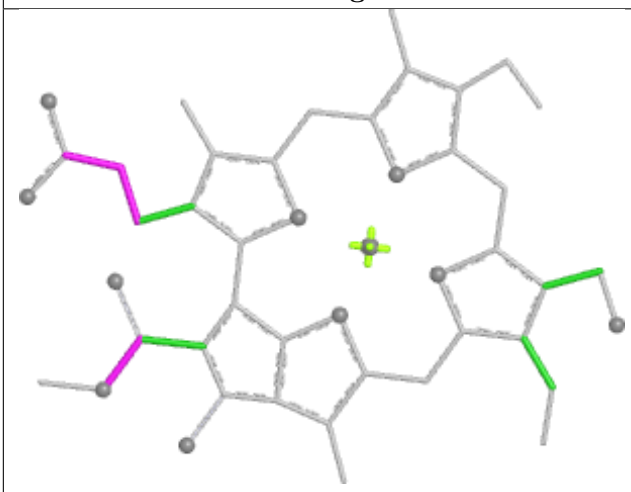
## Ligand CHL 4 606



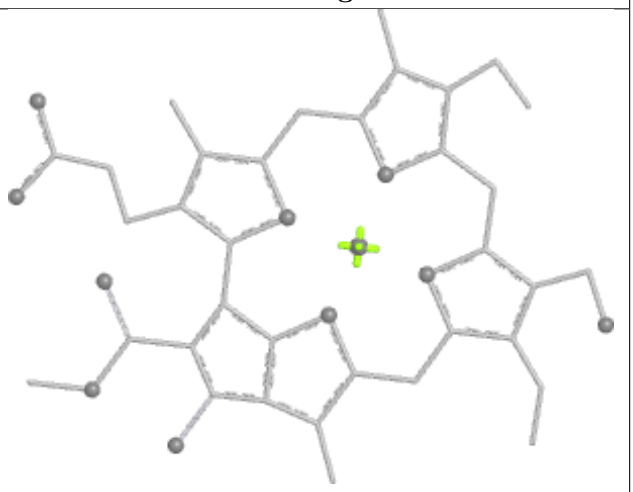
Bond lengths



Bond angles

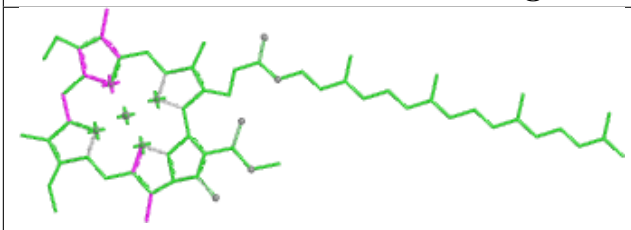


Torsions

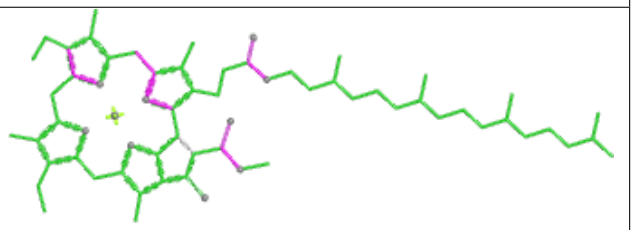


Rings

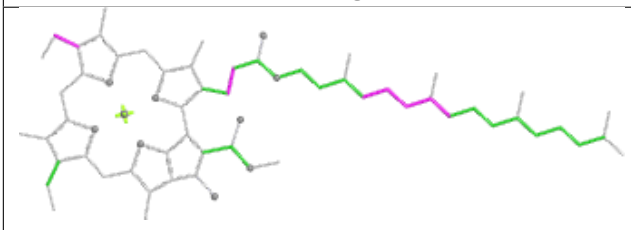
## Ligand CLA B 838



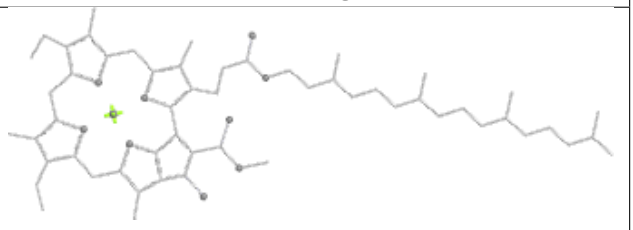
Bond lengths



Bond angles

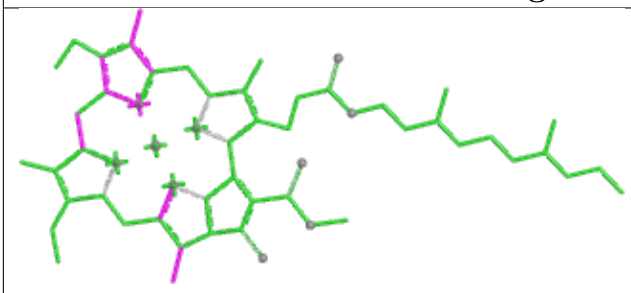


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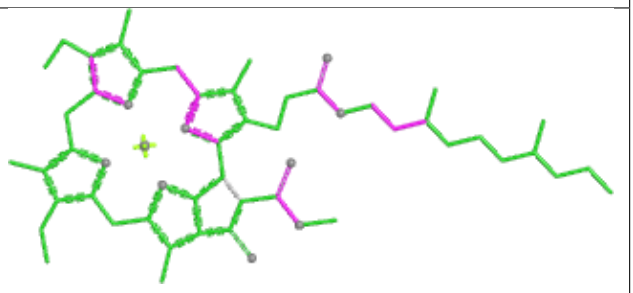


Rings

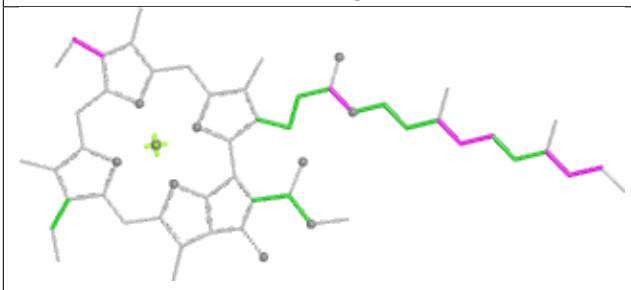
**Ligand CLA 9 611**



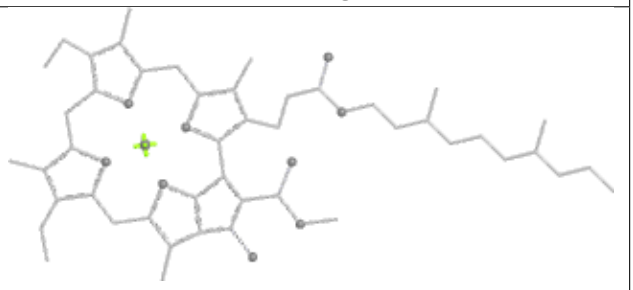
**Bond lengths**



**Bond angles**

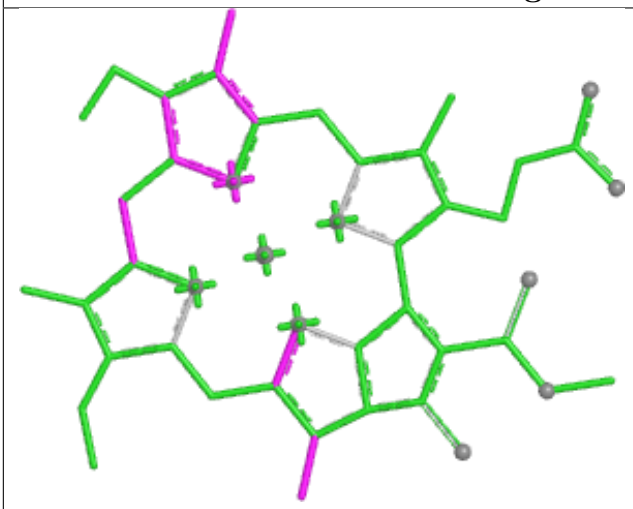


**Torsions**

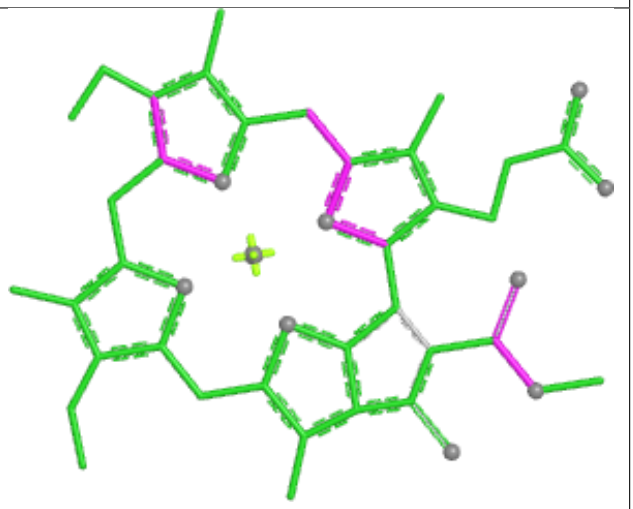


**Rings**

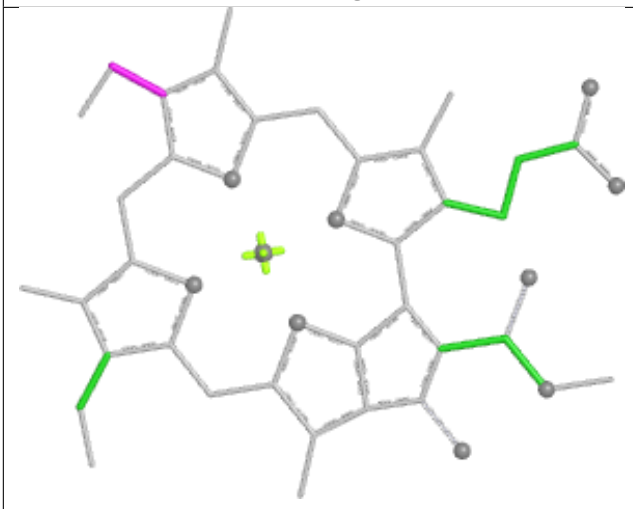
**Ligand CLA B 833**



**Bond lengths**



**Bond angles**

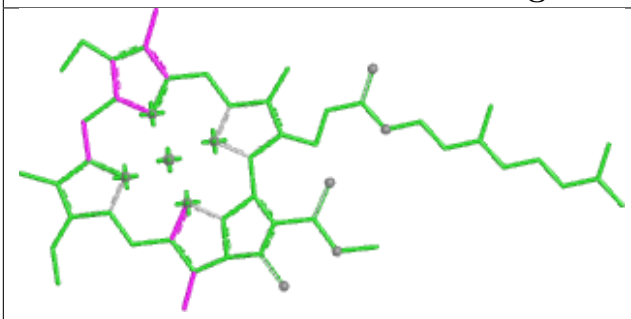


**Torsions**

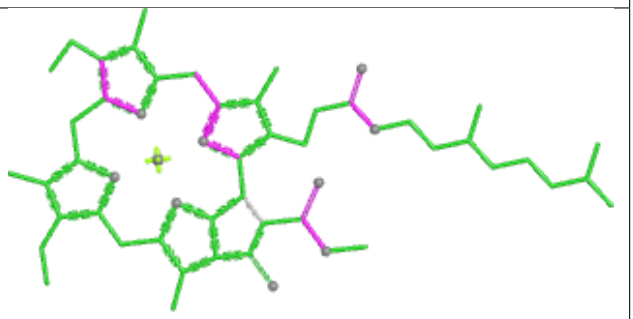


**Rings**

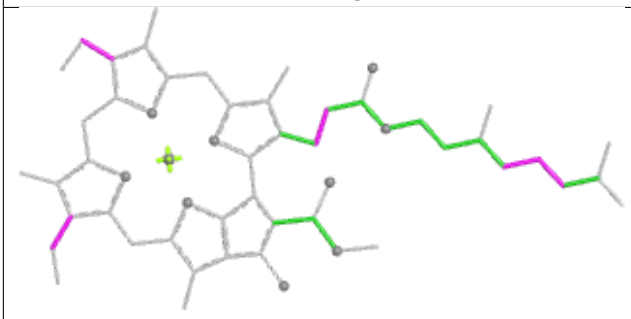
**Ligand CLA 4 612**



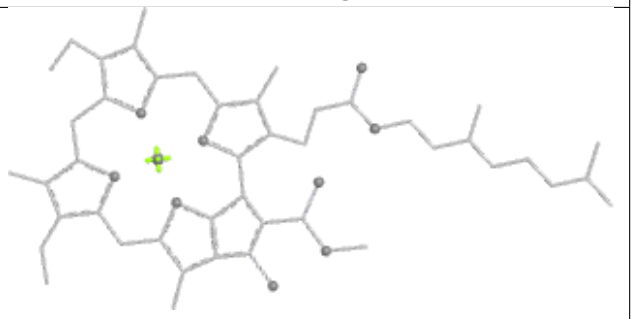
**Bond lengths**



**Bond angles**

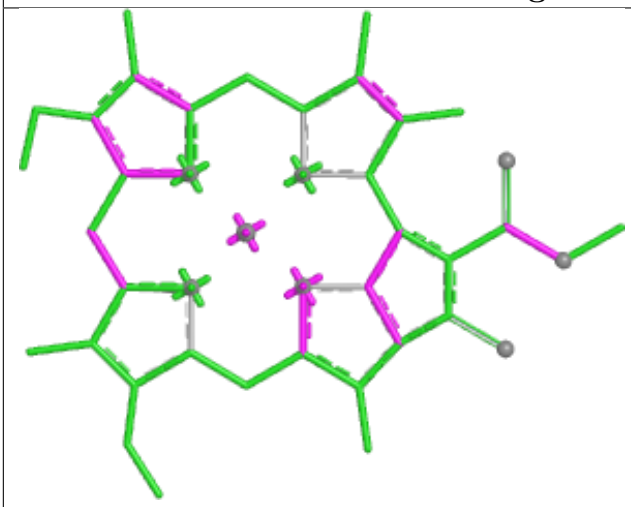


**Torsions**

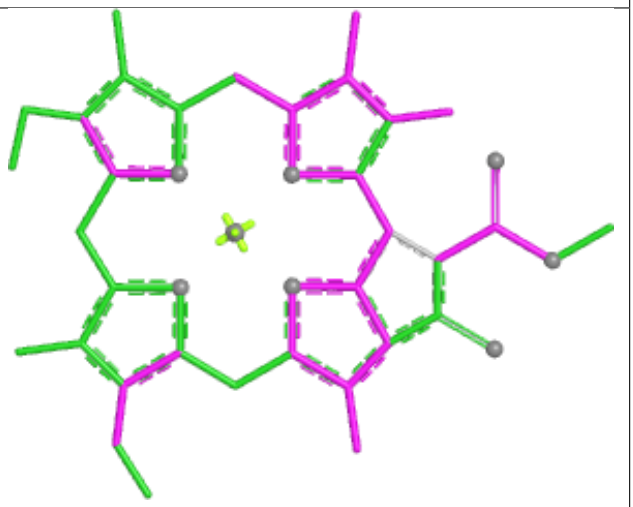


**Rings**

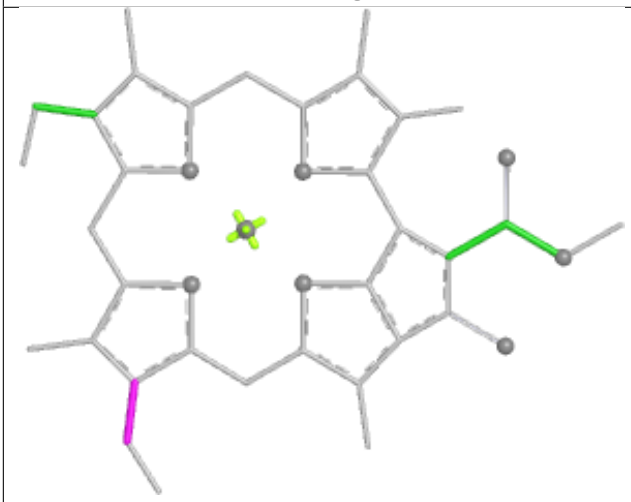
**Ligand CLA 1 309**



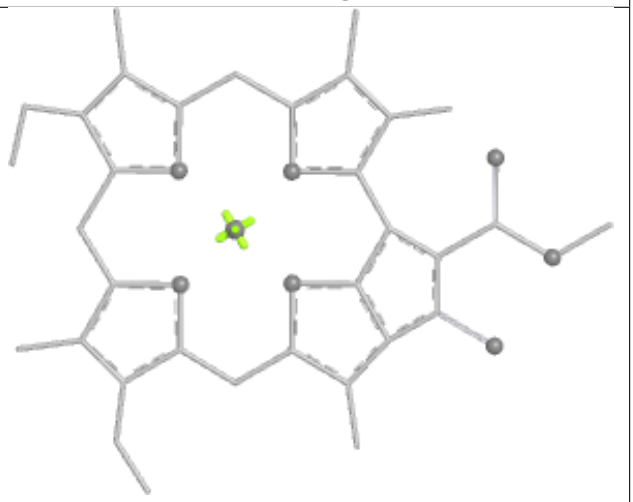
**Bond lengths**



**Bond angles**

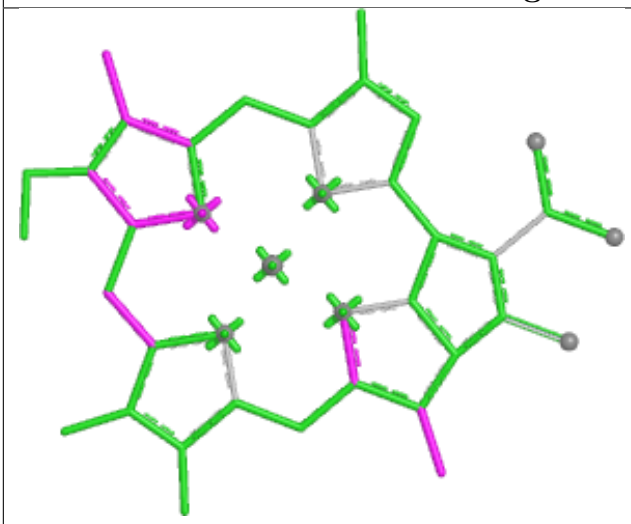


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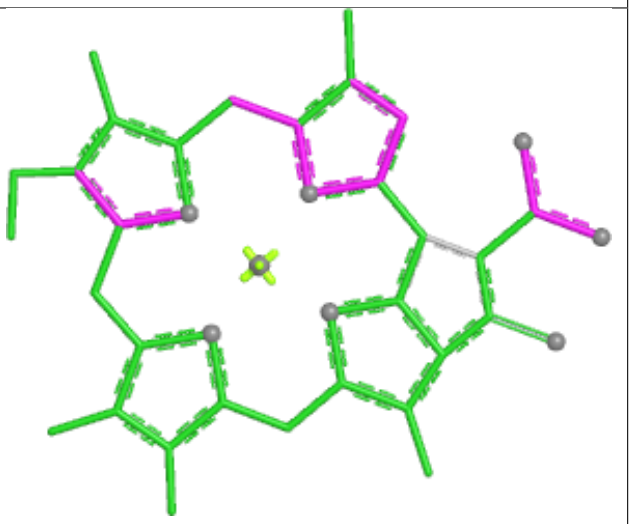


**Rings**

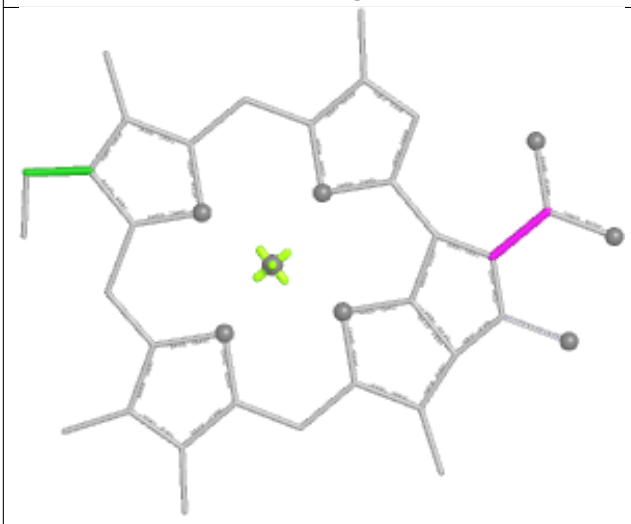
**Ligand CLA O 202**



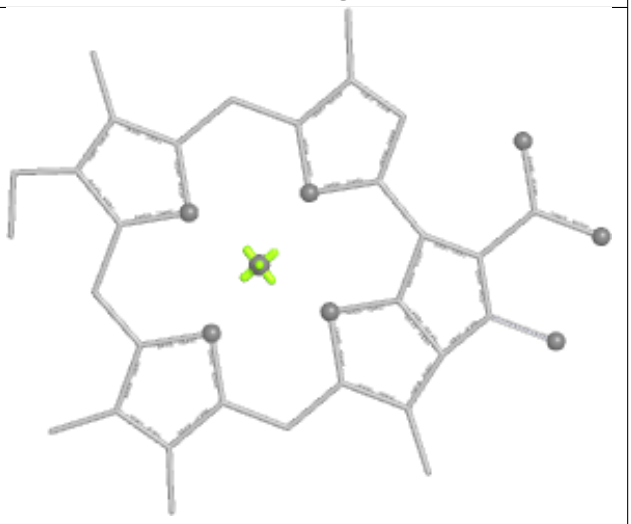
**Bond lengths**



**Bond angles**

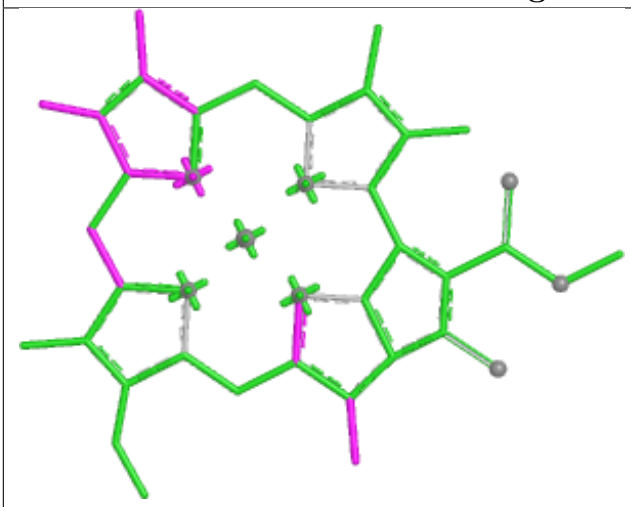


**Torsions**

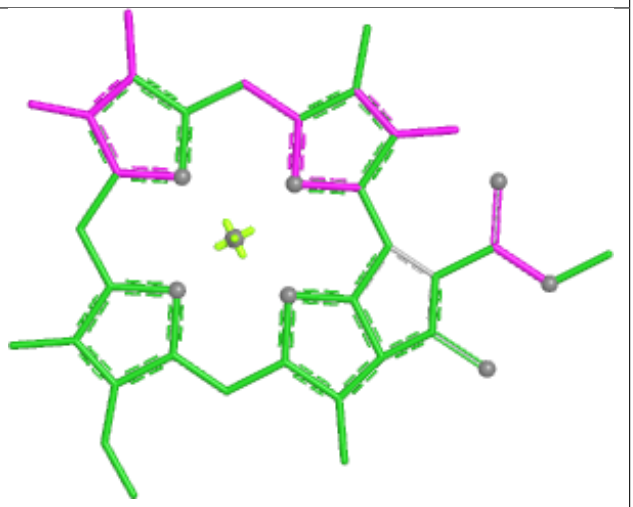


**Rings**

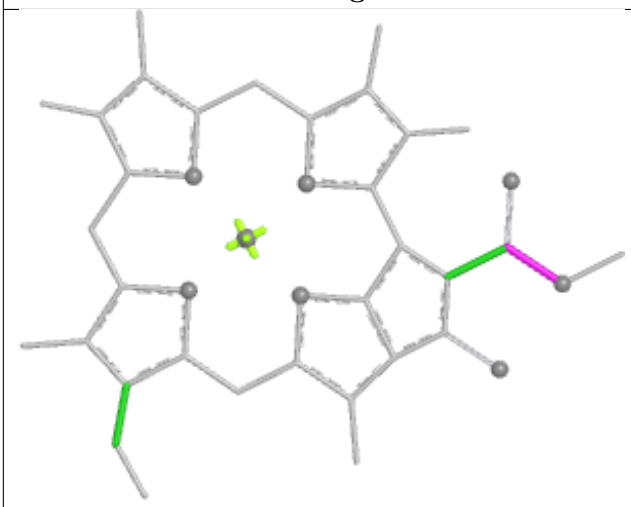
**Ligand CLA 5 608**



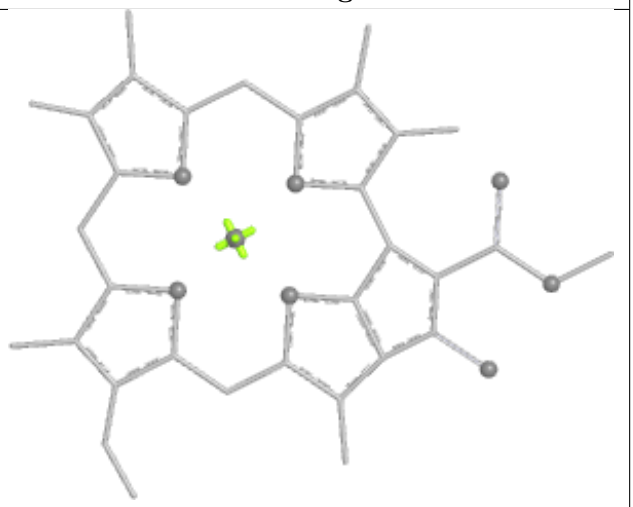
**Bond lengths**



**Bond angles**

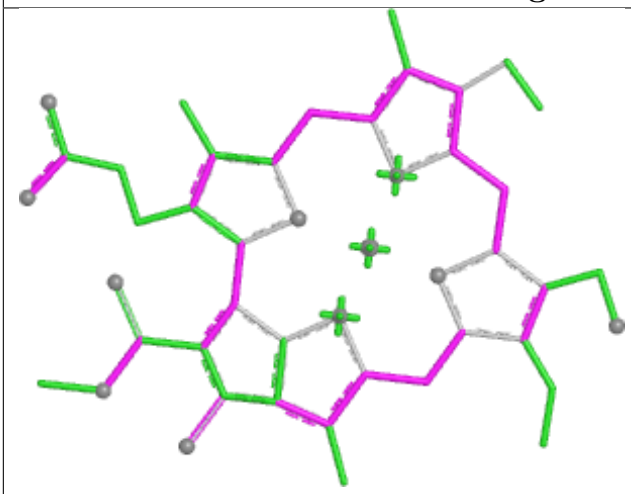


**Torsions**

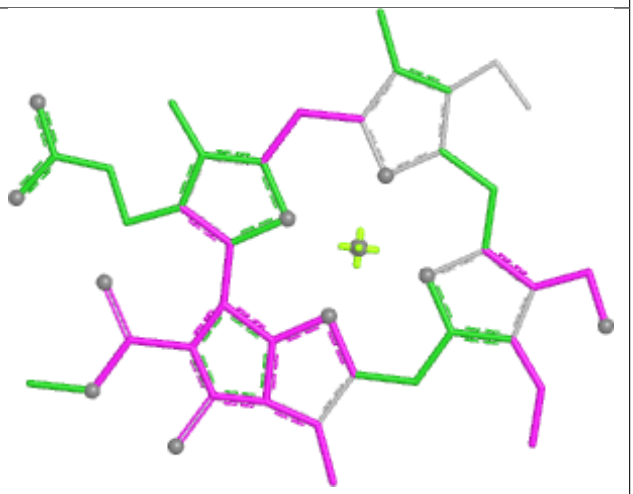


**Rings**

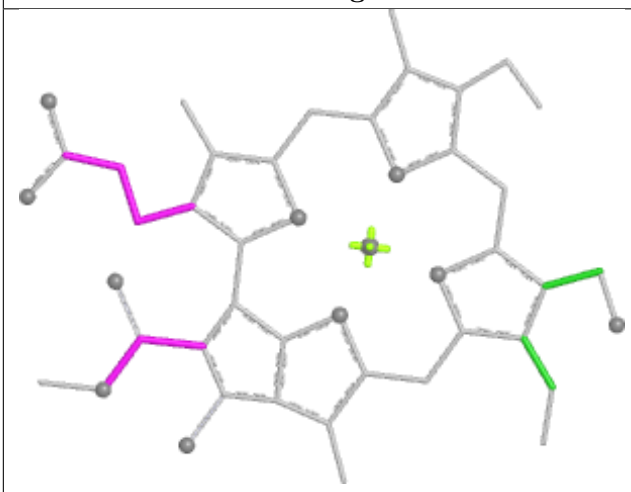
**Ligand CHL c 608**



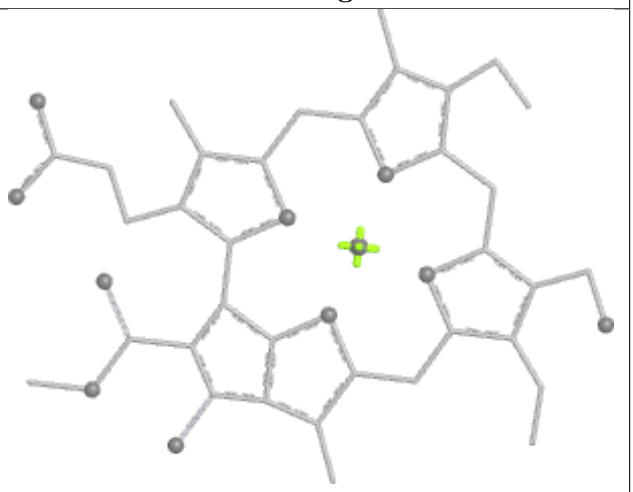
**Bond lengths**



**Bond angles**

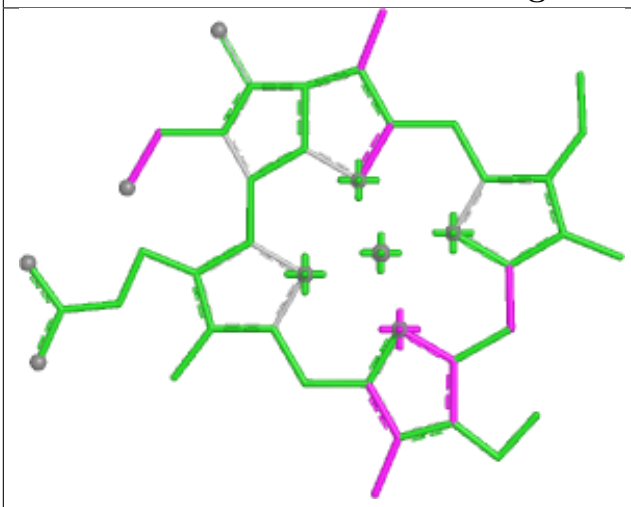


**Torsions**

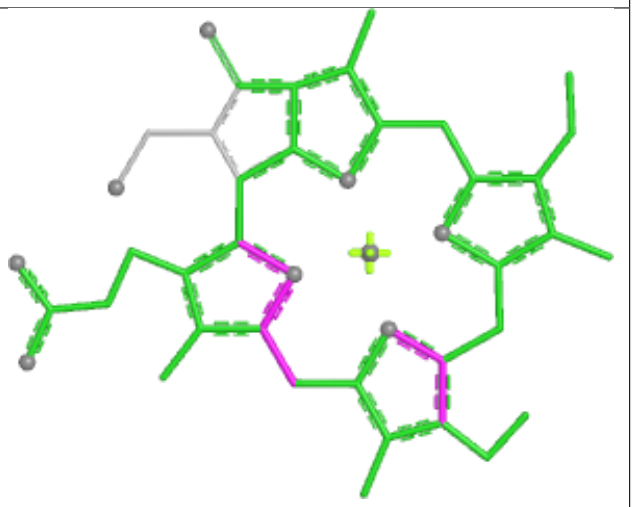


**Rings**

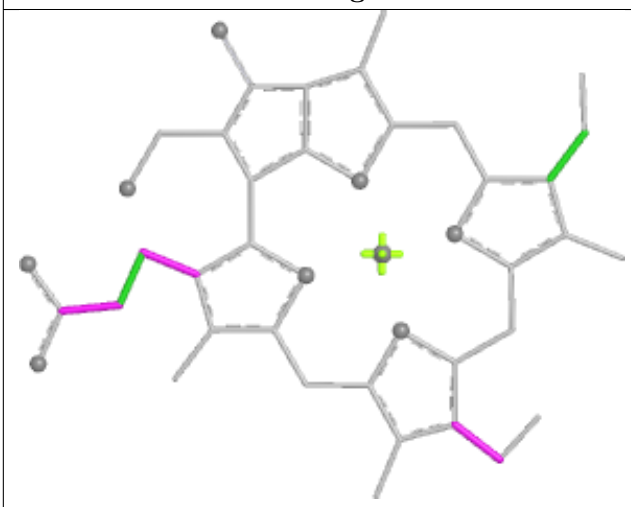
## Ligand CLA 8 608



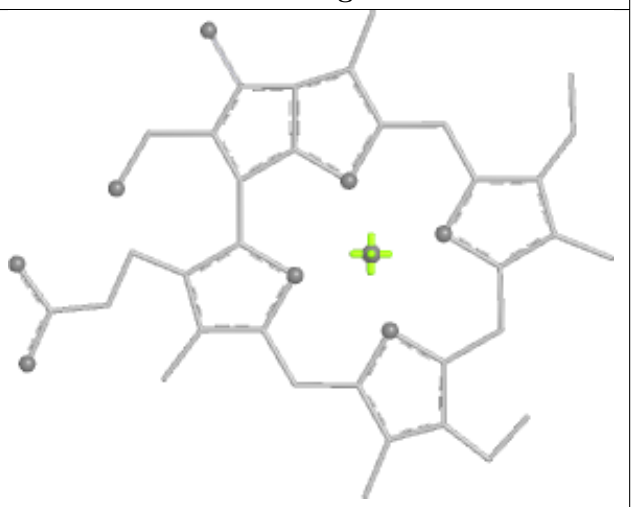
Bond lengths



Bond angles

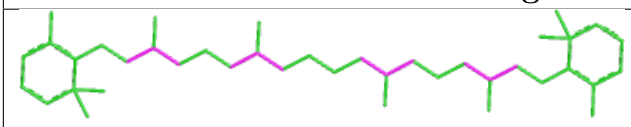


Torsions

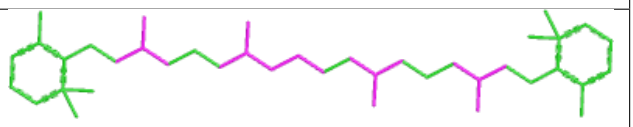


Rings

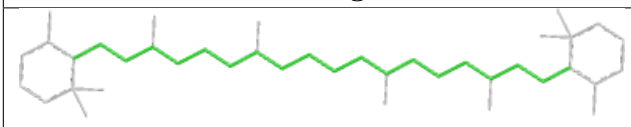
## Ligand BCR A 847



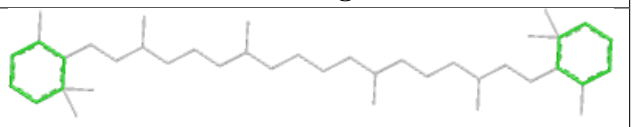
Bond lengths



Bond angles

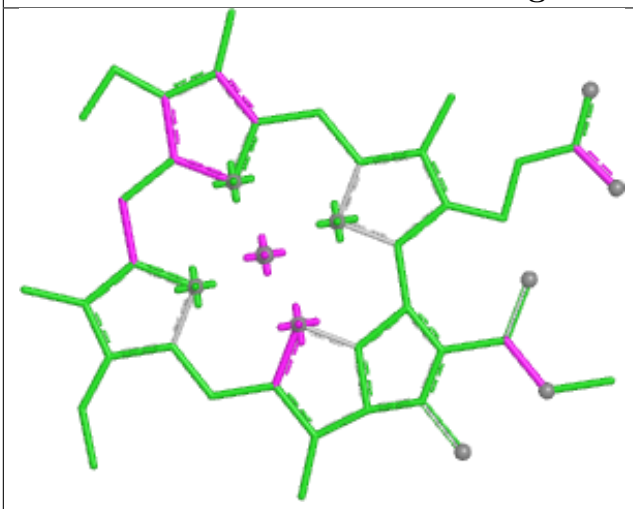


Torsions

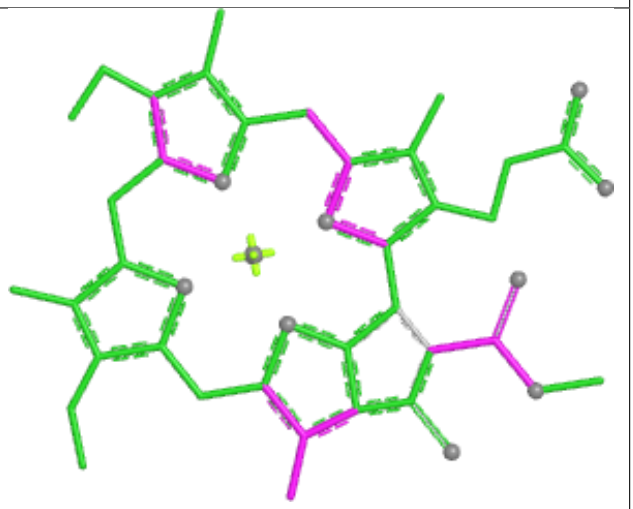


Rings

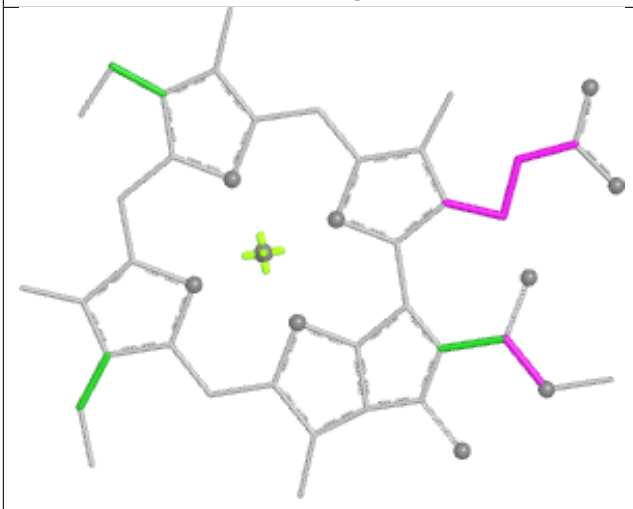
**Ligand CLA 8 609**



**Bond lengths**



**Bond angles**

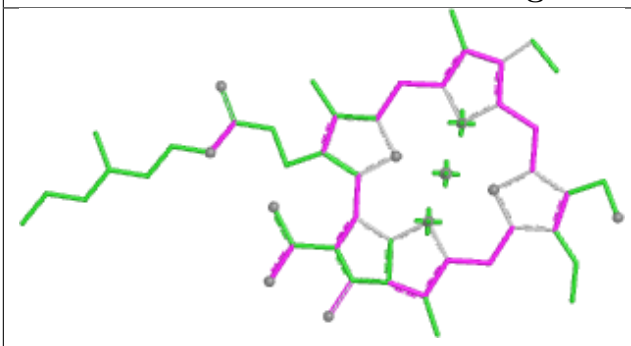


**Torsions**

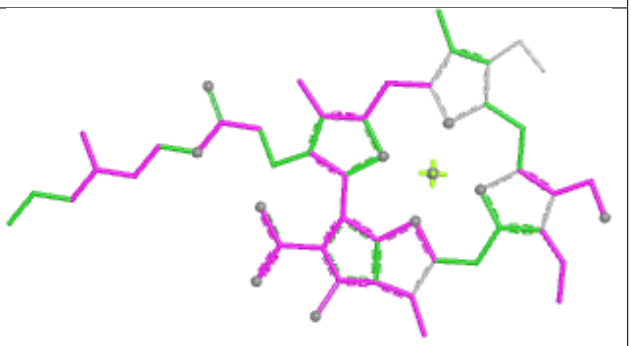


**Rings**

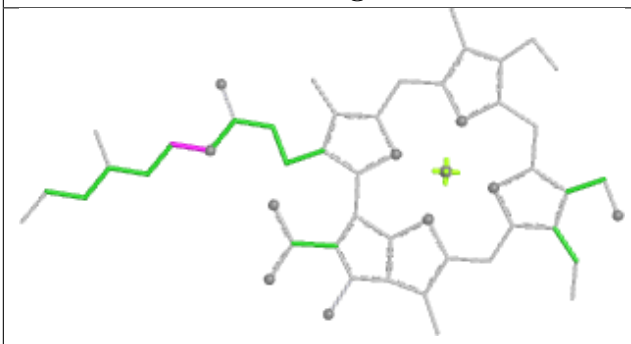
**Ligand CHL b 310**



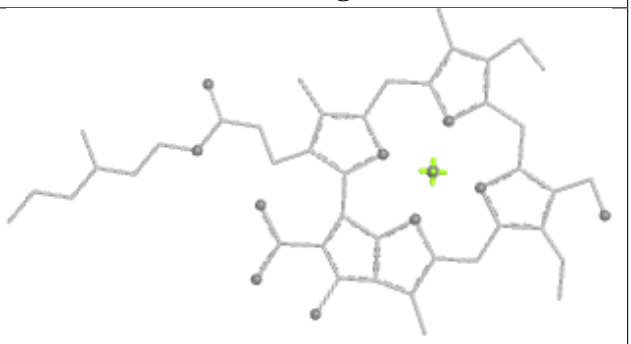
**Bond lengths**



**Bond angles**

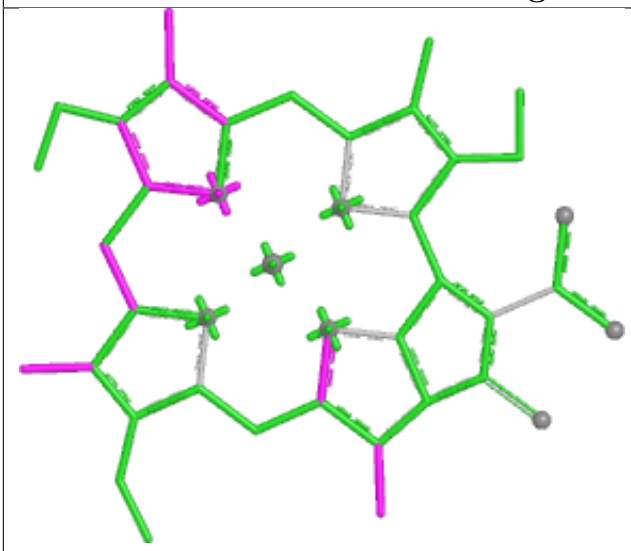


**Torsions**

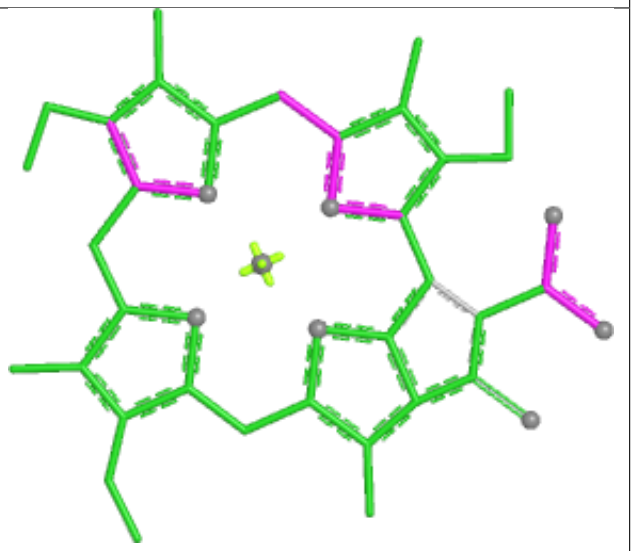


**Rings**

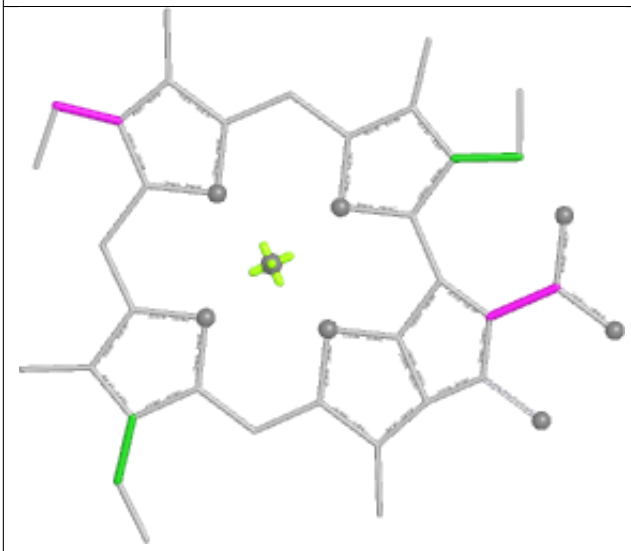
**Ligand CLA 3 405**



**Bond lengths**



**Bond angles**

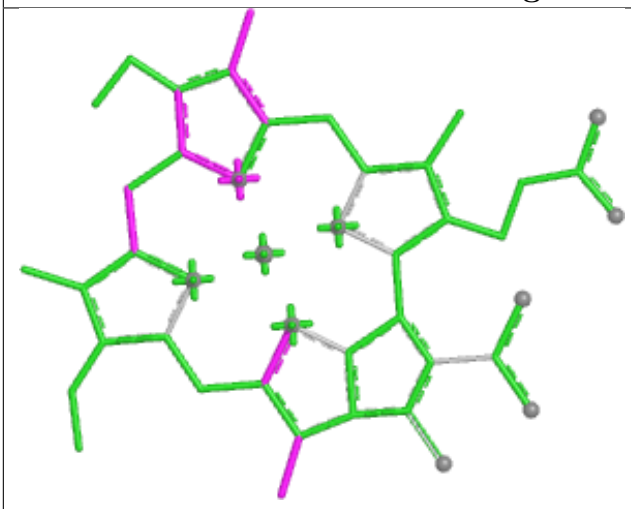


**Torsions**

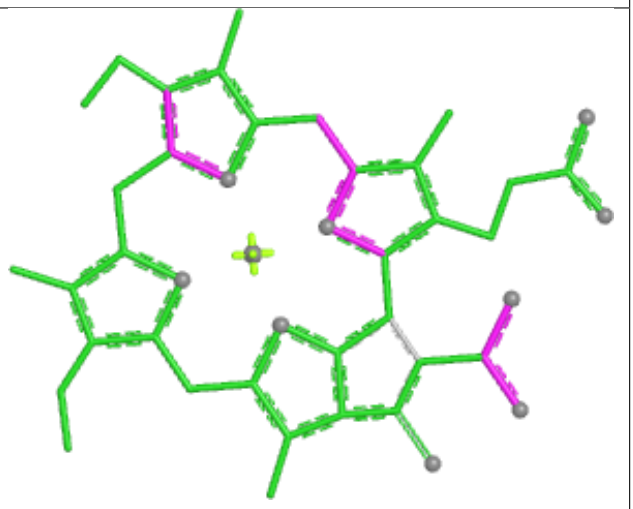


**Rings**

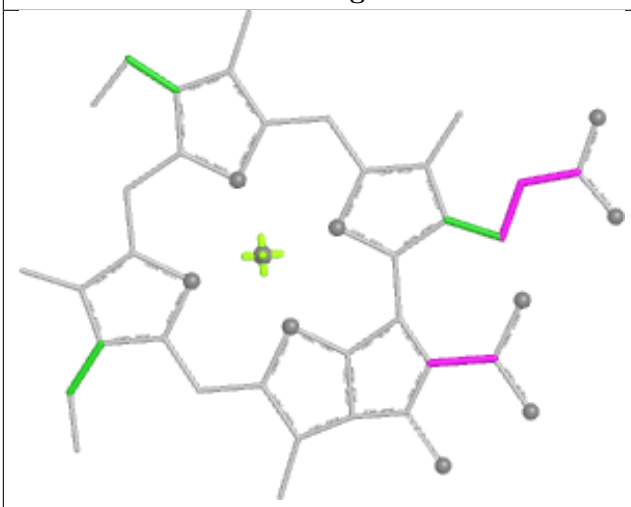
## Ligand CLA G 204



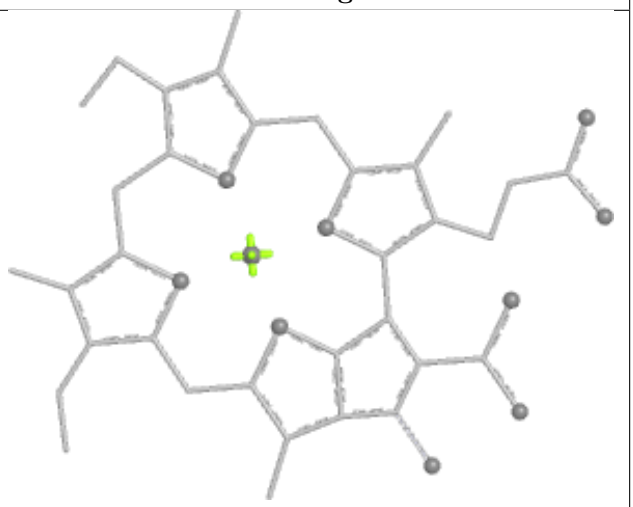
Bond lengths



Bond angles

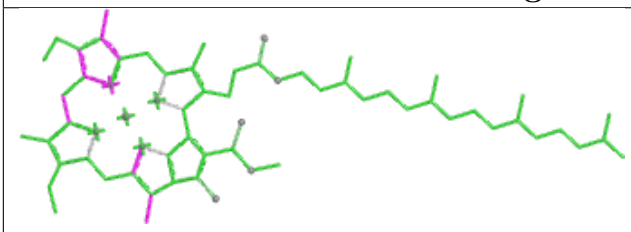


Torsions

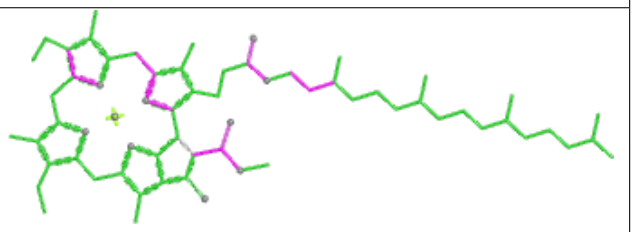


Rings

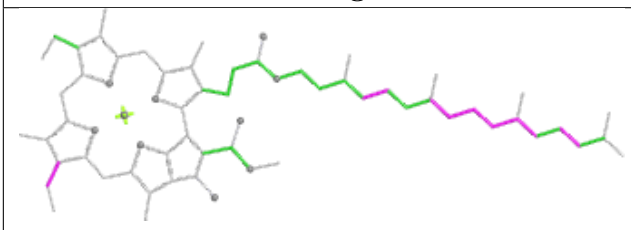
## Ligand CLA B 823



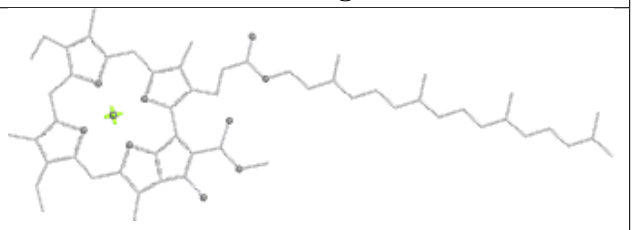
Bond lengths



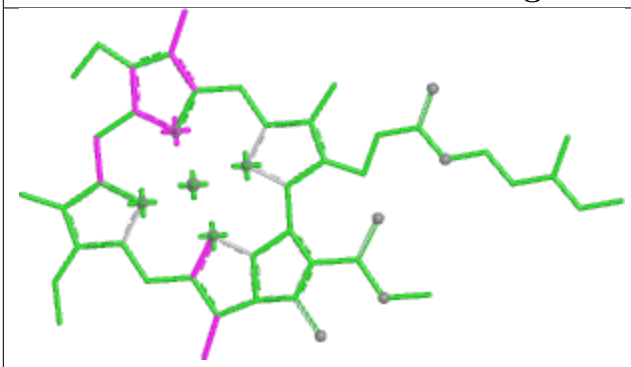
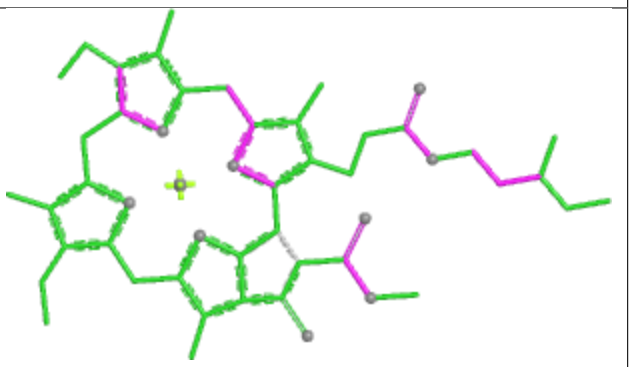
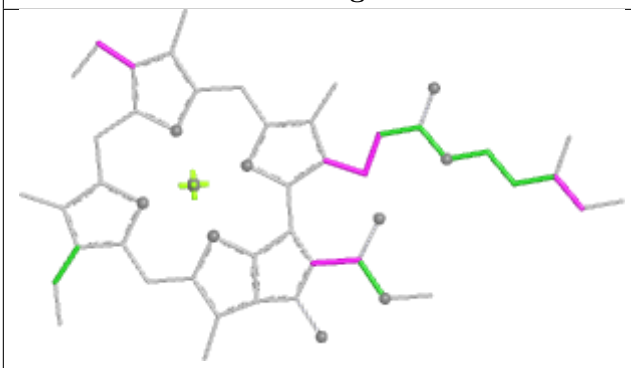
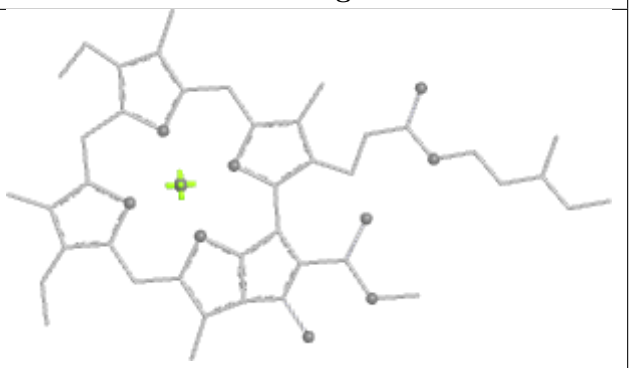
Bond angles

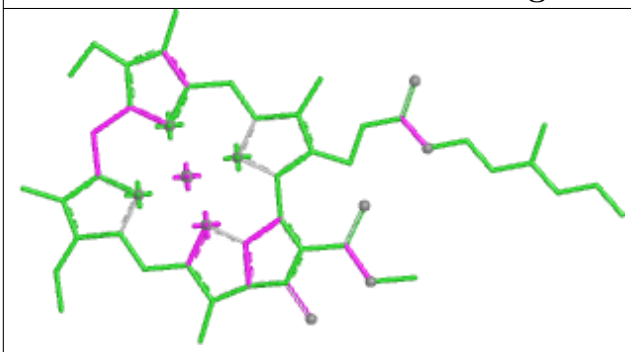
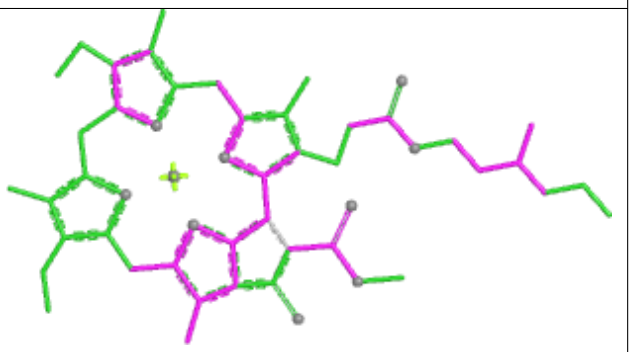
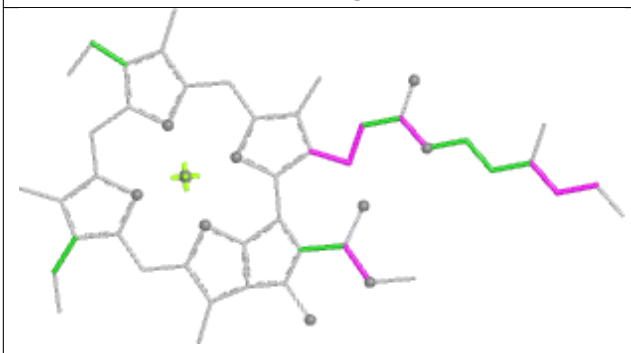
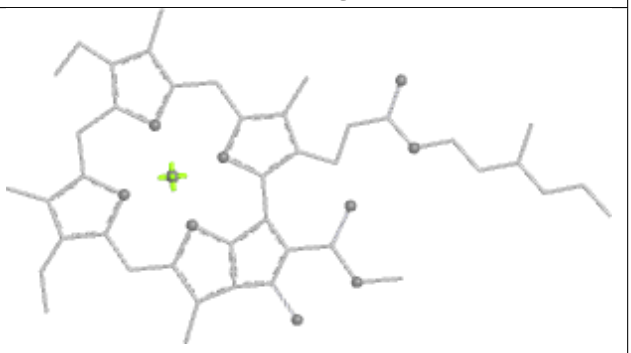


Torsions



Rings

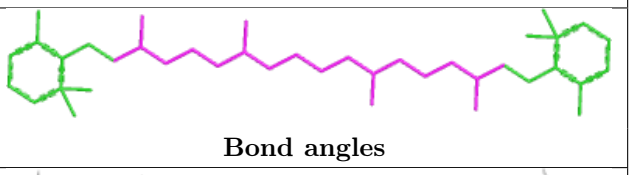
| Ligand CLA A 837 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 4 609 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

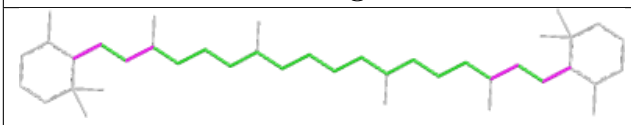
## Ligand BCR M 101



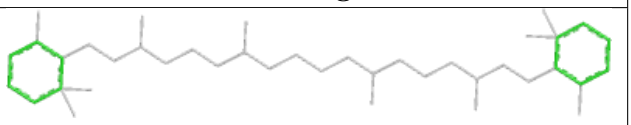
Bond lengths



Bond angles

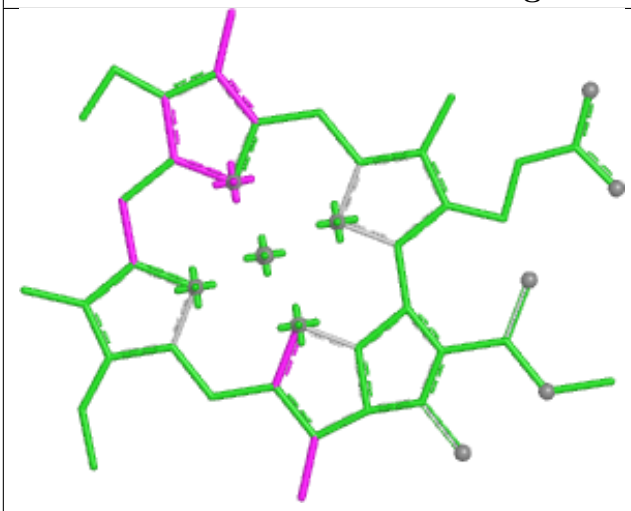


Torsions

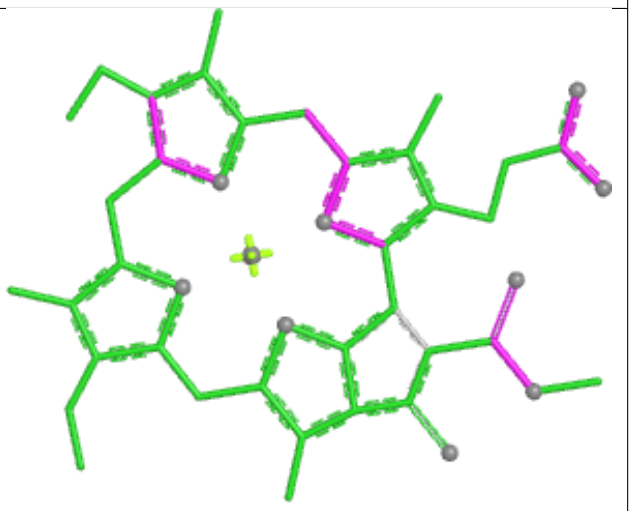


Rings

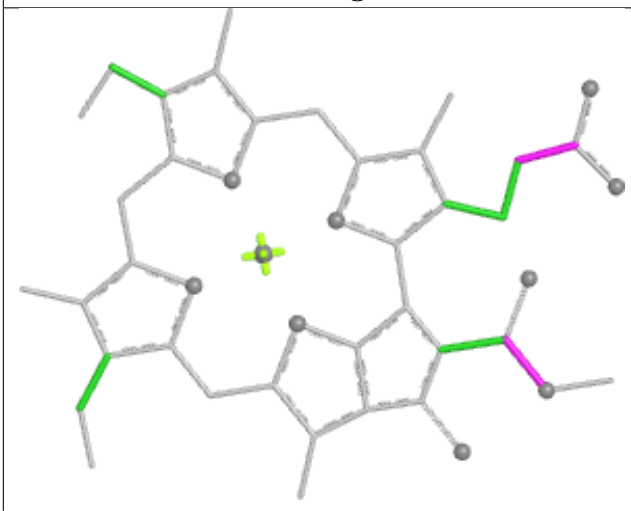
## Ligand CLA A 810



Bond lengths



Bond angles

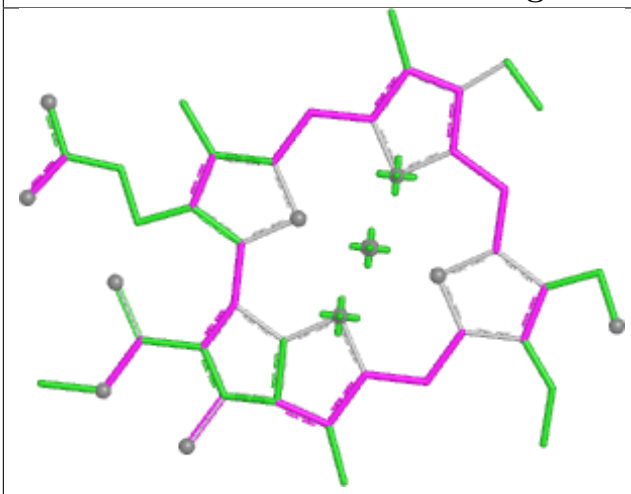


Torsions

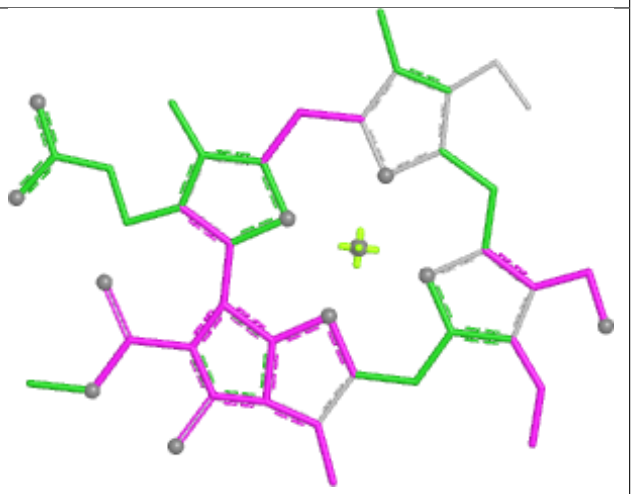


Rings

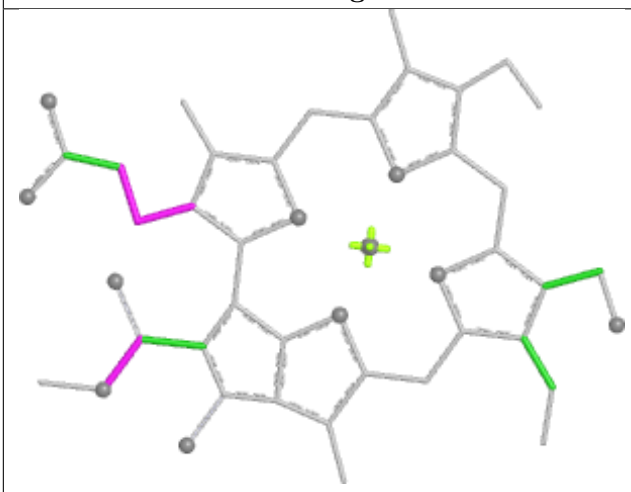
**Ligand CHL b 302**



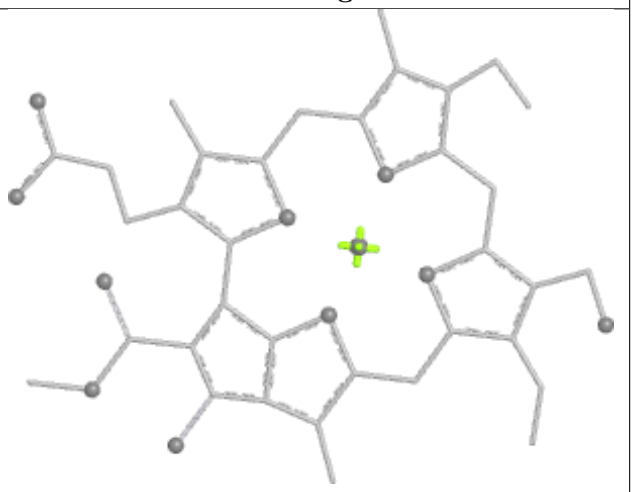
**Bond lengths**



**Bond angles**

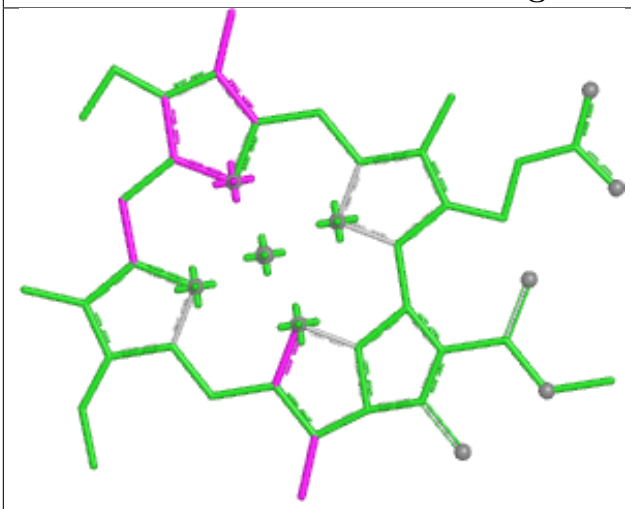


**Torsions**

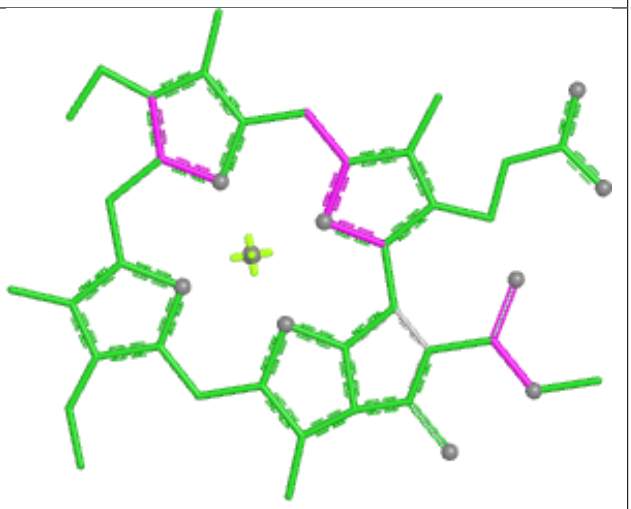


**Rings**

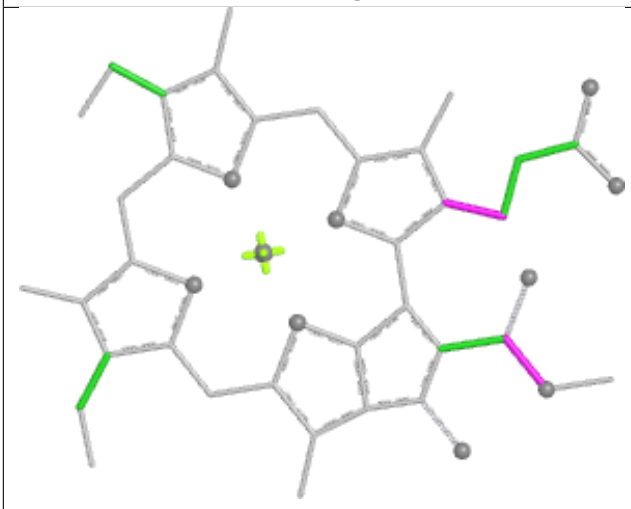
**Ligand CLA 6 604**



**Bond lengths**



**Bond angles**

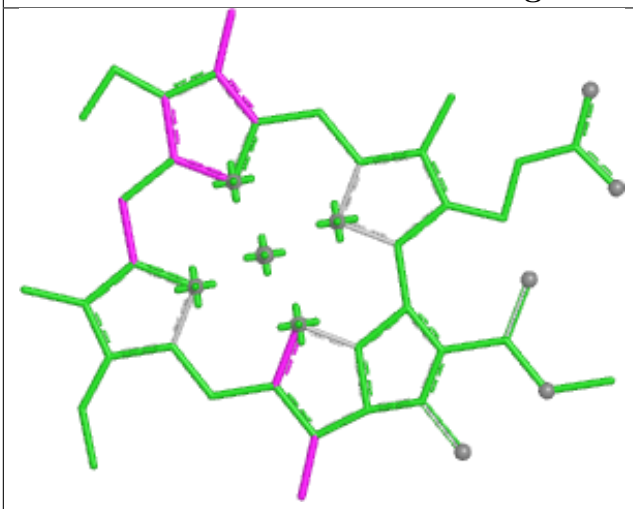


**Torsions**

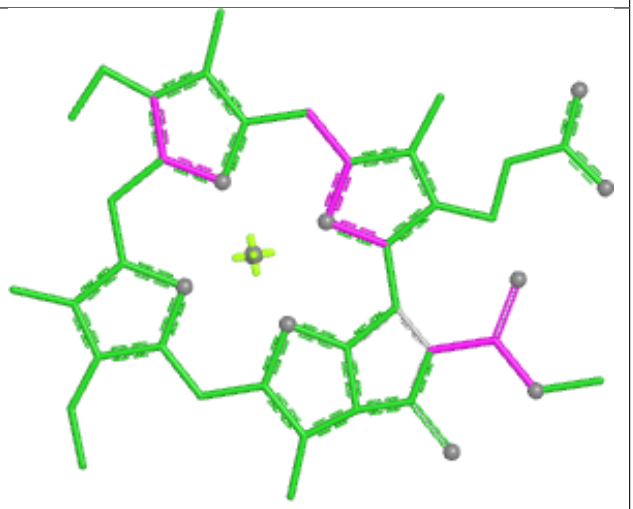


**Rings**

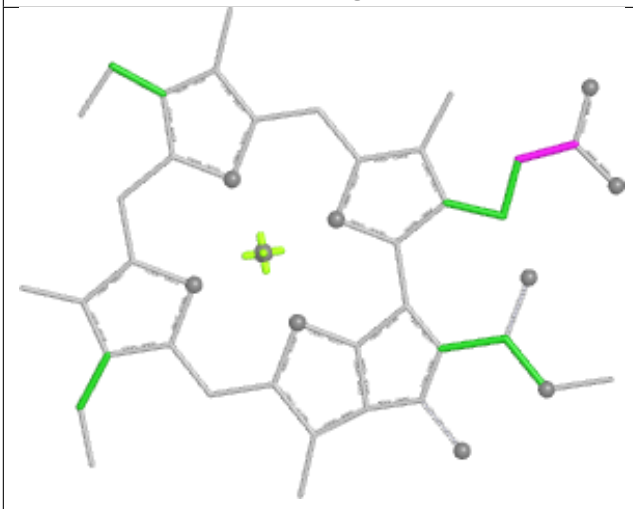
**Ligand CLA B 829**



**Bond lengths**



**Bond angles**

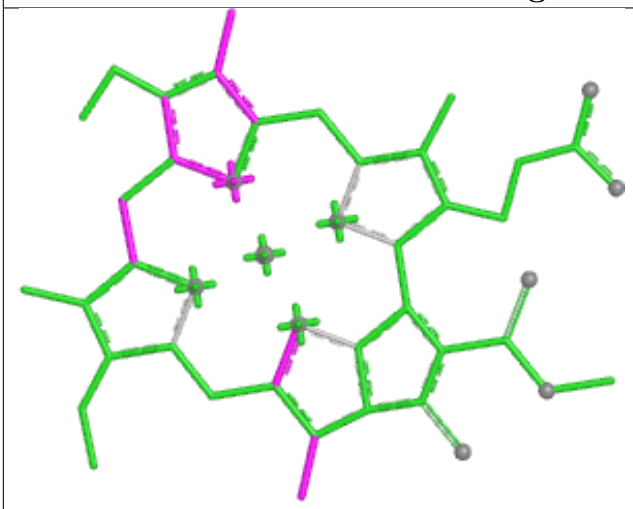


**Torsions**

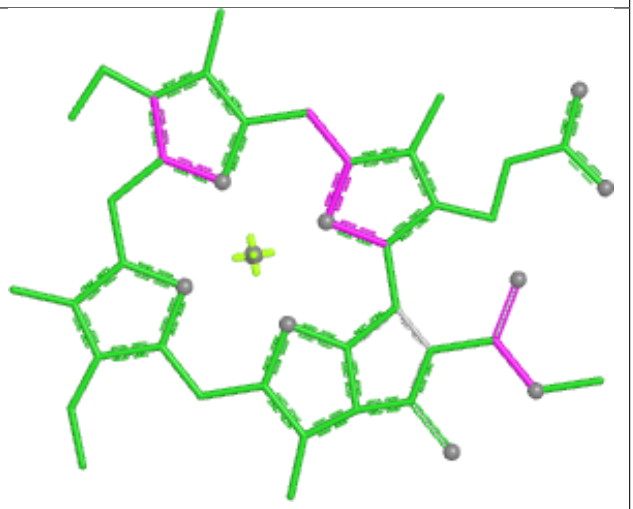


**Rings**

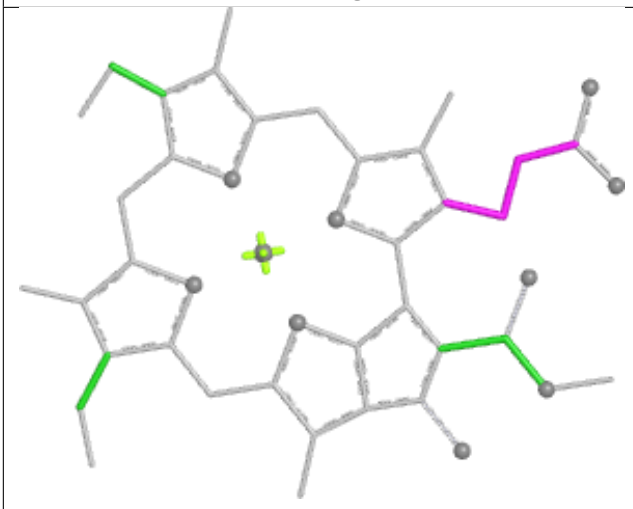
**Ligand CLA a 610**



**Bond lengths**



**Bond angles**

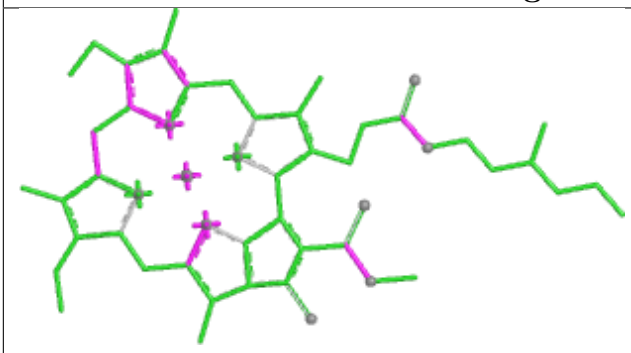


**Torsions**

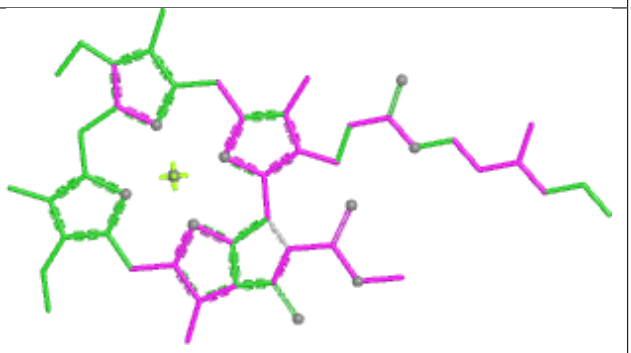


**Rings**

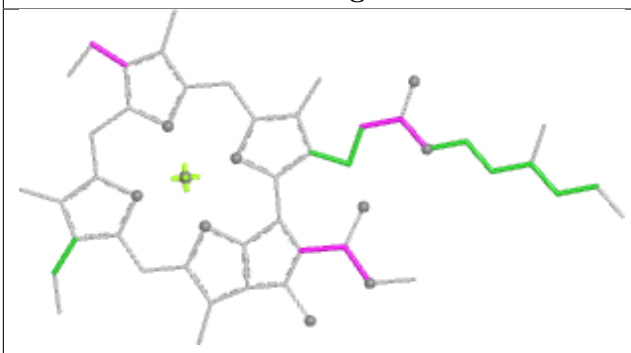
**Ligand CLA A 801**



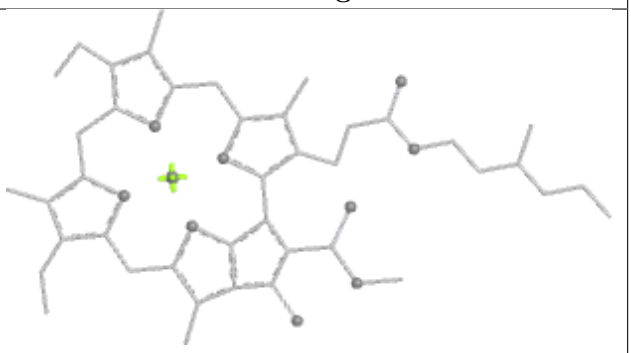
**Bond lengths**



**Bond angles**

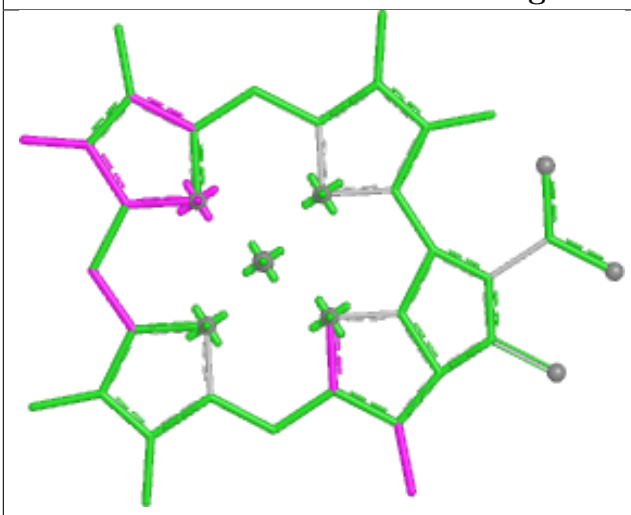


**Torsions**



**Rings**

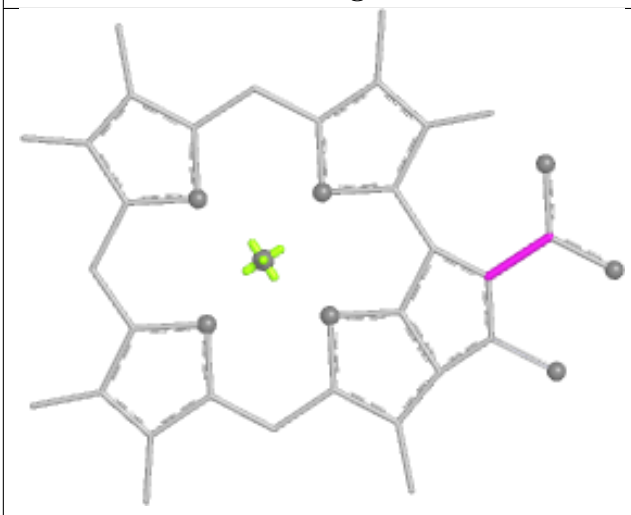
**Ligand CLA 5 613**



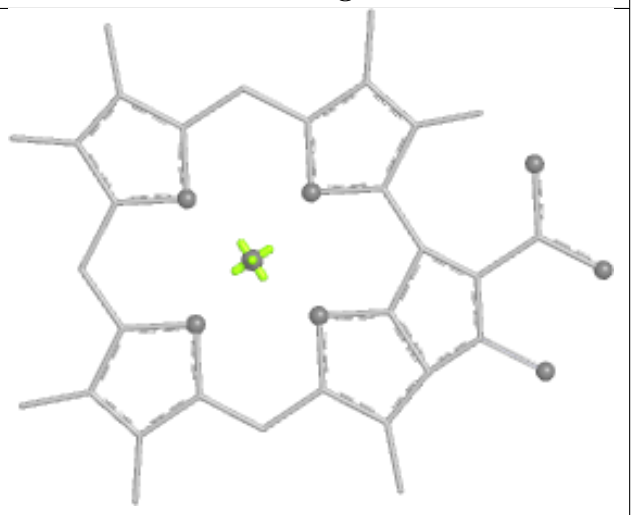
**Bond lengths**



**Bond angles**

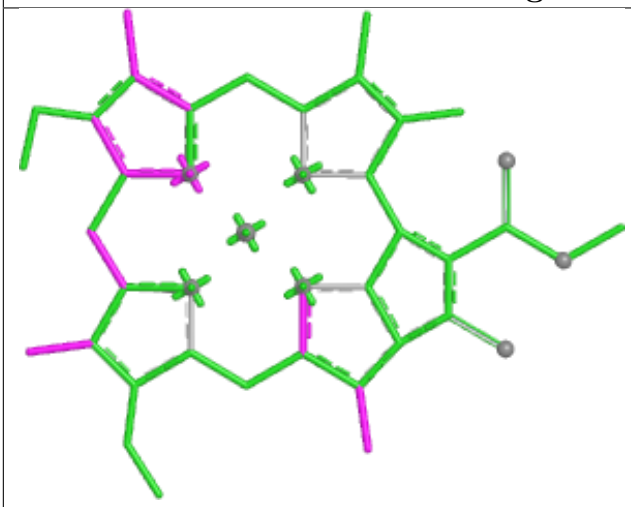


**Torsions**

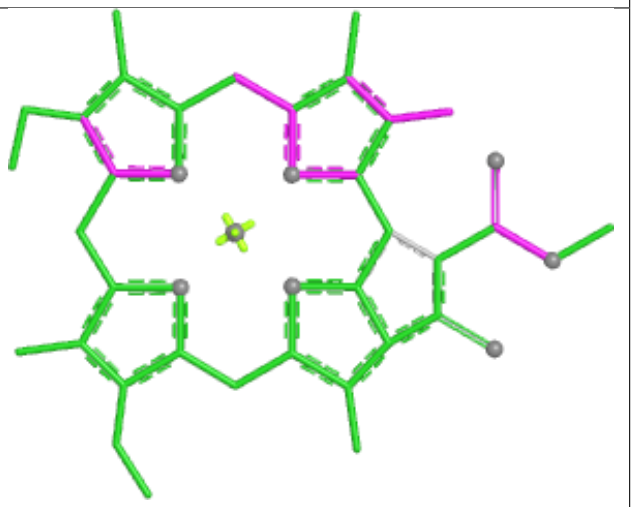


**Rings**

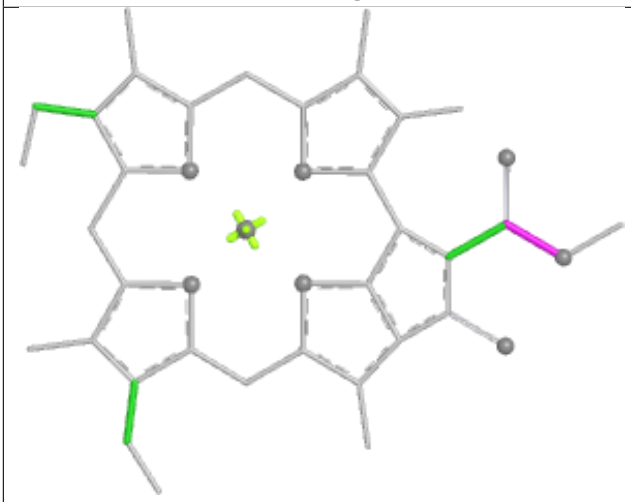
**Ligand CLA F 305**



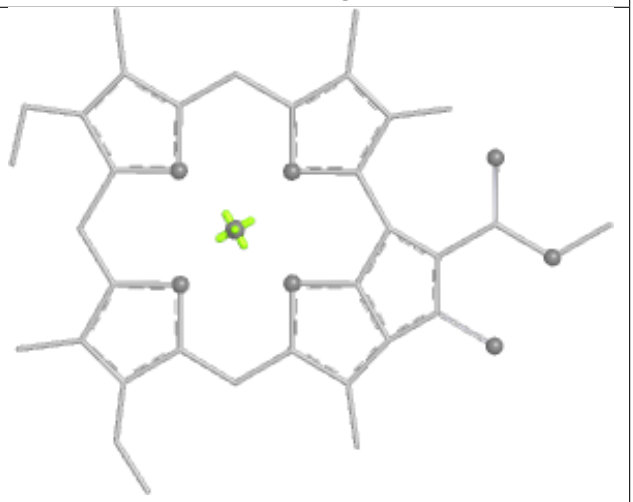
**Bond lengths**



**Bond angles**

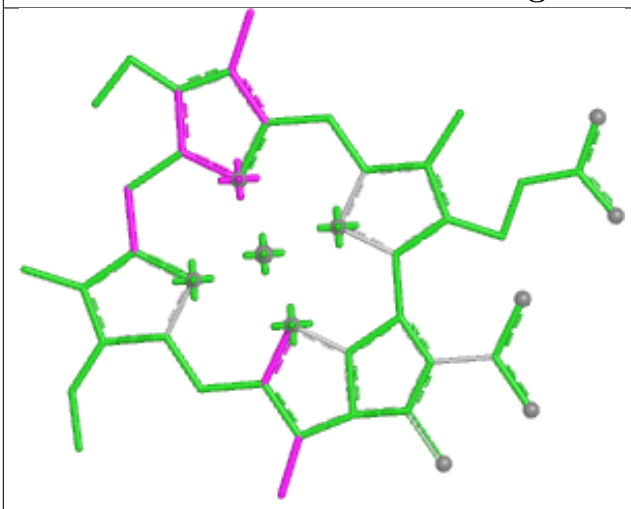


**Torsions**

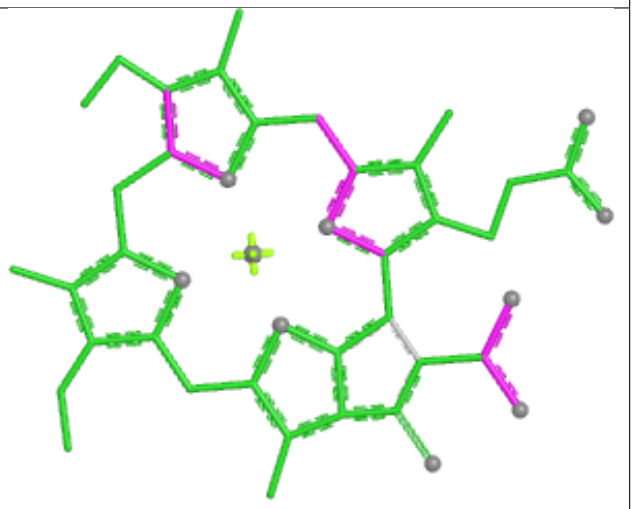


**Rings**

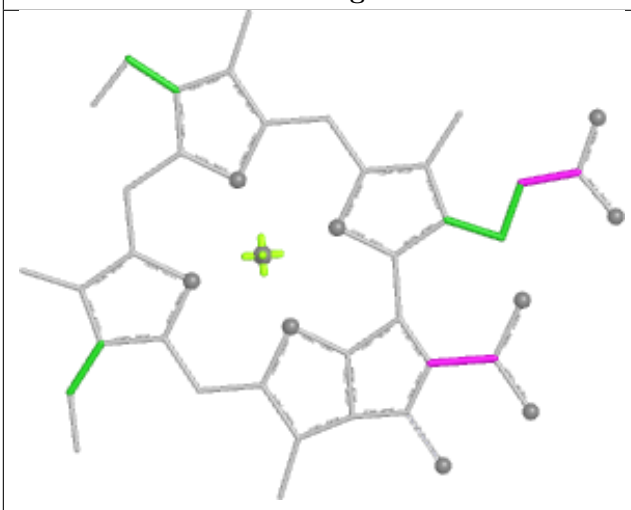
**Ligand CLA 8 603**



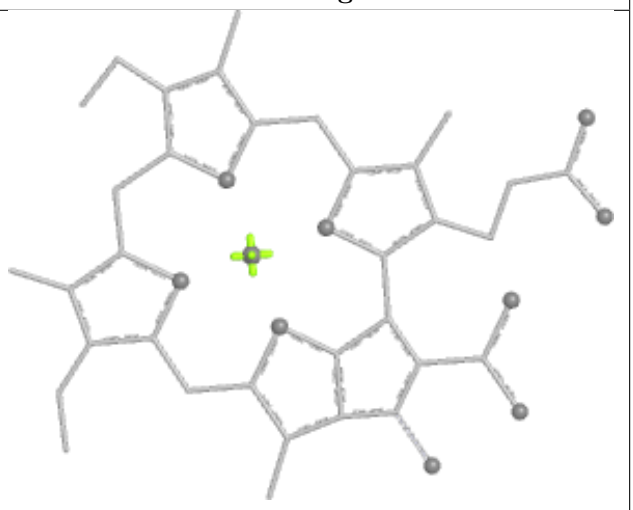
**Bond lengths**



**Bond angles**

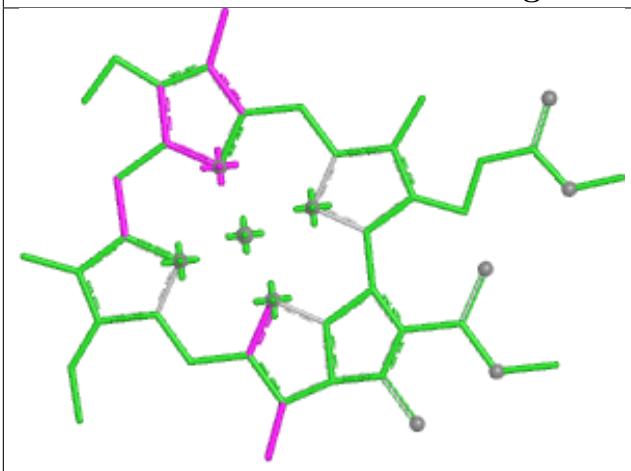


**Torsions**

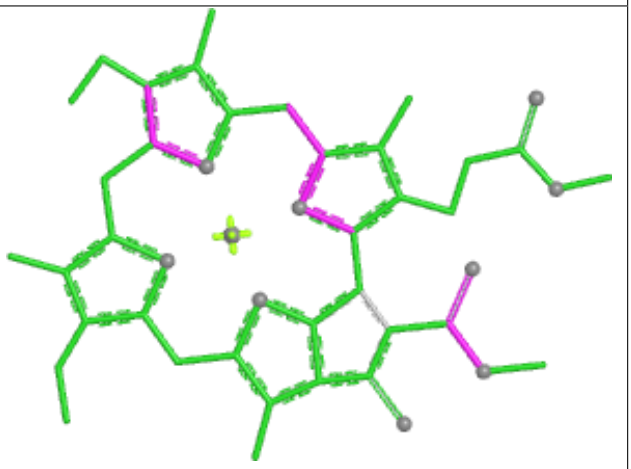


**Rings**

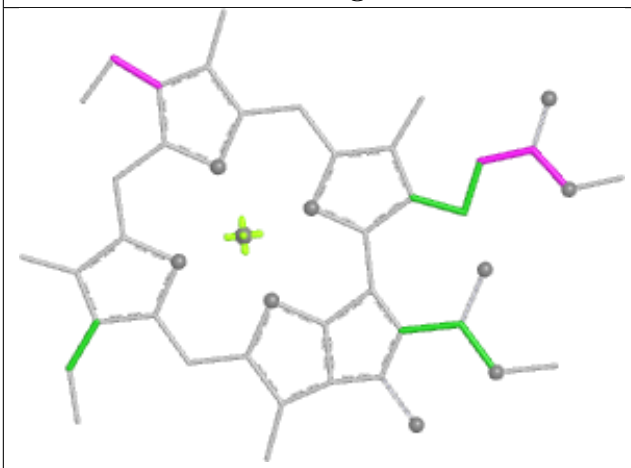
## Ligand CLA K 201



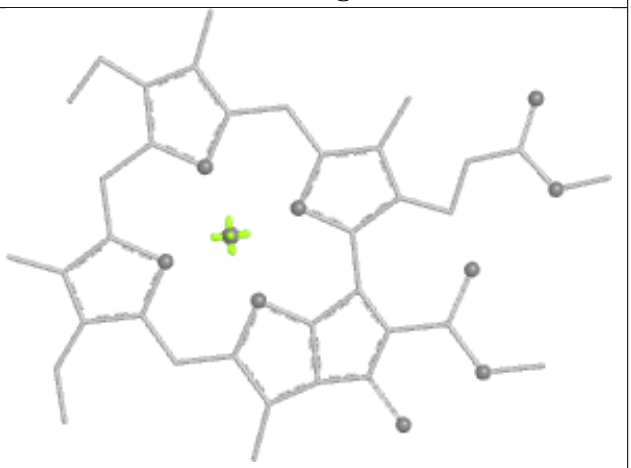
Bond lengths



Bond angles

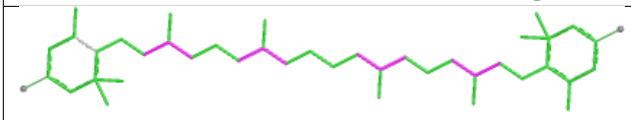


Torsions



Rings

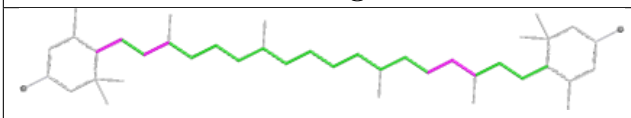
## Ligand LUT 7 415



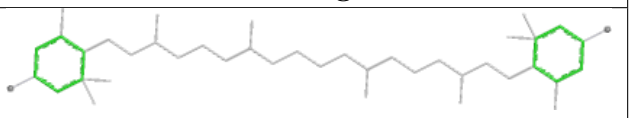
Bond lengths



Bond angles

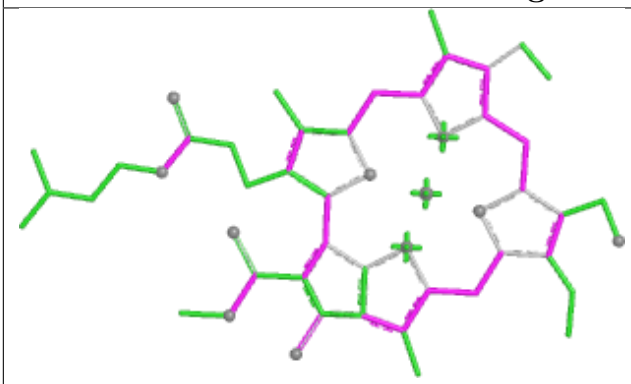


Torsions

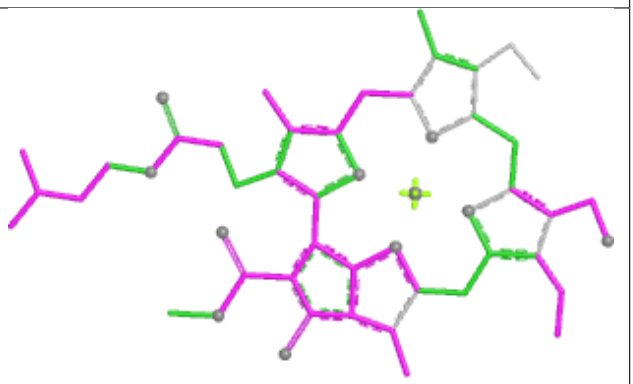


Rings

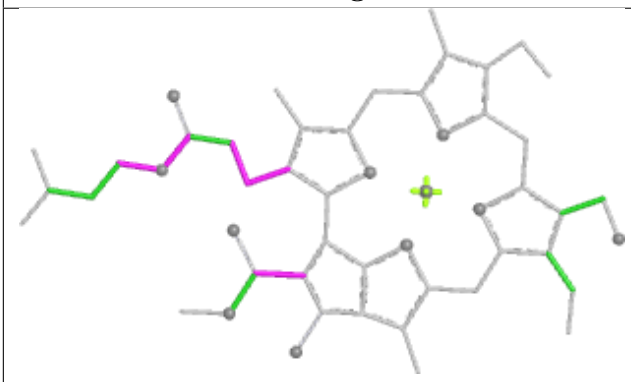
## Ligand CHL 1 302



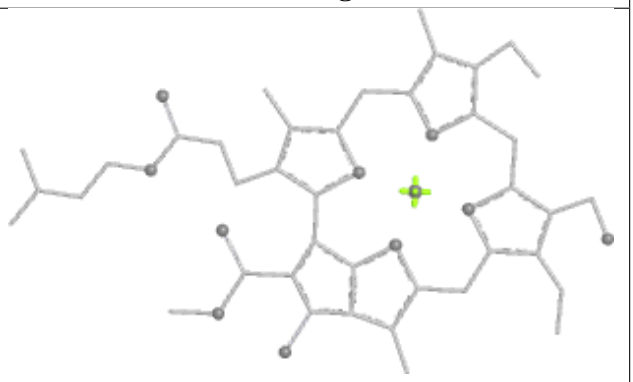
Bond lengths



Bond angles

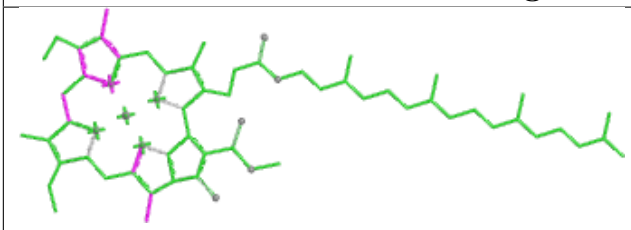


Torsions

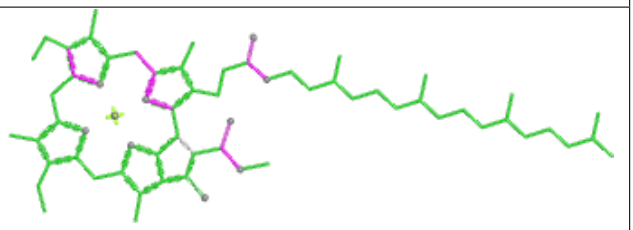


Rings

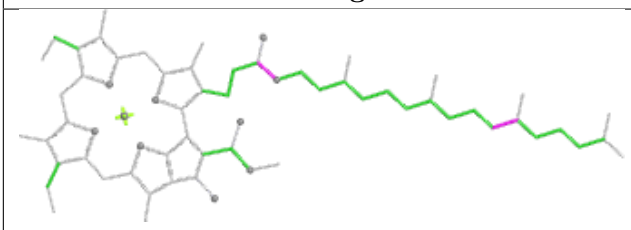
## Ligand CLA A 812



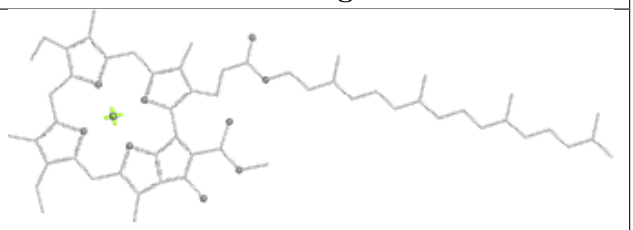
Bond lengths



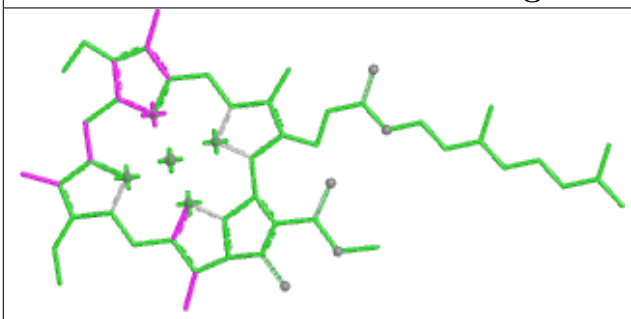
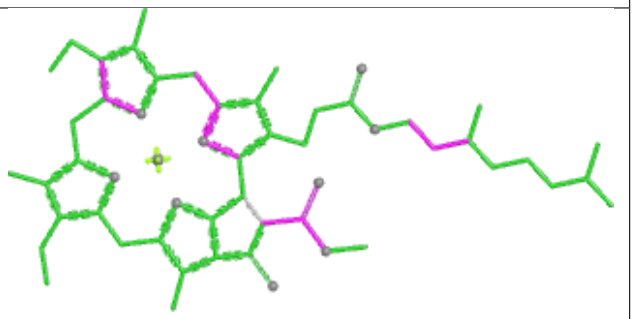
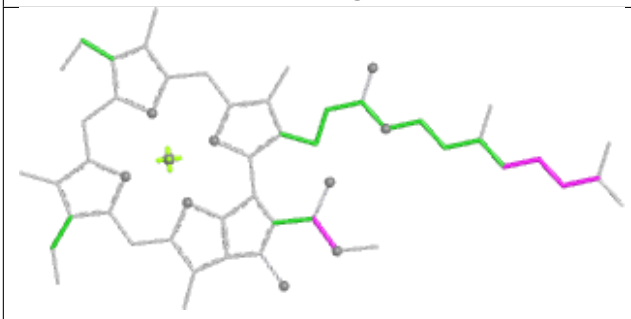
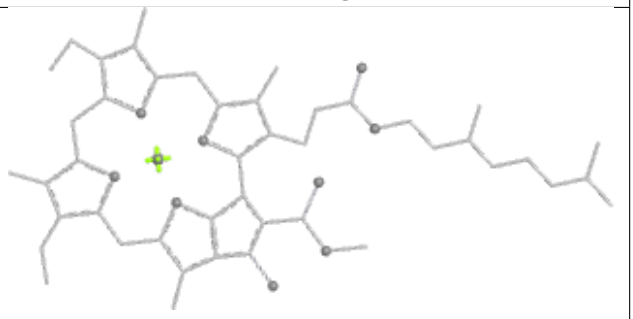
Bond angles



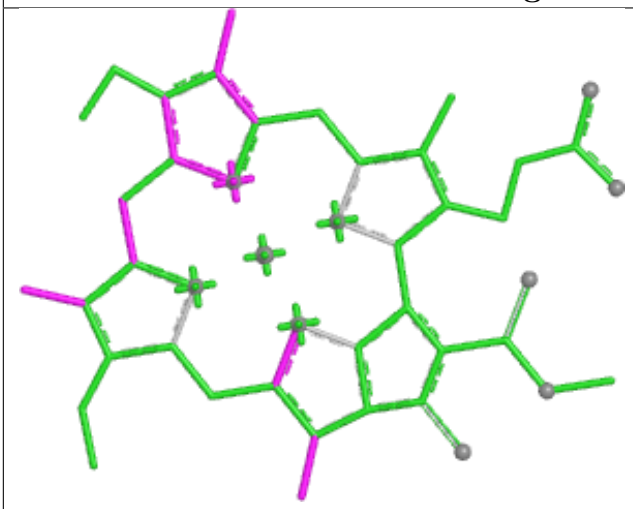
Torsions



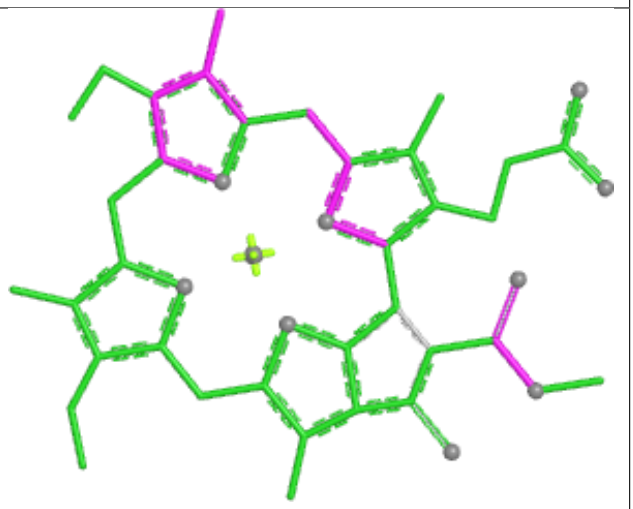
Rings

| Ligand CLA A 831 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

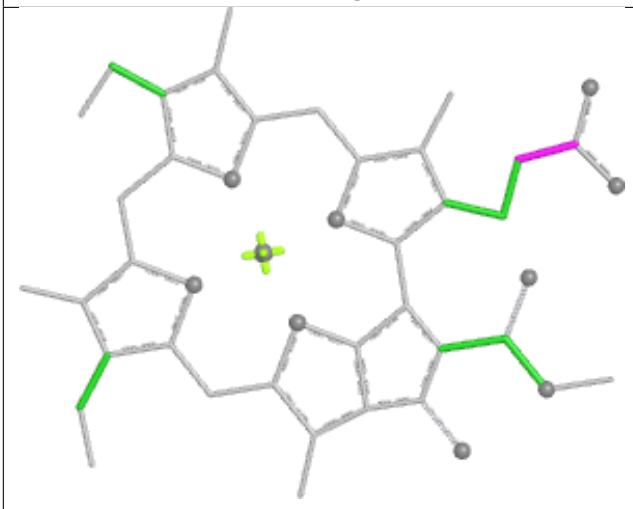
**Ligand CLA A 808**



**Bond lengths**



**Bond angles**

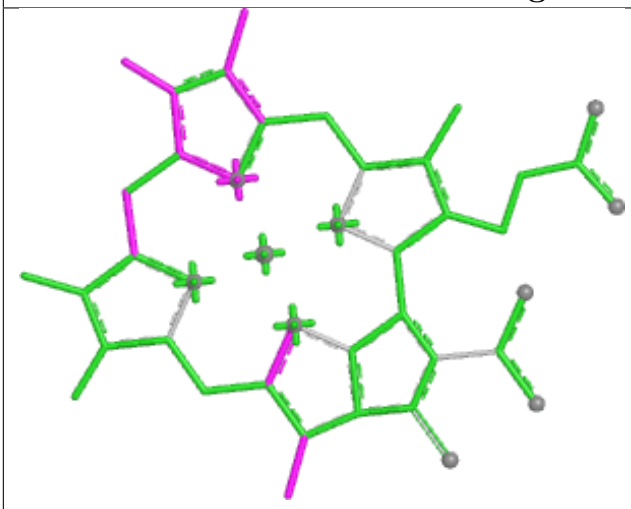


**Torsions**

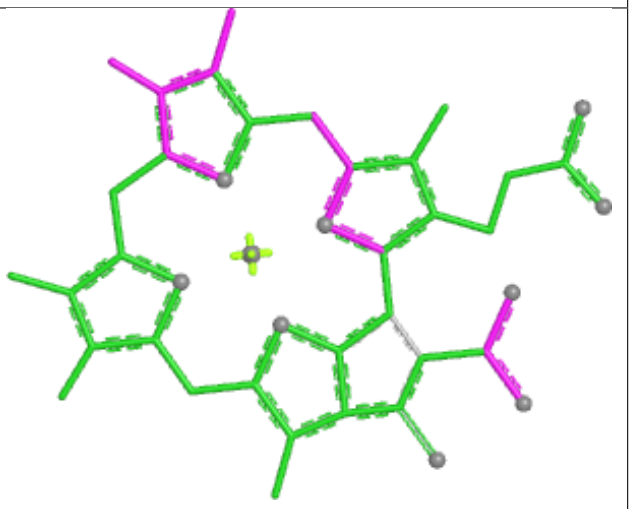


**Rings**

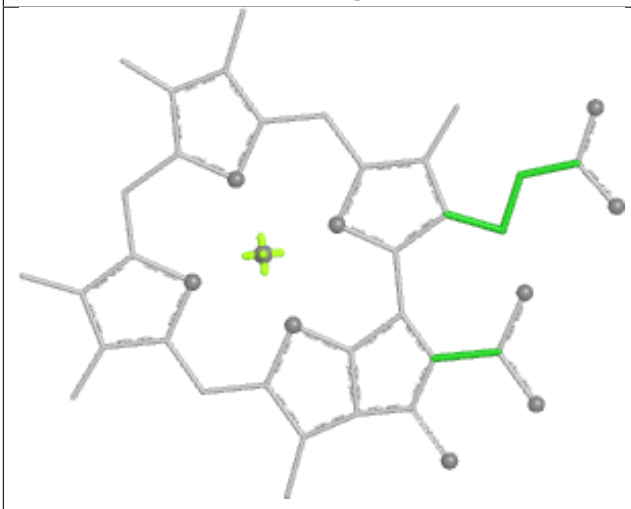
**Ligand CLA 3 404**



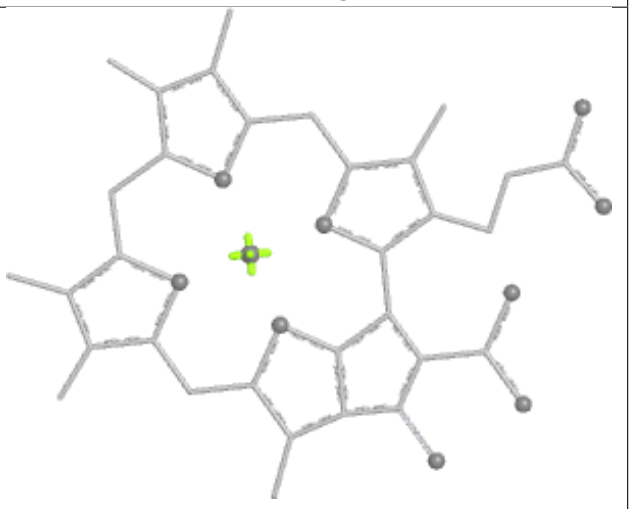
**Bond lengths**



**Bond angles**

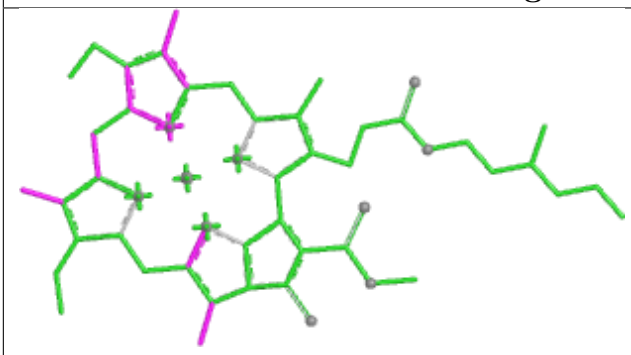


**Torsions**

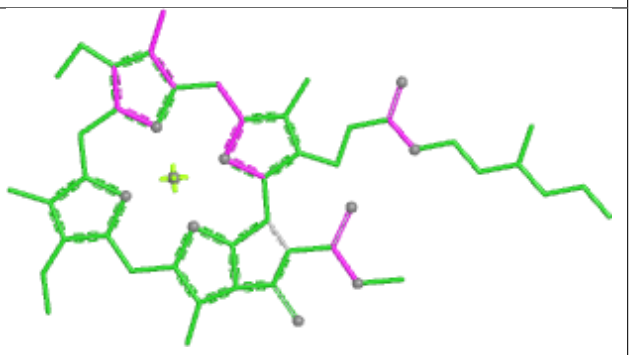


**Rings**

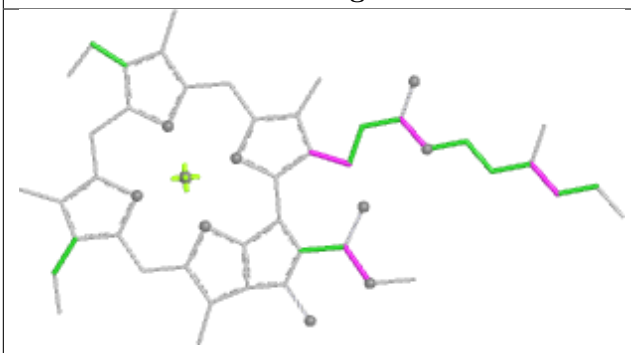
**Ligand CLA B 828**



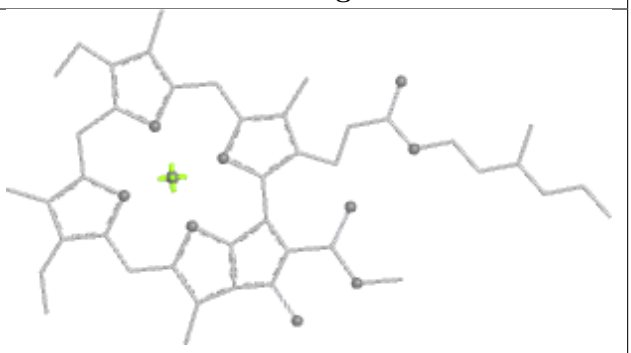
**Bond lengths**



**Bond angles**

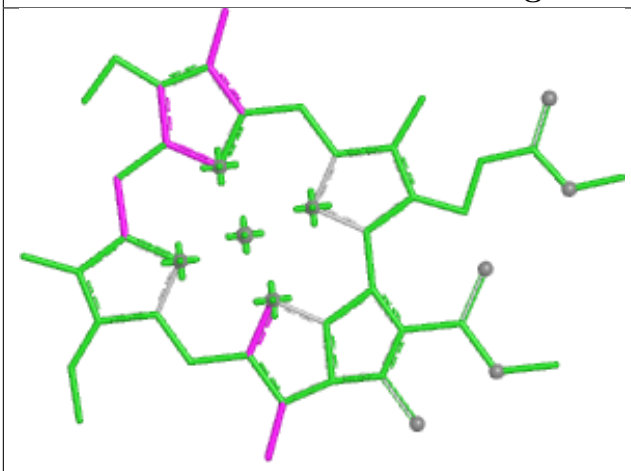


**Torsions**

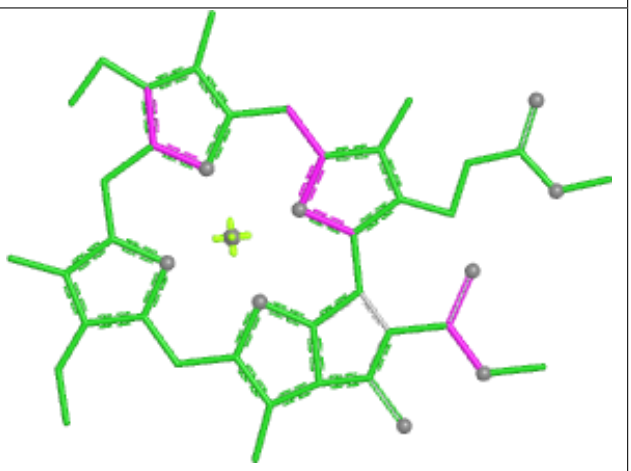


**Rings**

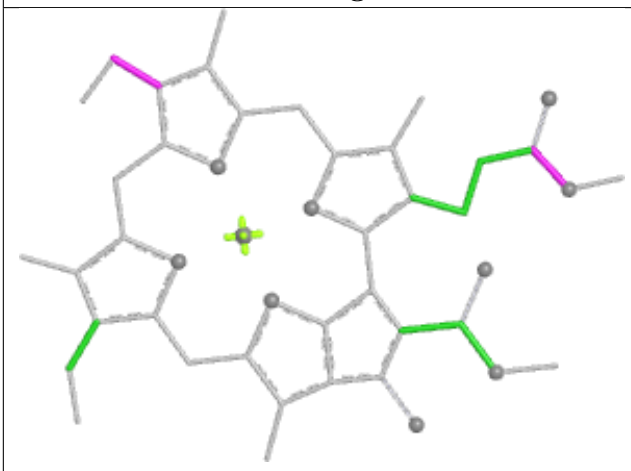
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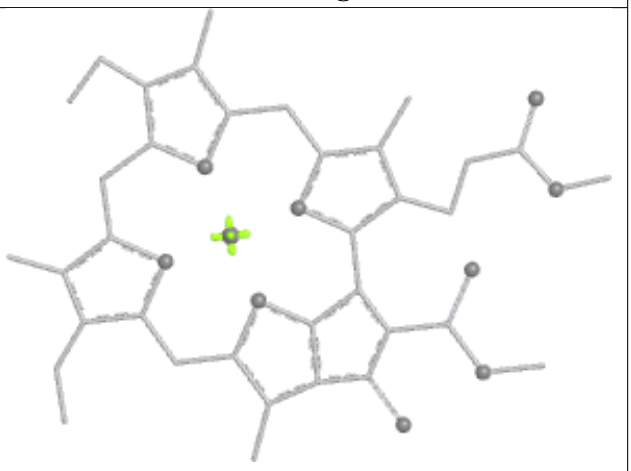
**Bond lengths**



**Bond angles**

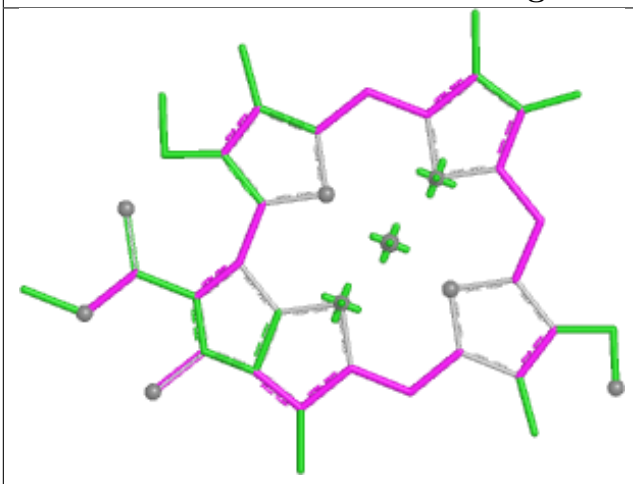


**Torsions**

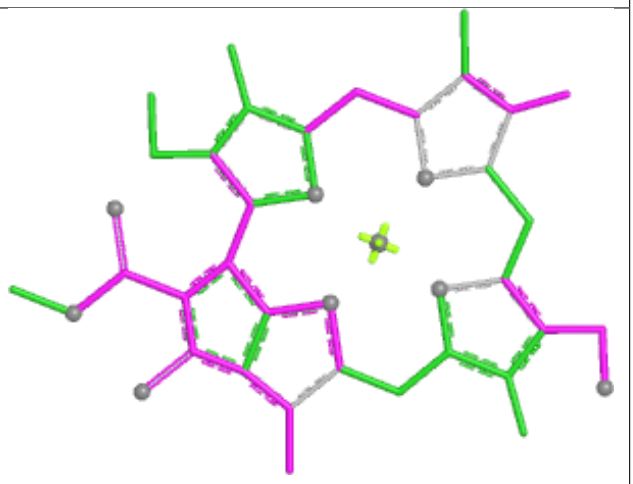


**Rings**

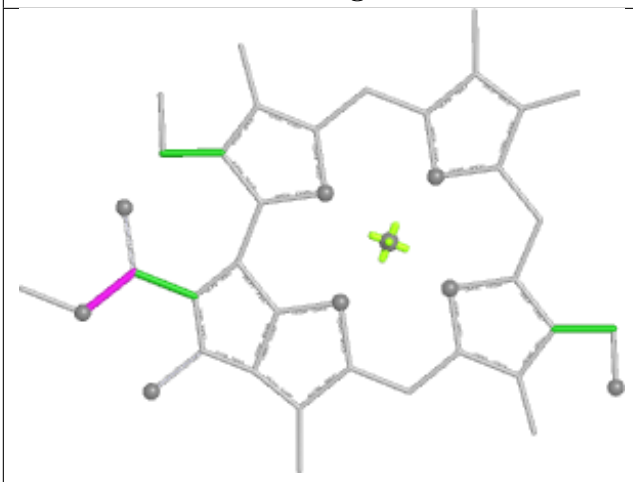
## Ligand CHL 4 605



Bond lengths



Bond angles

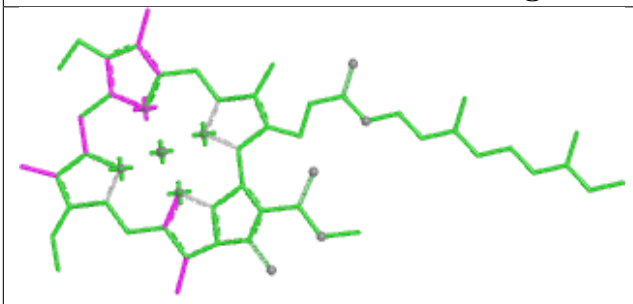


Torsions

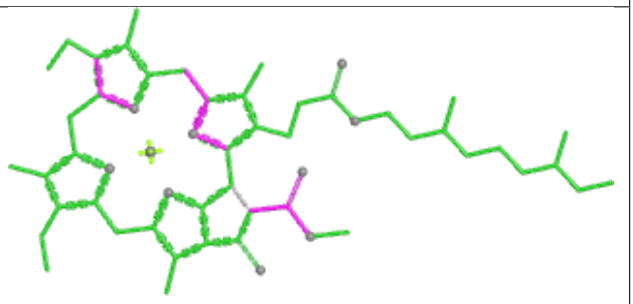


Rings

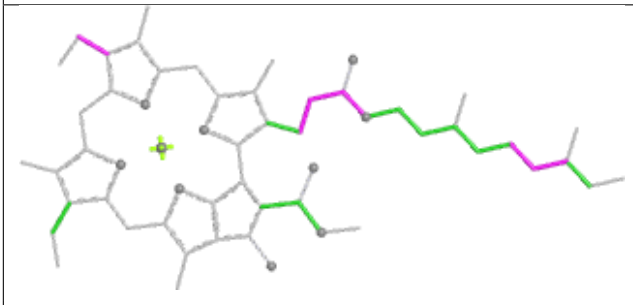
## Ligand CLA A 823



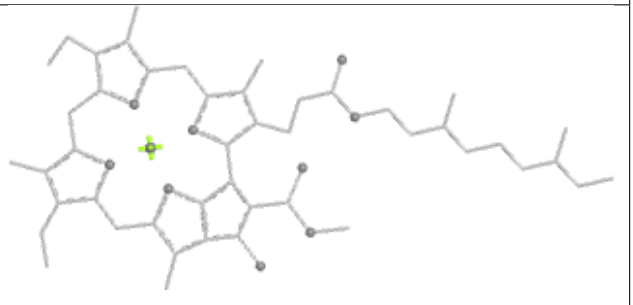
Bond lengths



Bond angles



Torsions

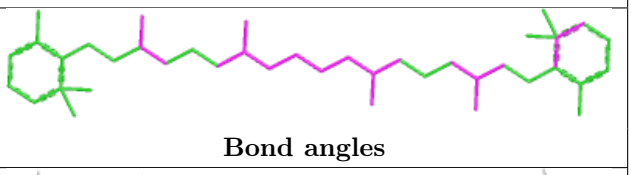


Rings

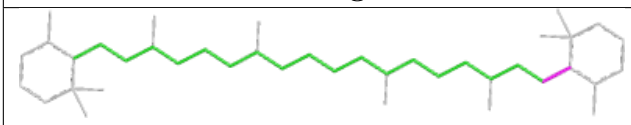
## Ligand BCR 2 618



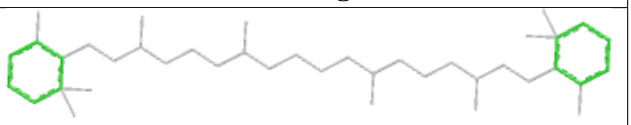
Bond lengths



Bond angles

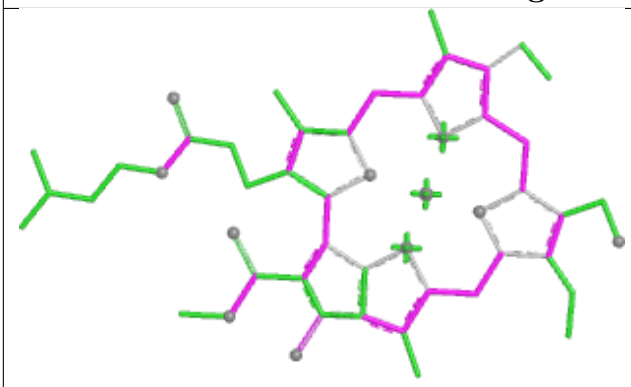


Torsions

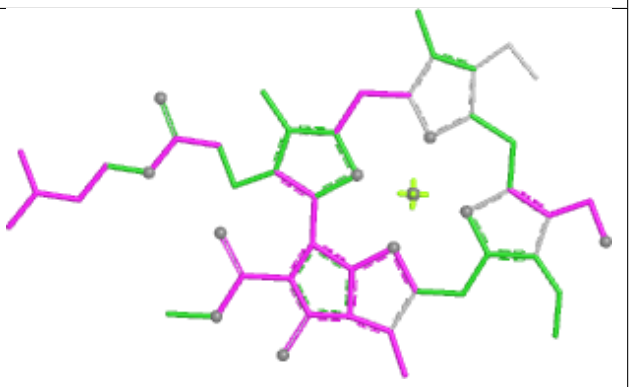


Rings

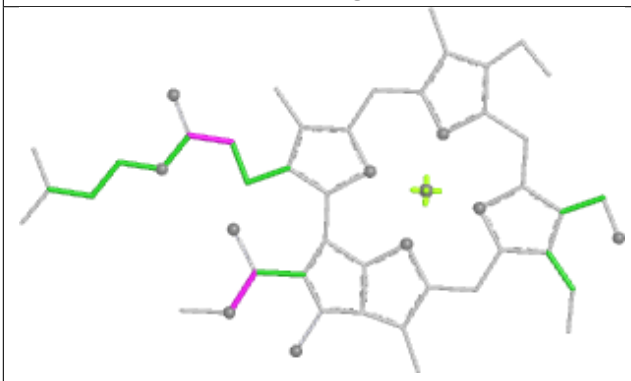
## Ligand CHL 6 607



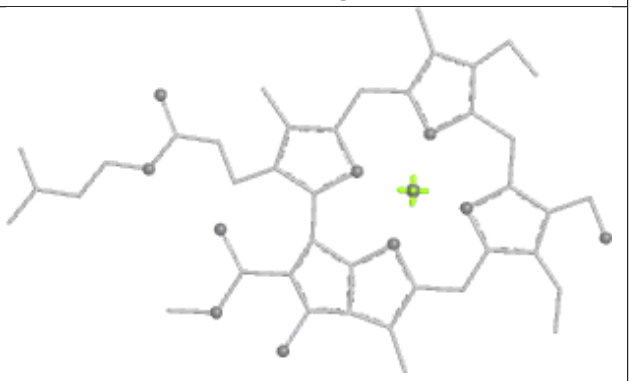
Bond lengths



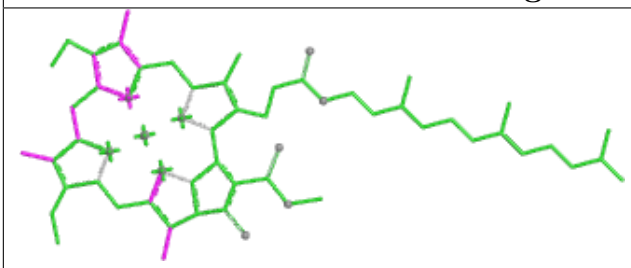
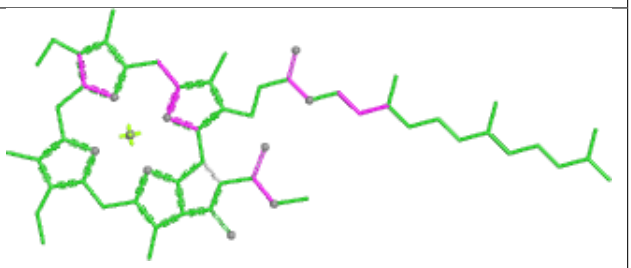
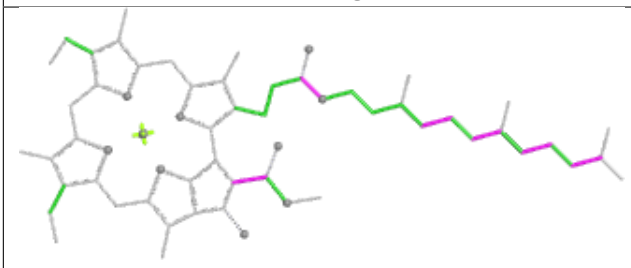
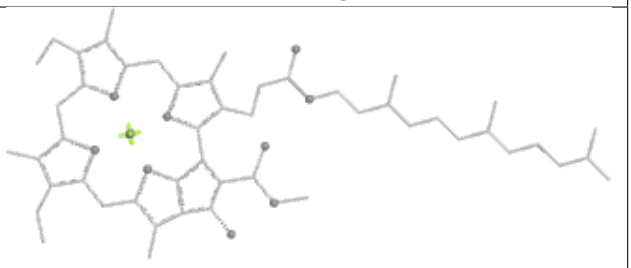
Bond angles

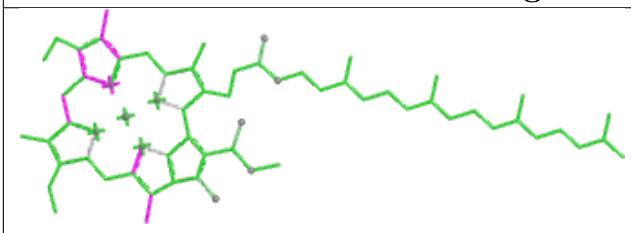
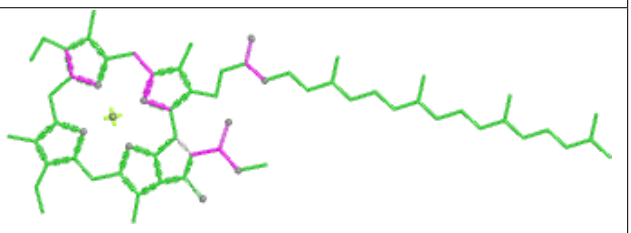
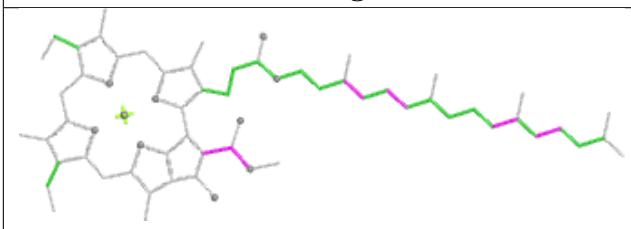
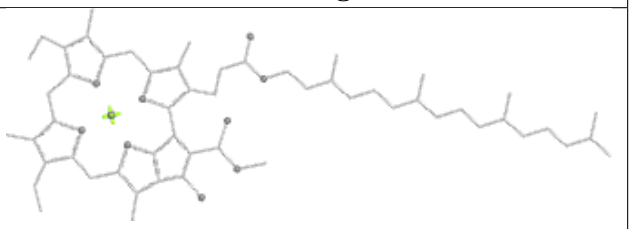


Torsions

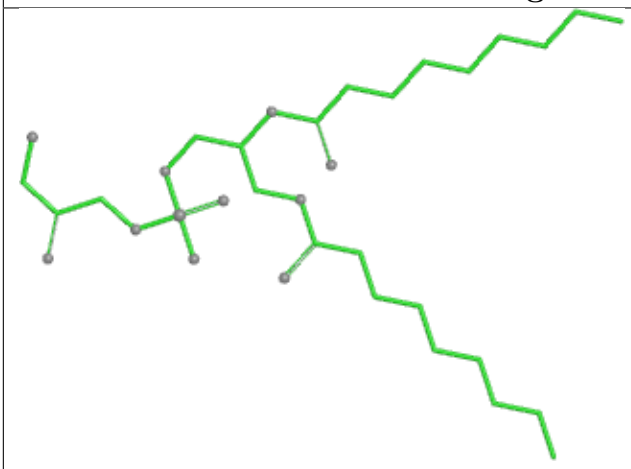


Rings

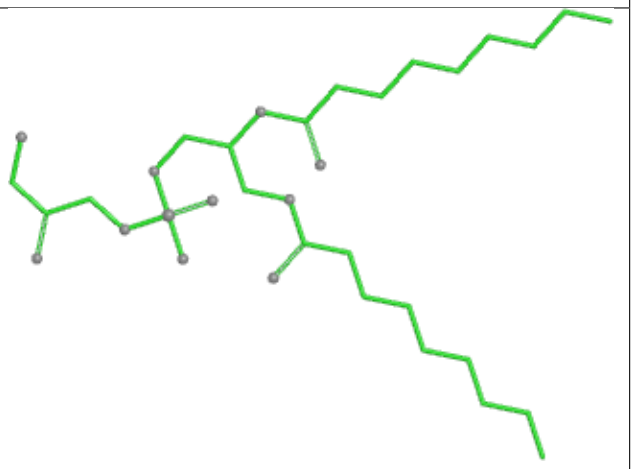
| Ligand CLA B 814 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA A 834 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

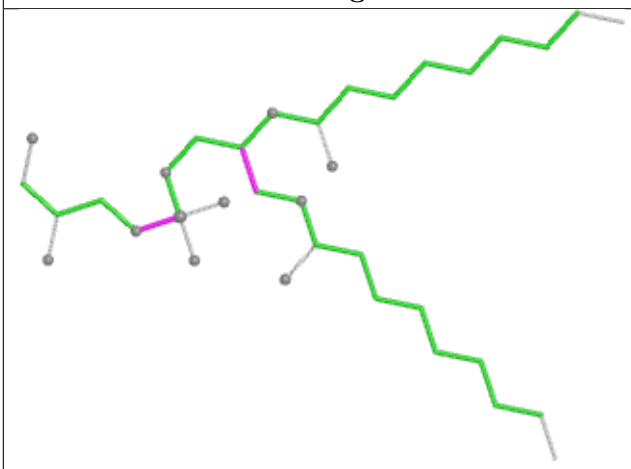
**Ligand LHG 6 619**



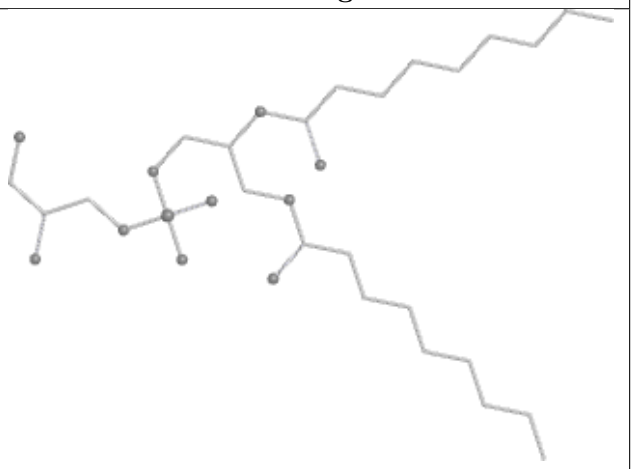
**Bond lengths**



**Bond angles**

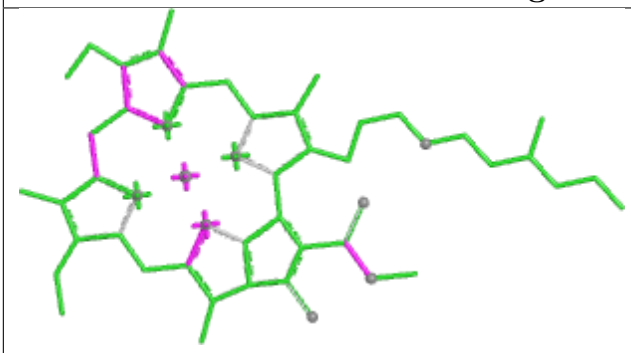


**Torsions**

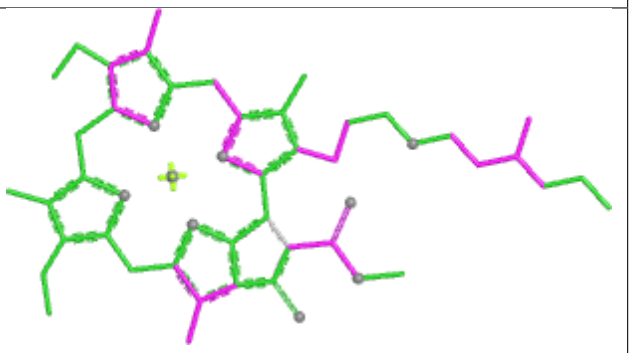


**Rings**

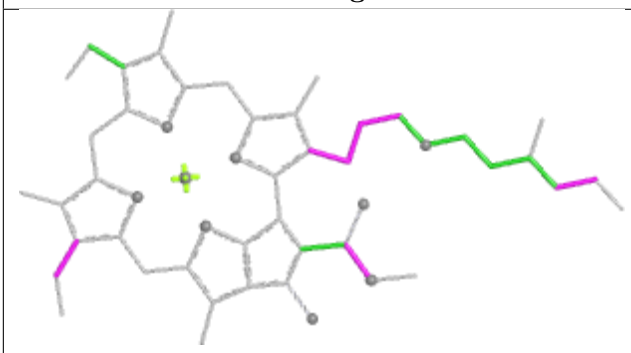
**Ligand CLA 2 609**



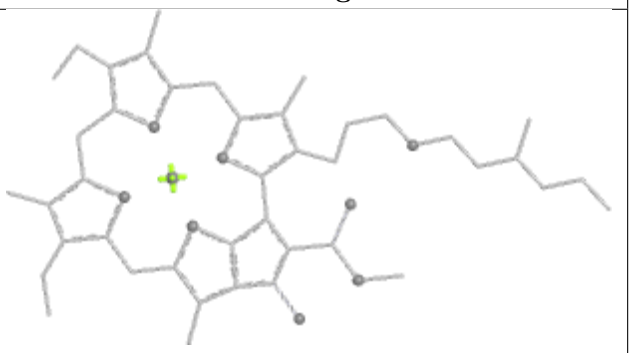
**Bond lengths**



**Bond angles**

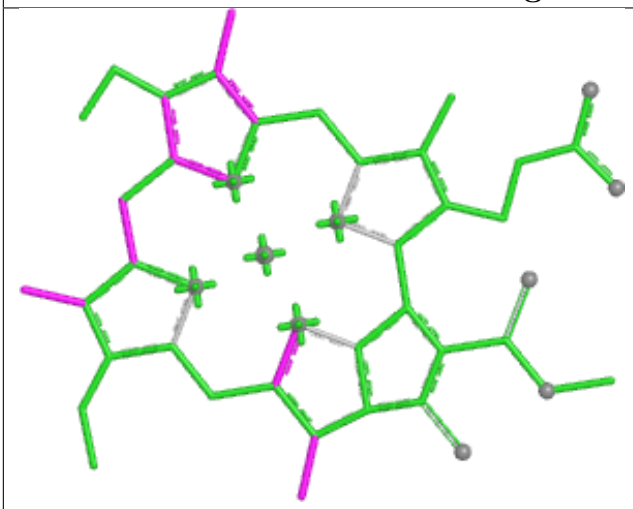


**Torsions**

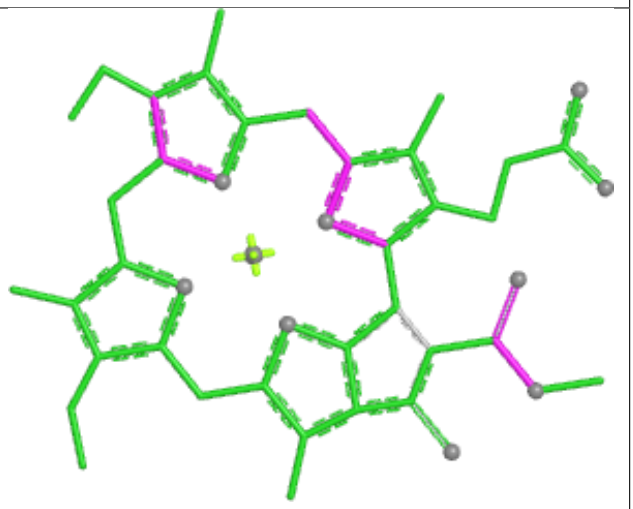


**Rings**

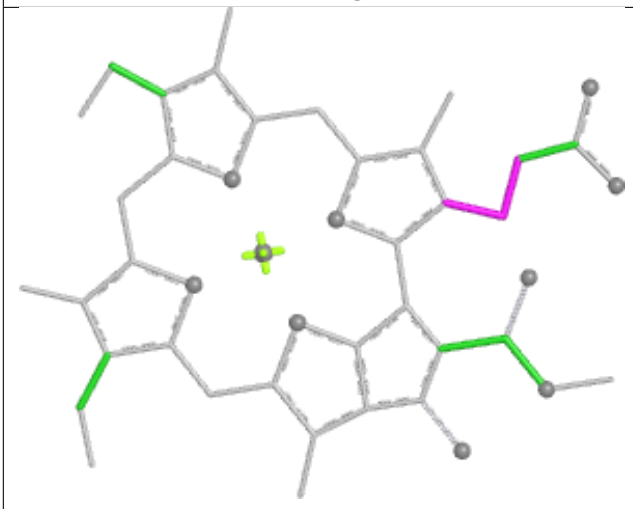
**Ligand CLA B 811**



**Bond lengths**



**Bond angles**

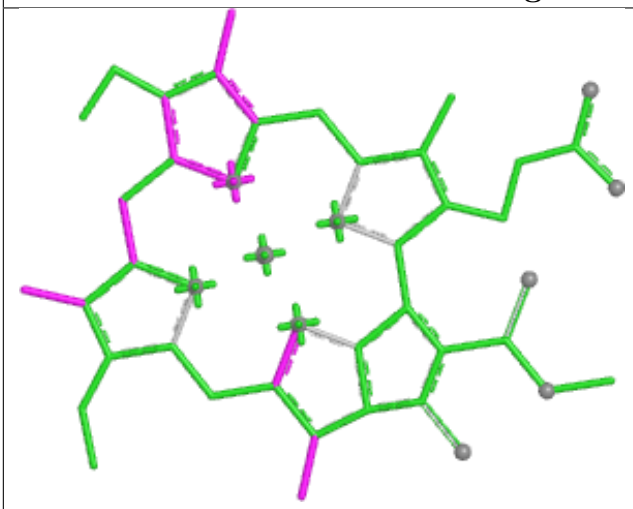


**Torsions**

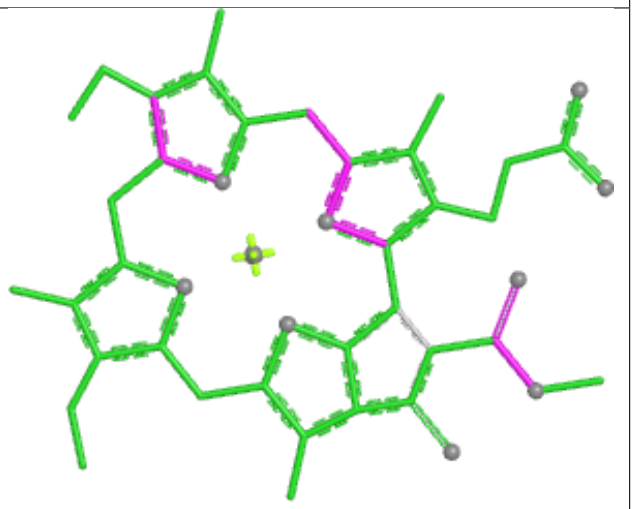


**Rings**

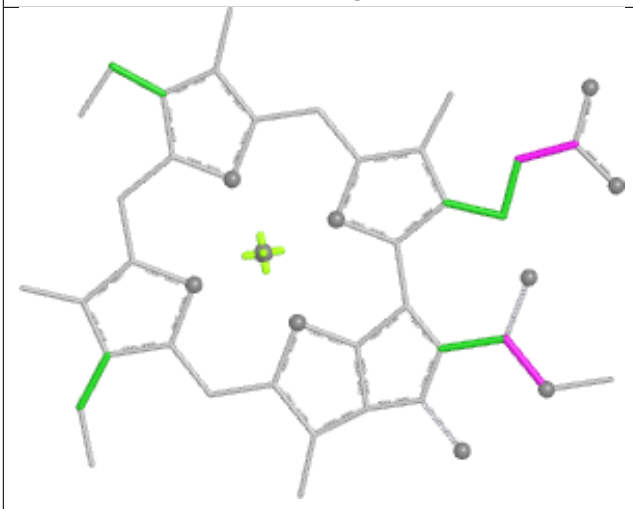
**Ligand CLA B 822**



**Bond lengths**



**Bond angles**

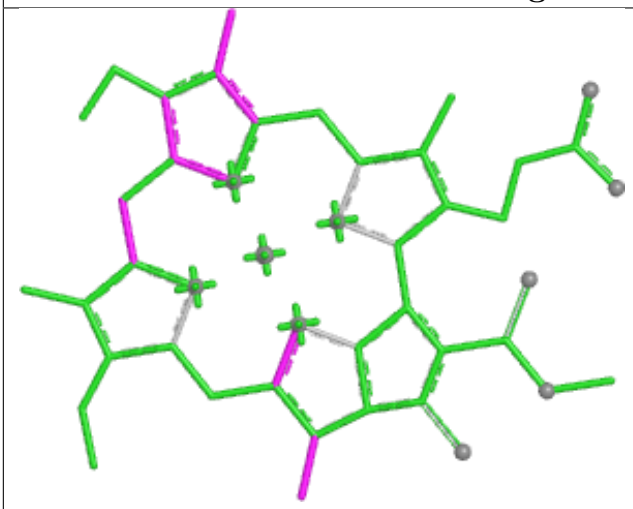


**Torsions**

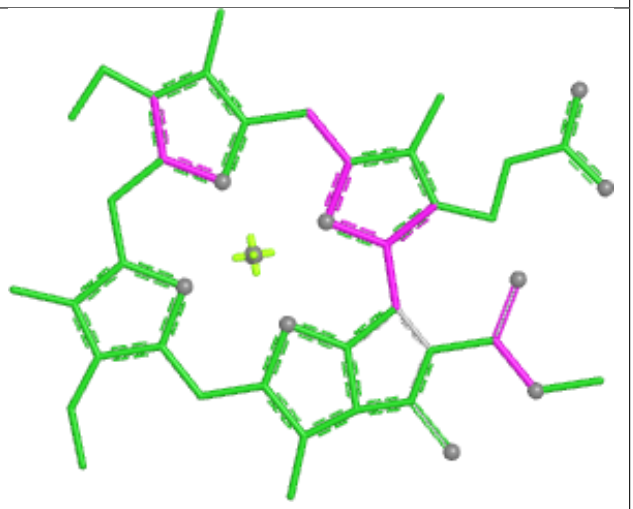


**Rings**

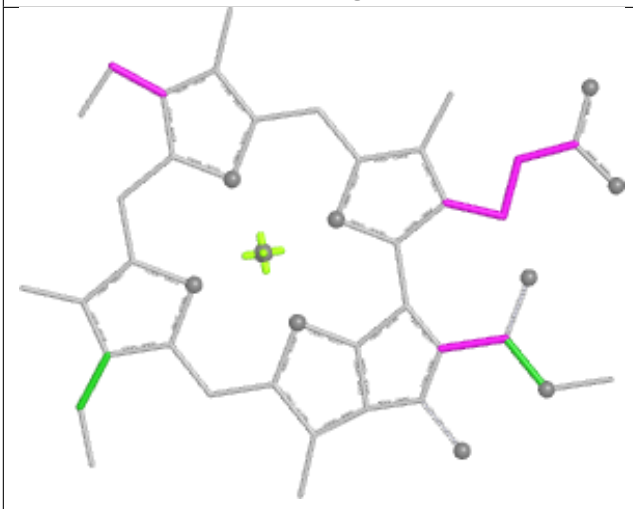
**Ligand CLA 7 402**



**Bond lengths**



**Bond angles**

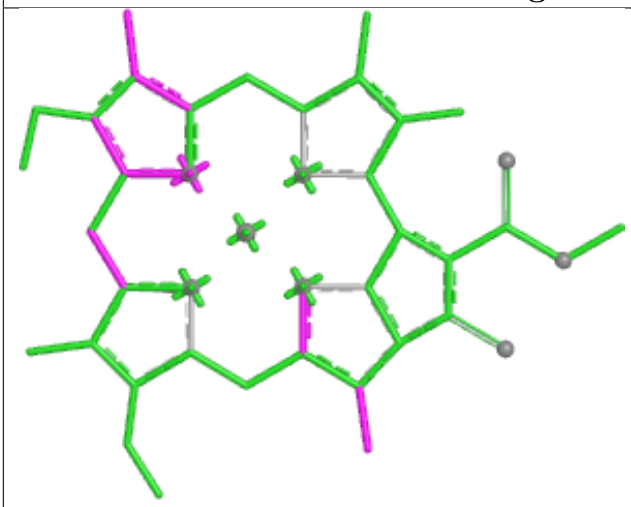


**Torsions**

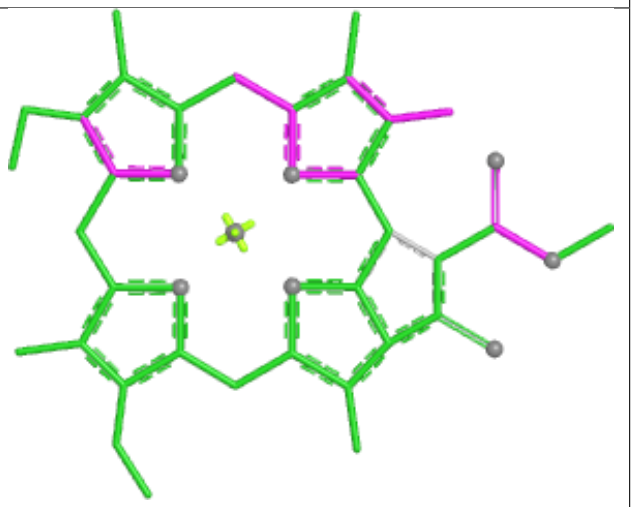


**Rings**

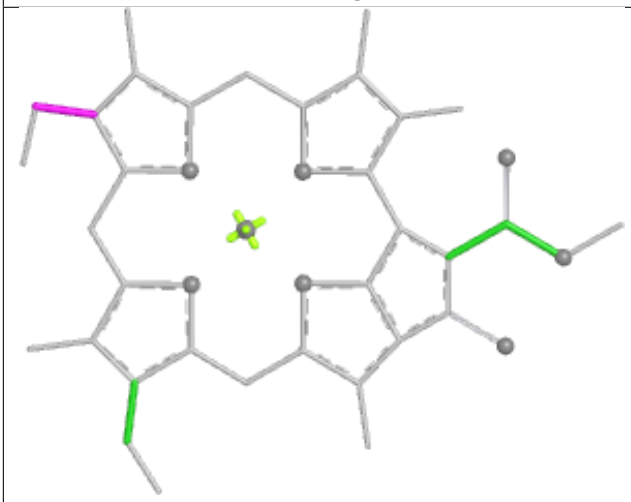
**Ligand CLA a 614**



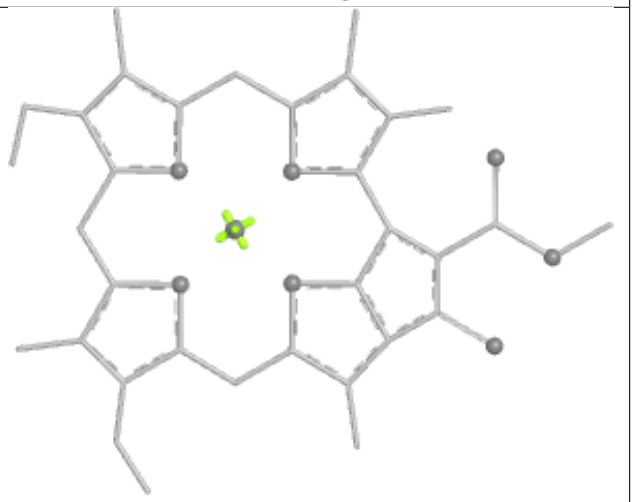
**Bond lengths**



**Bond angles**

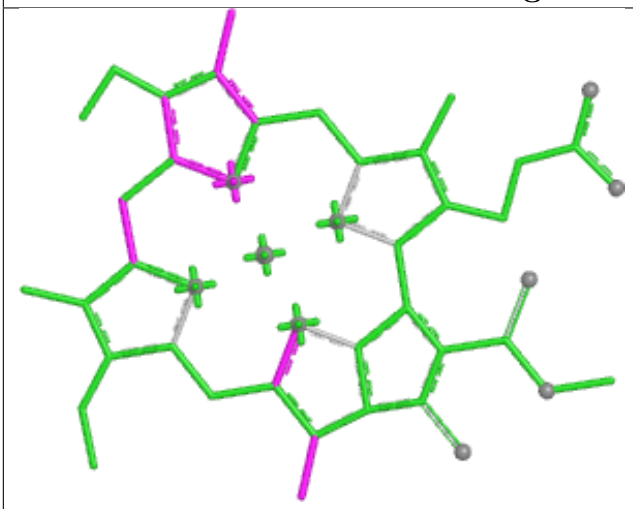


**Torsions**

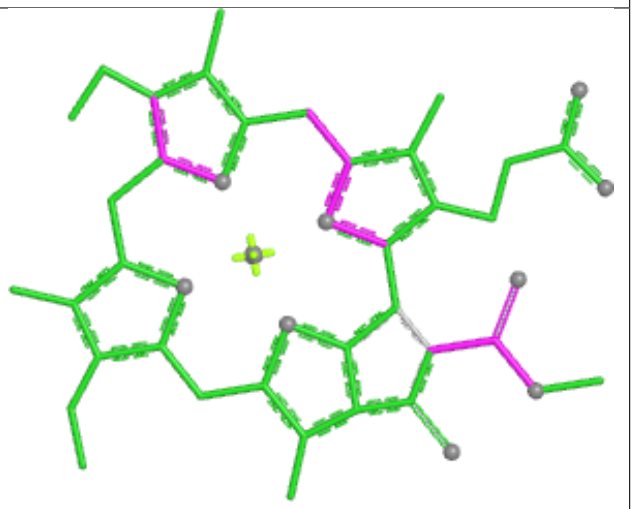


**Rings**

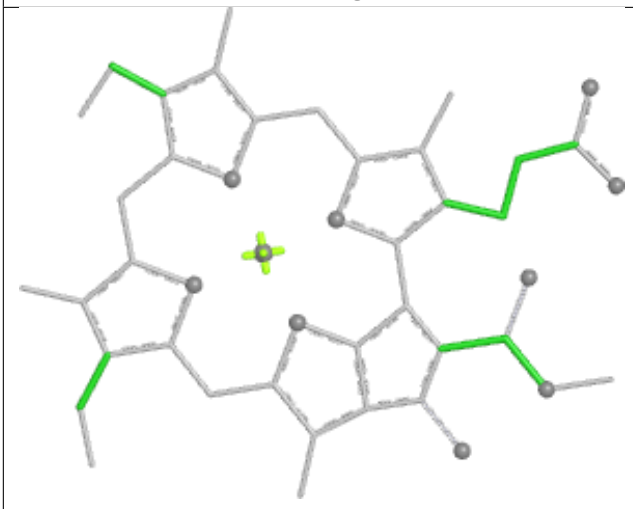
**Ligand CLA A 839**



**Bond lengths**



**Bond angles**

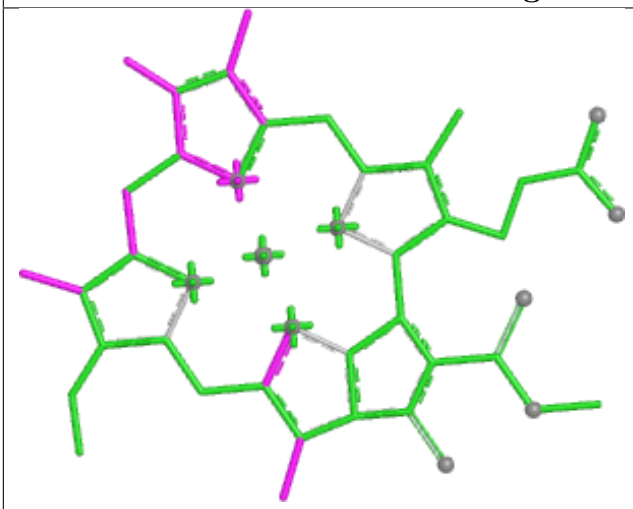


**Torsions**

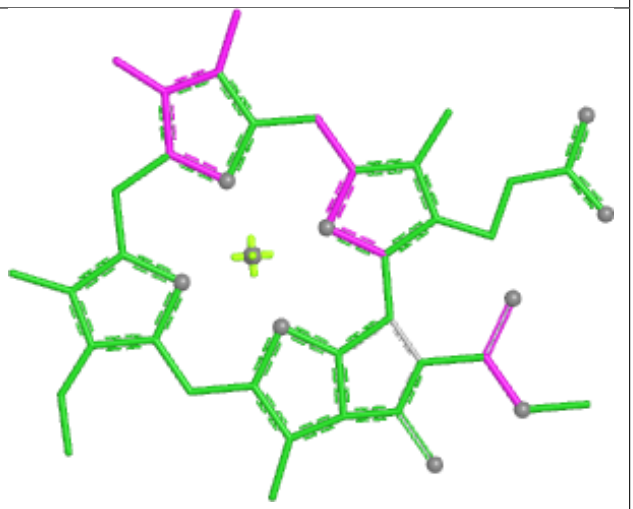


**Rings**

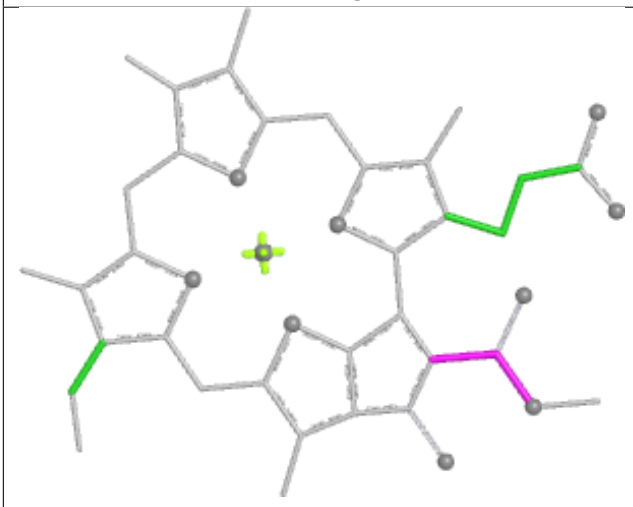
## Ligand CLA K 203



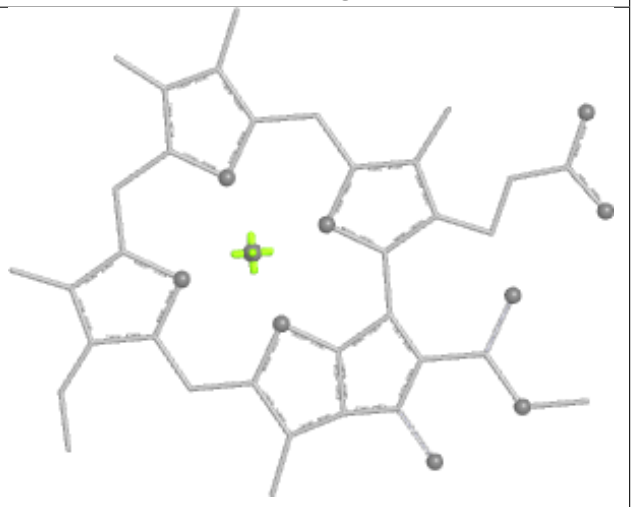
Bond lengths



Bond angles

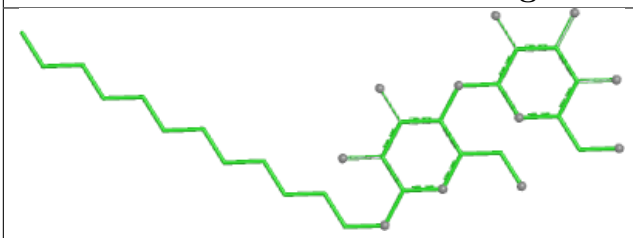


Torsions

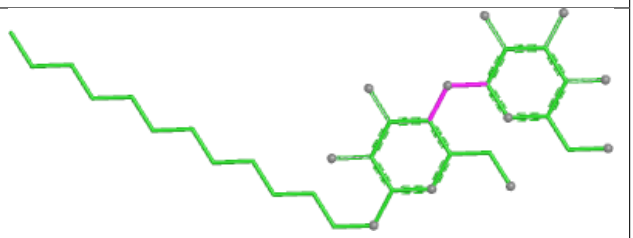


Rings

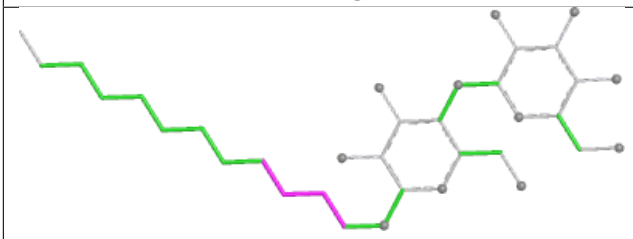
## Ligand LMU A 856



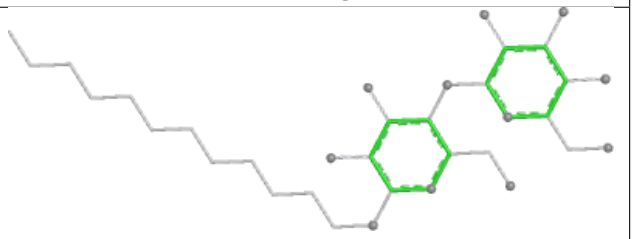
Bond lengths



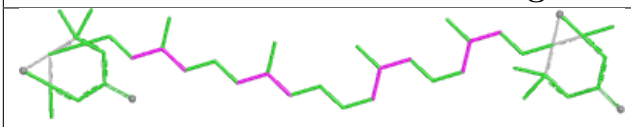
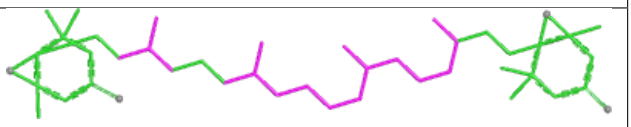
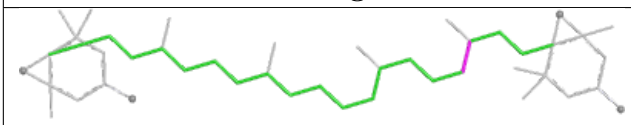
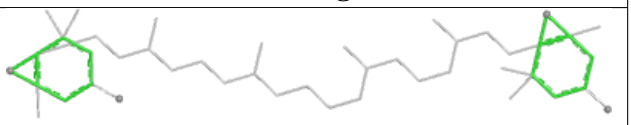
Bond angles

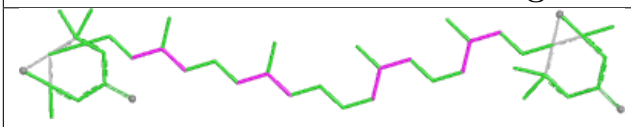
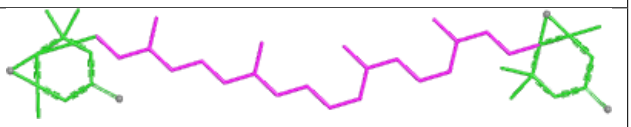
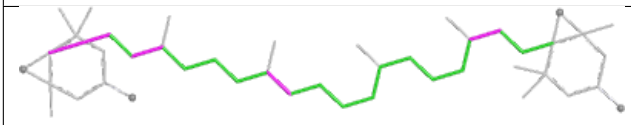
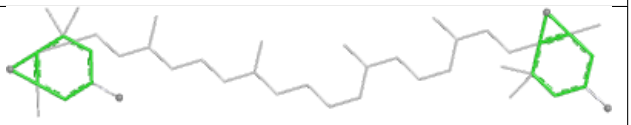


Torsions

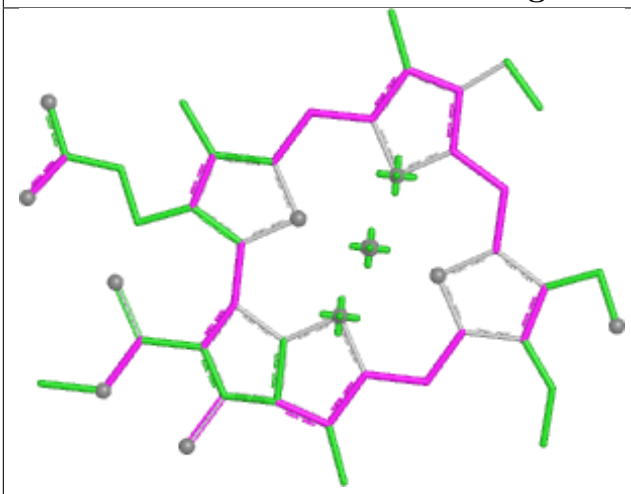


Rings

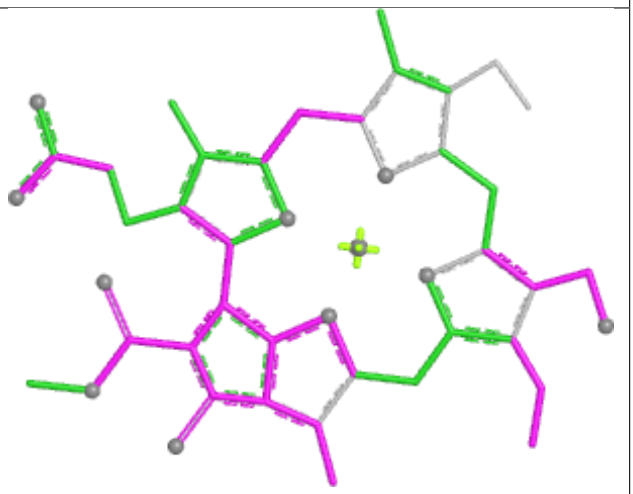
| Ligand XAT a 618 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand XAT 9 616 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

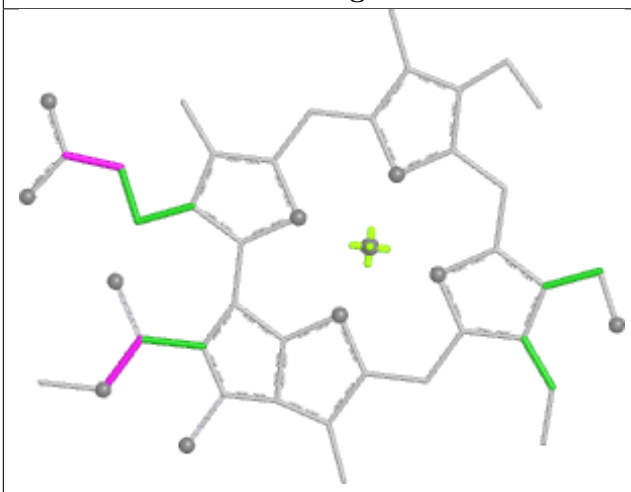
## Ligand CHL a 606



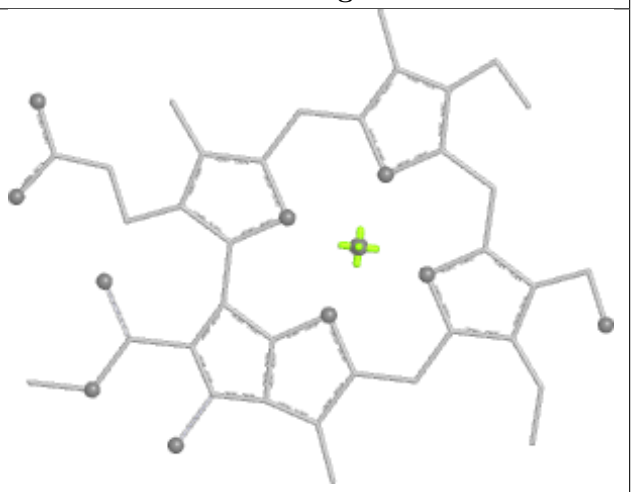
Bond lengths



Bond angles

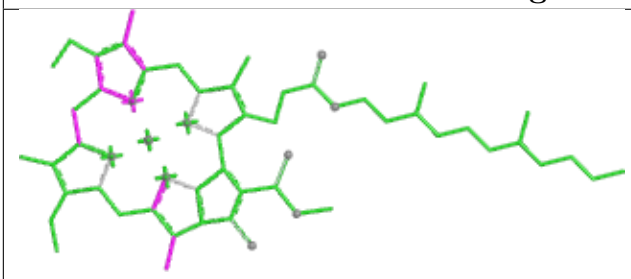


Torsions

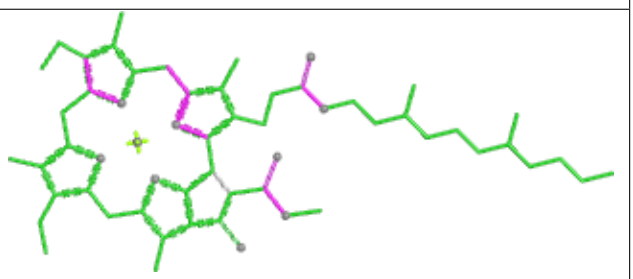


Rings

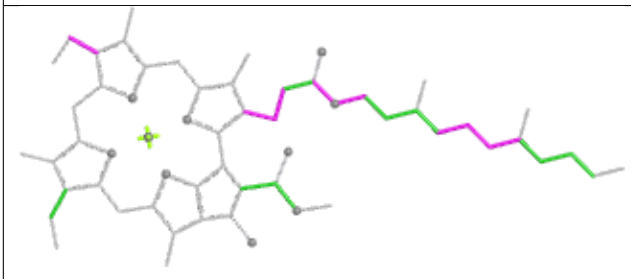
## Ligand CLA c 611



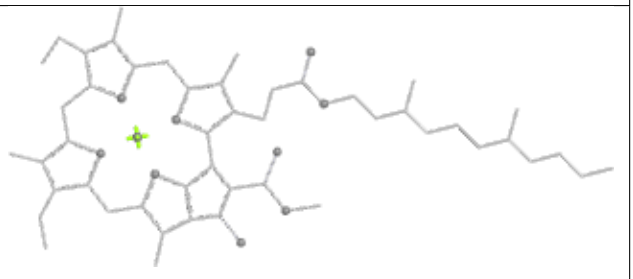
Bond lengths



Bond angles

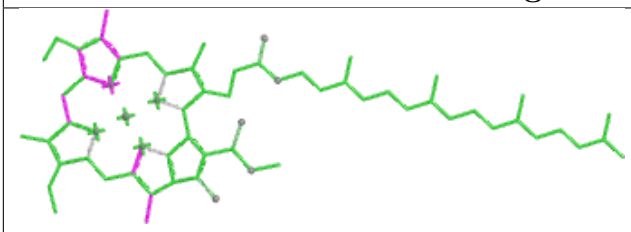


Torsions

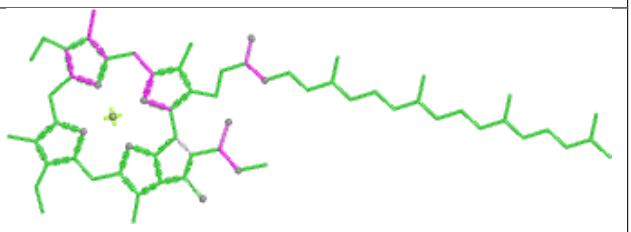


Rings

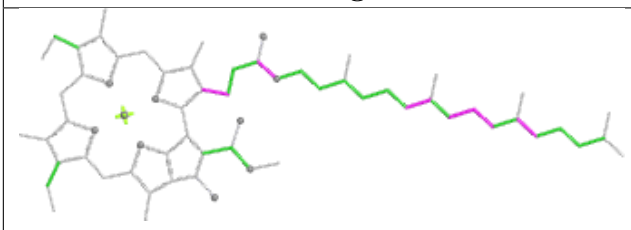
## Ligand CLA B 824



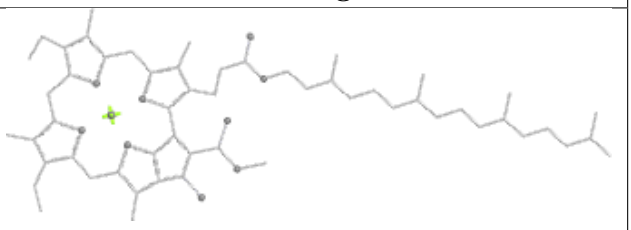
Bond lengths



Bond angles

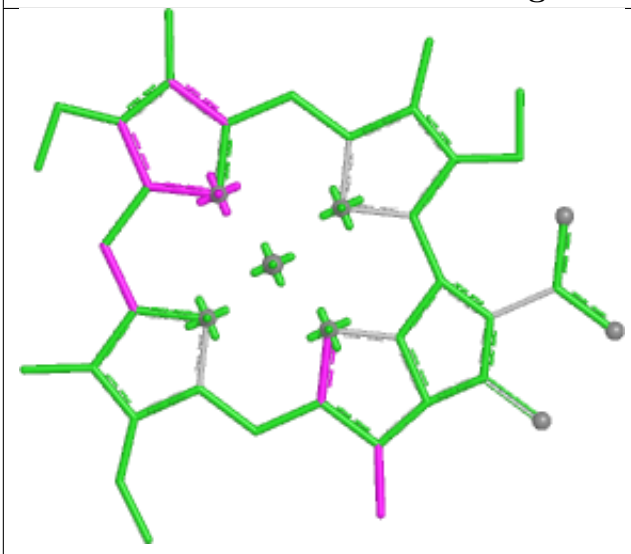


Torsions

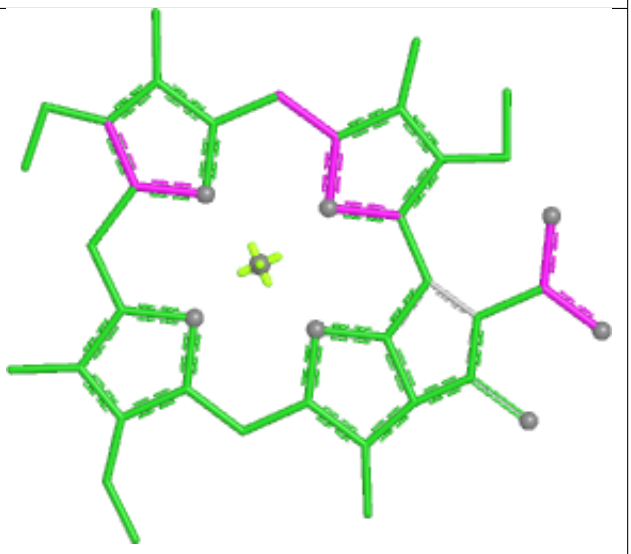


Rings

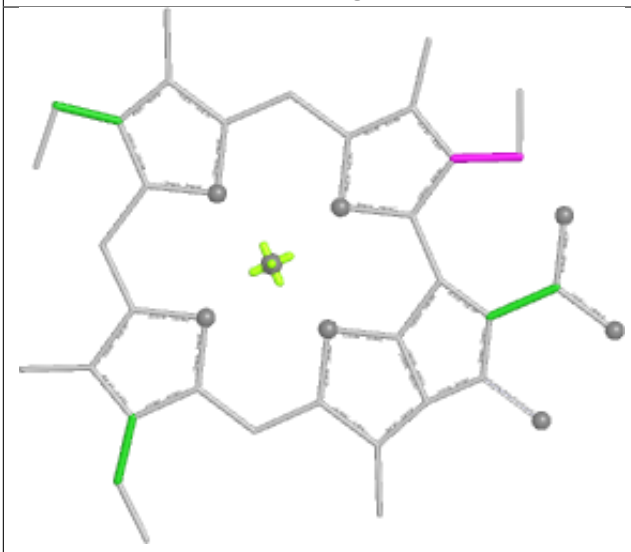
## Ligand CLA 7 404



Bond lengths



Bond angles

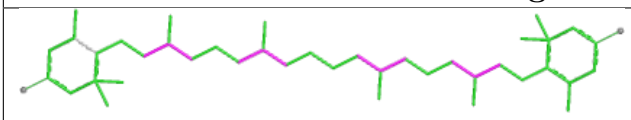


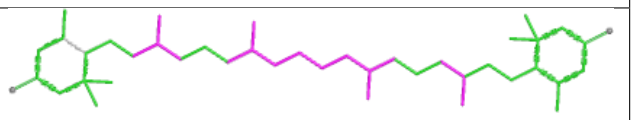
Torsions

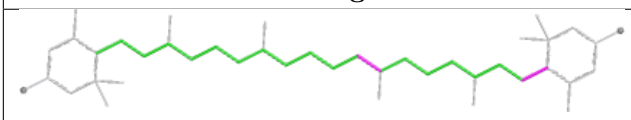


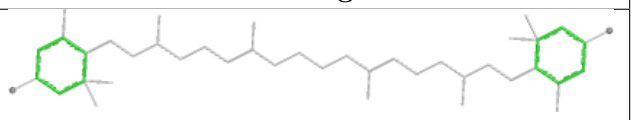
Rings

## Ligand LUT 8 614

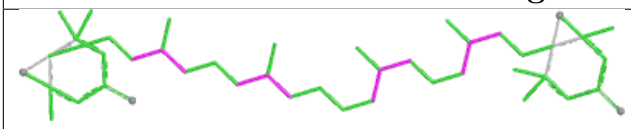

Bond lengths

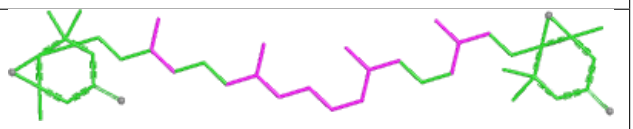

Bond angles

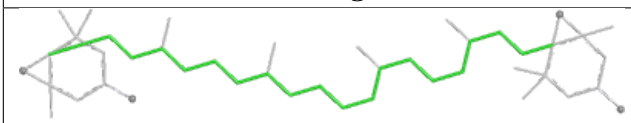

Torsions

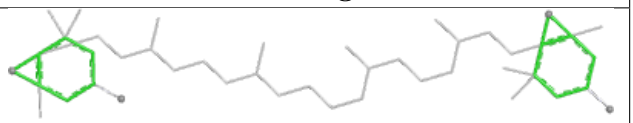

Rings

## Ligand XAT 8 615

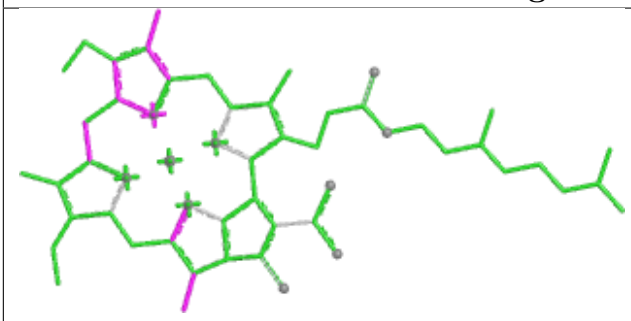

Bond lengths

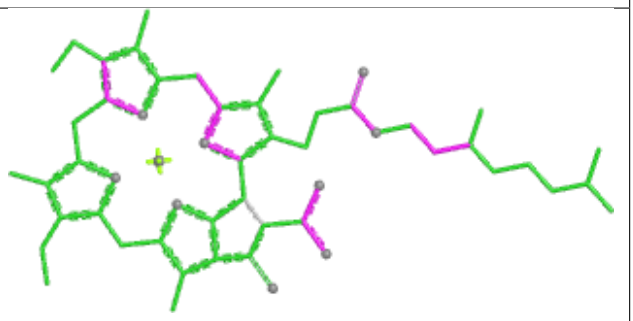

Bond angles

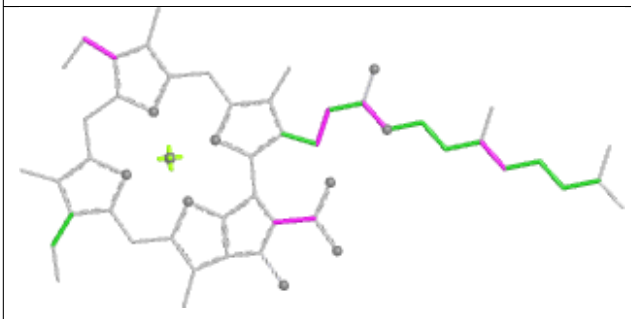

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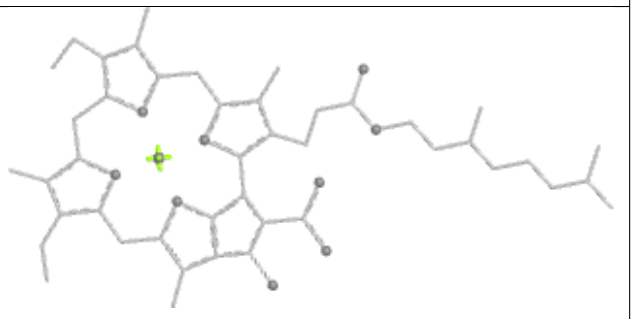

Rings

## Ligand CLA 7 411

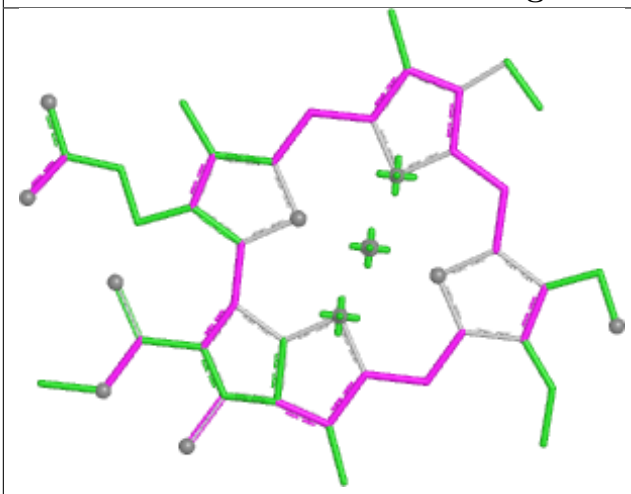

Bond lengths


Bond angles

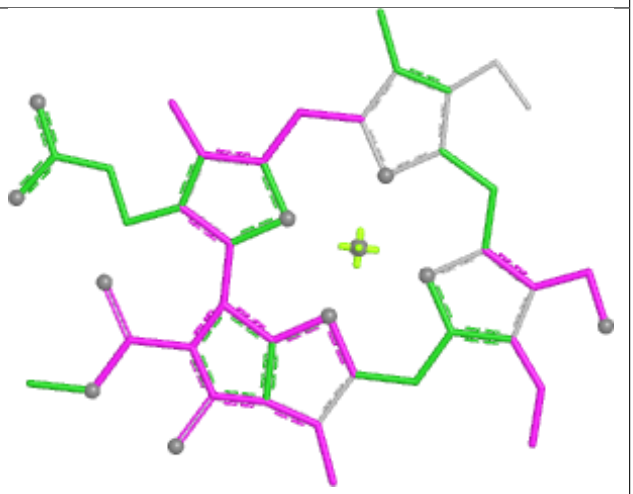

Torsions


Rings

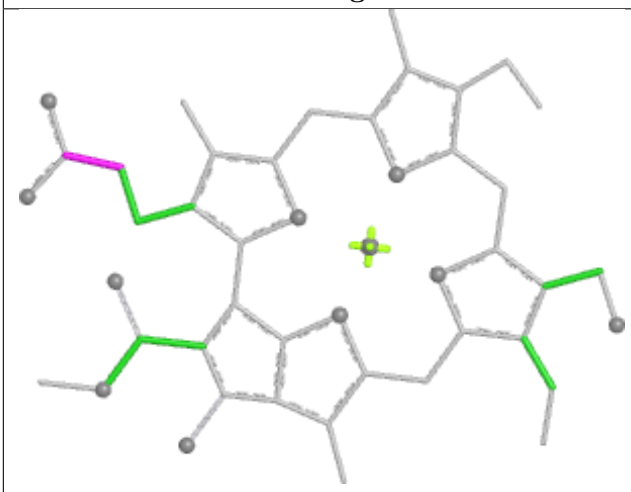
**Ligand CHL b 307**



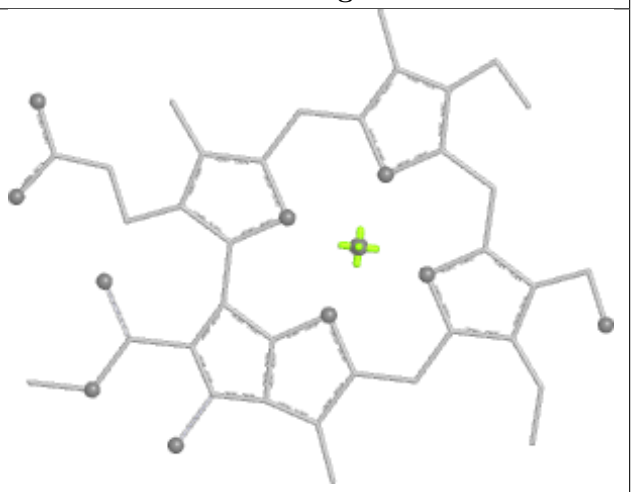
**Bond lengths**



**Bond angles**

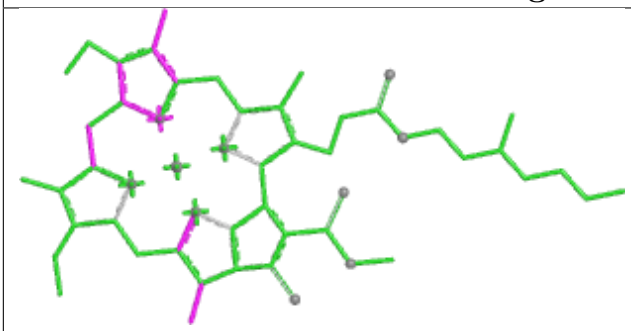


**Torsions**

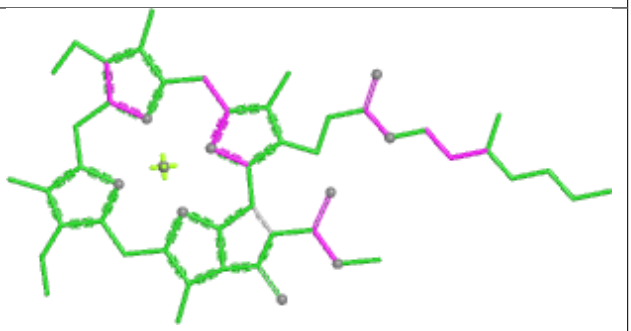


**Rings**

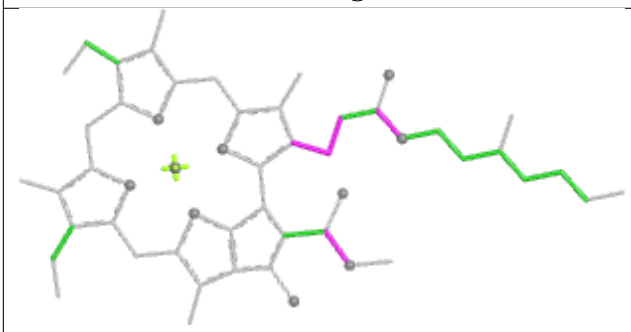
**Ligand CLA 9 613**



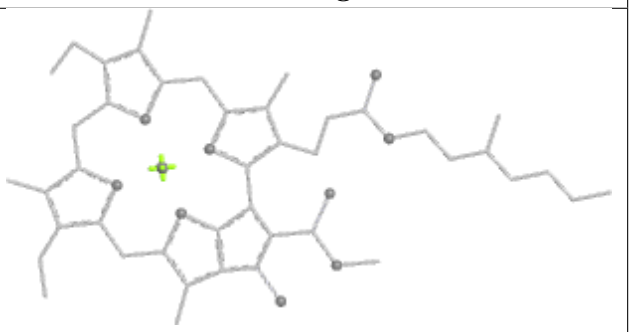
**Bond lengths**



**Bond angles**

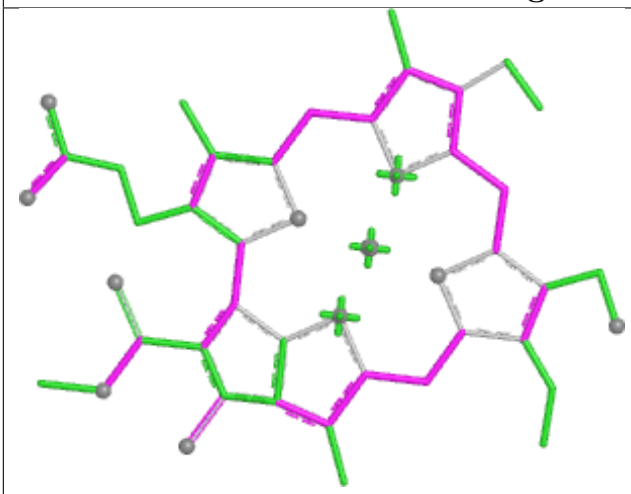


**Torsions**

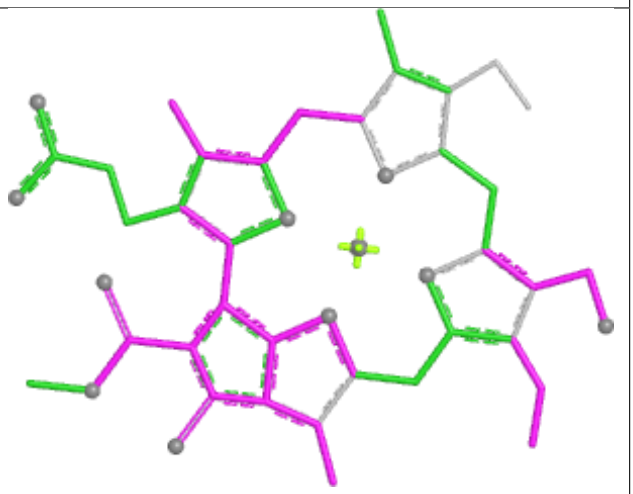


**Rings**

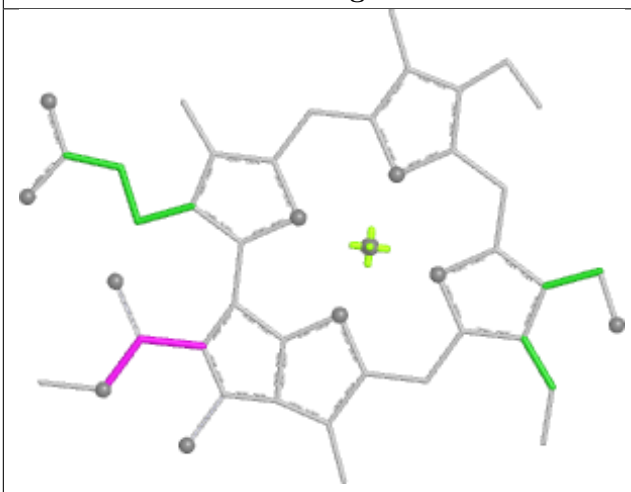
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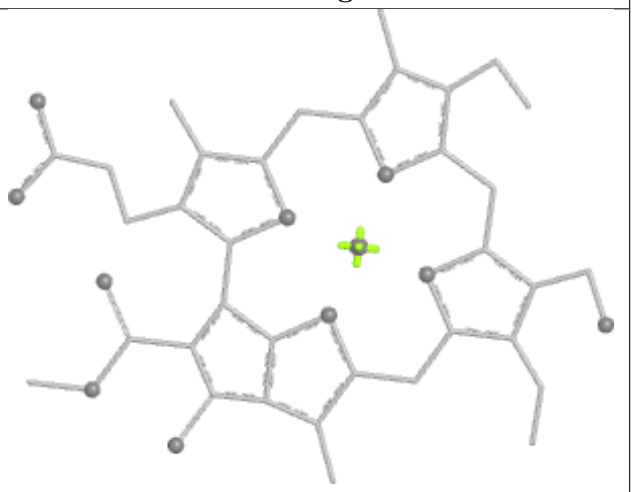
**Bond lengths**



**Bond angles**

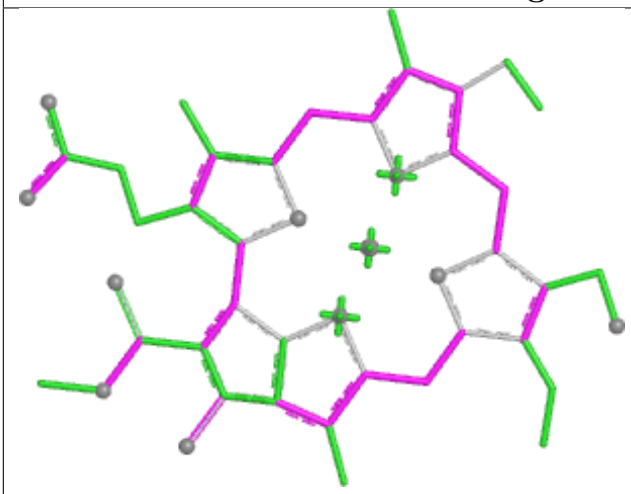


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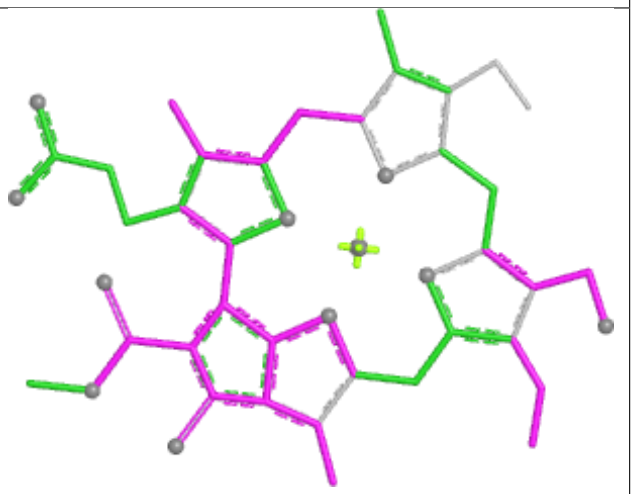


**Rings**

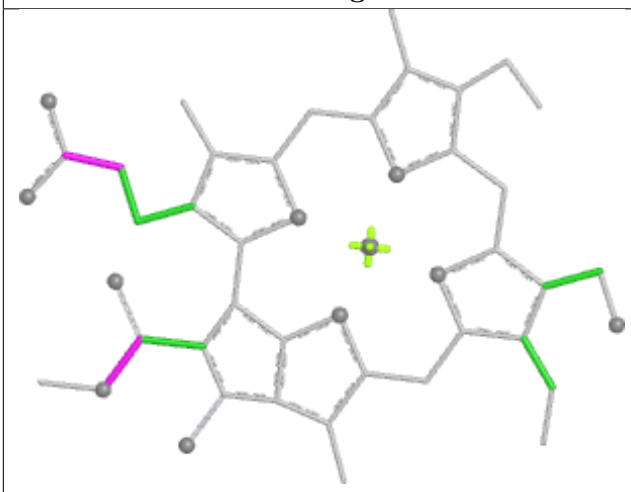
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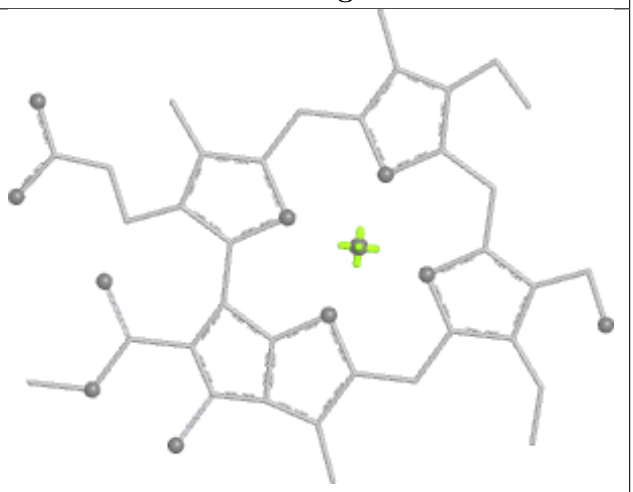
Bond lengths



Bond angles

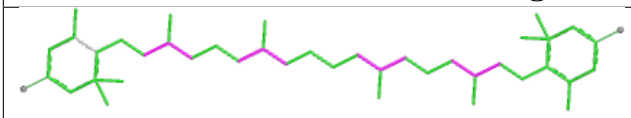


Torsions

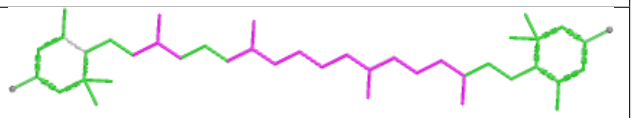


Rings

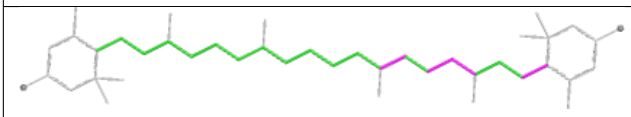
**Ligand LUT 5 615**



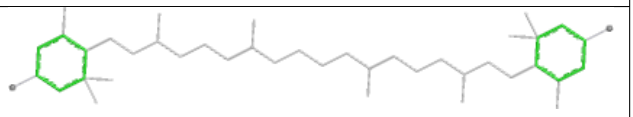
Bond lengths



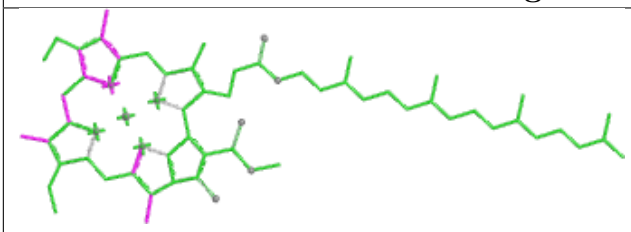
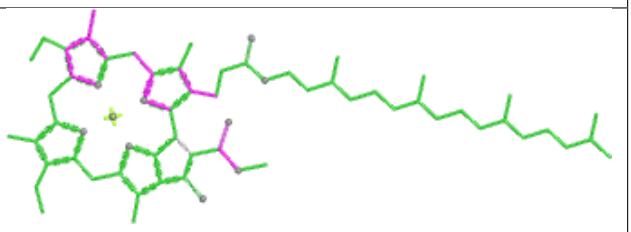
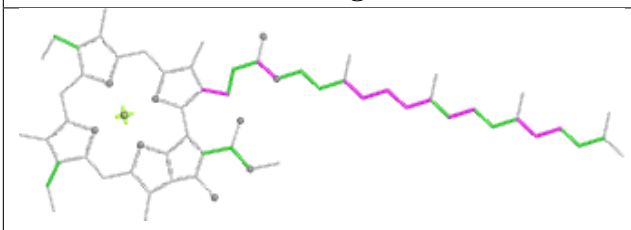
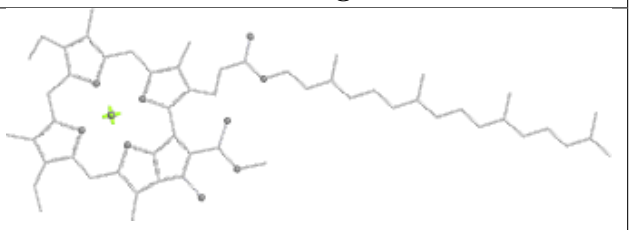
Bond angles

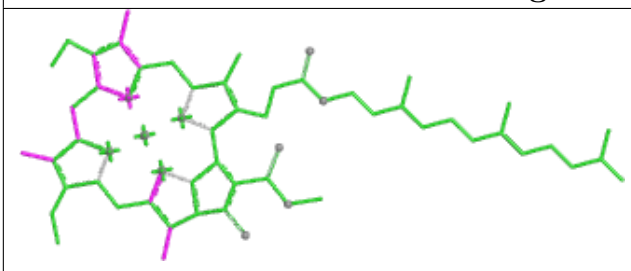
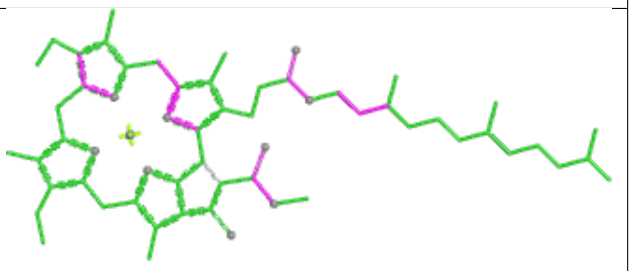
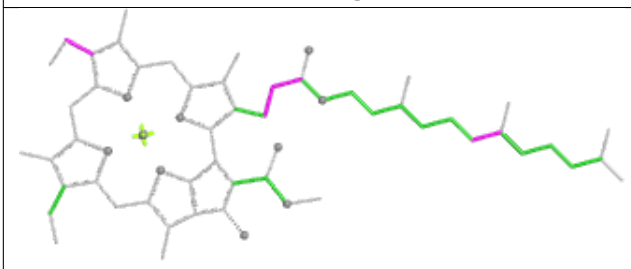
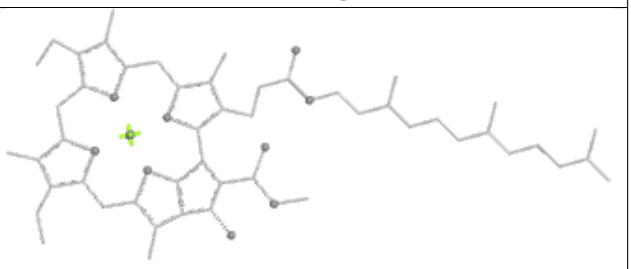


Torsions

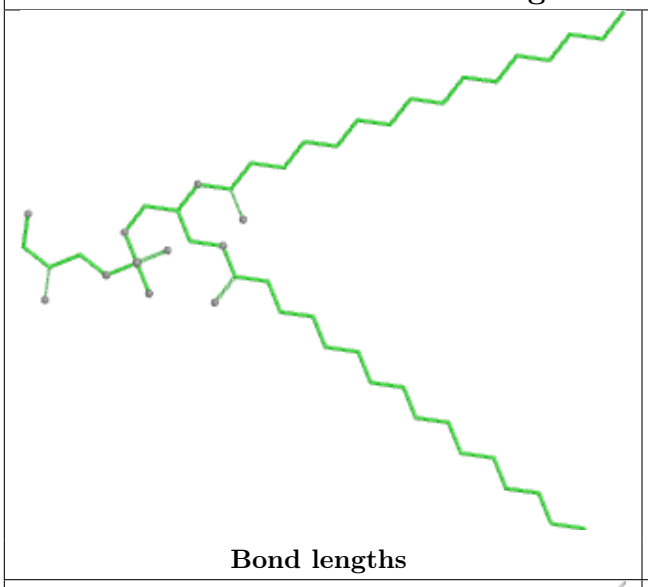


Rings

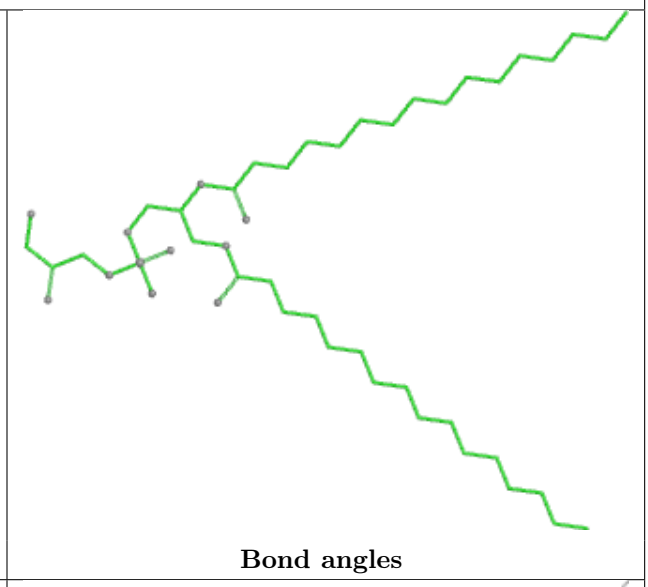
| Ligand CLA B 836 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

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

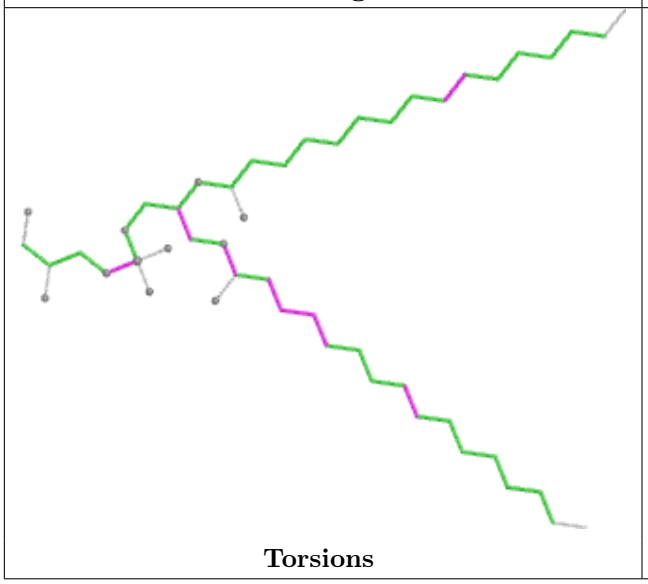
**Ligand LHG a 617**



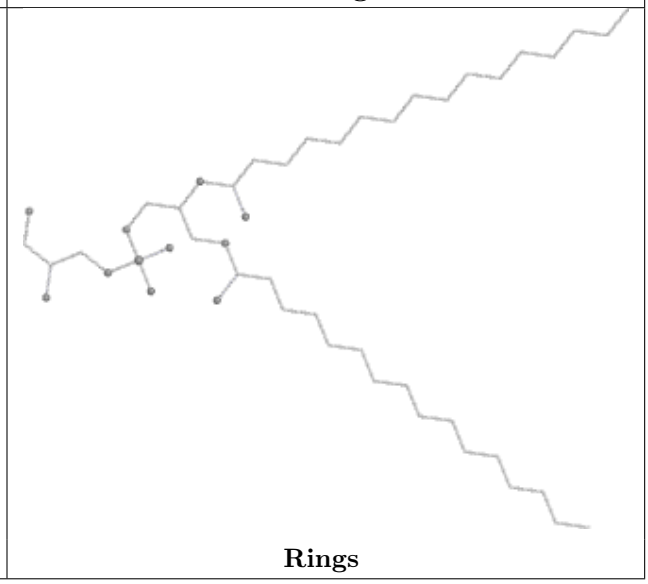
**Bond lengths**



**Bond angles**

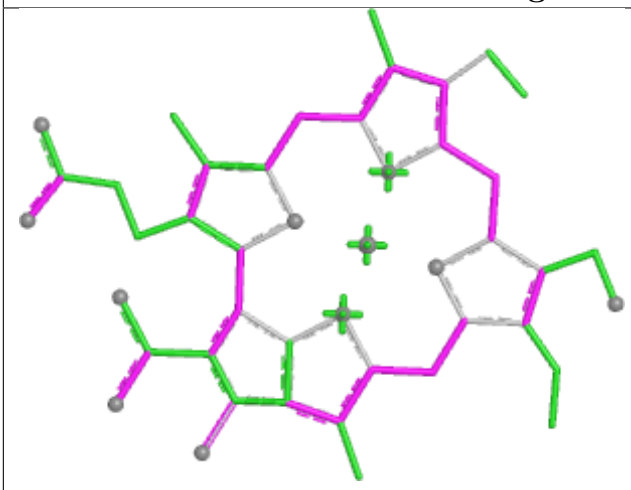


**Torsions**

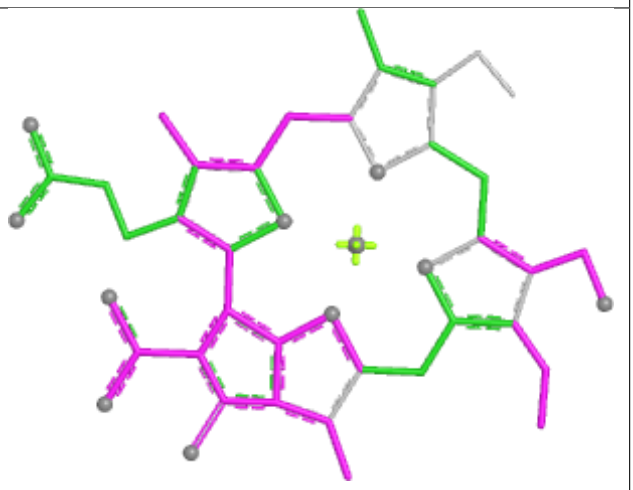


**Rings**

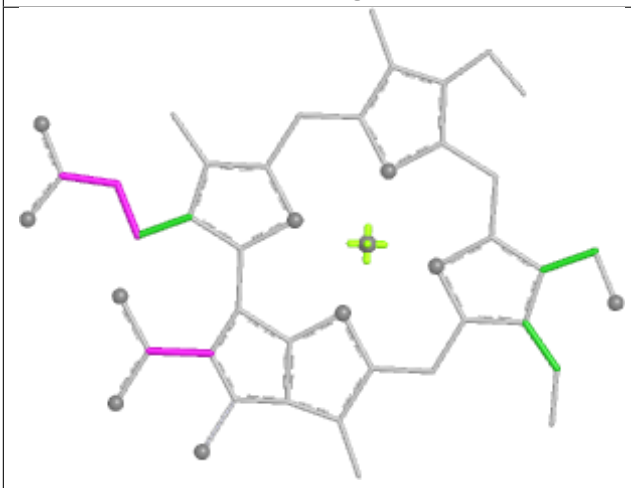
**Ligand CHL a 605**



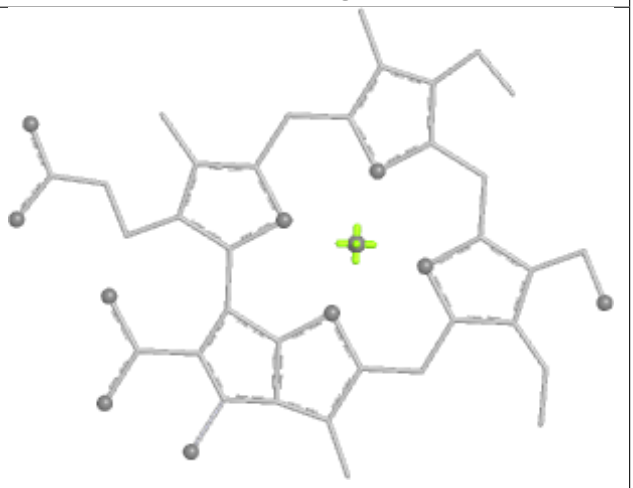
Bond lengths



Bond angles

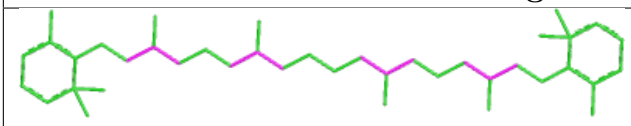


Torsions

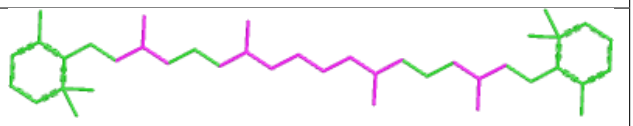


Rings

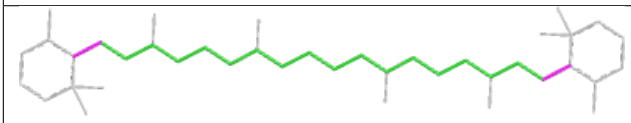
**Ligand BCR 6 618**



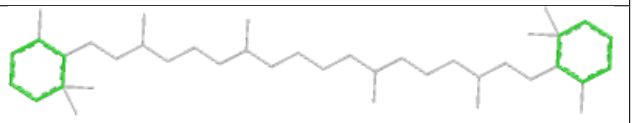
Bond lengths



Bond angles



Torsions

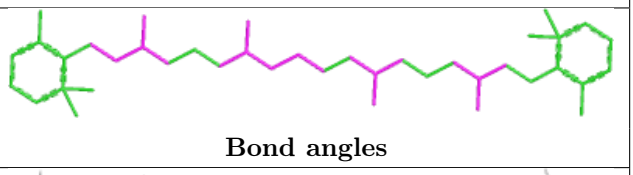


Rings

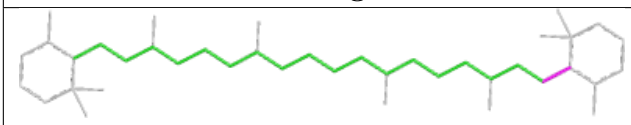
## Ligand BCR 4 617



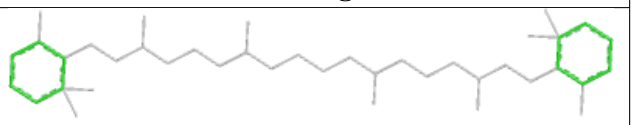
Bond lengths



Bond angles

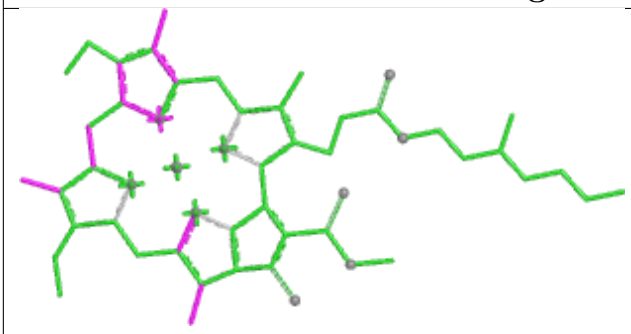


Torsions

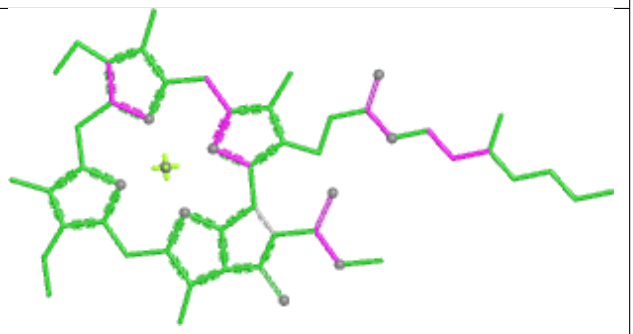


Rings

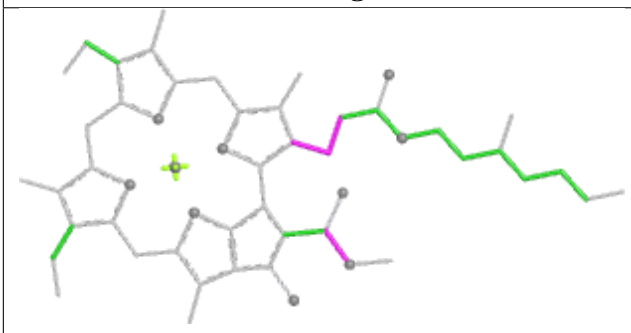
## Ligand CLA 9 602



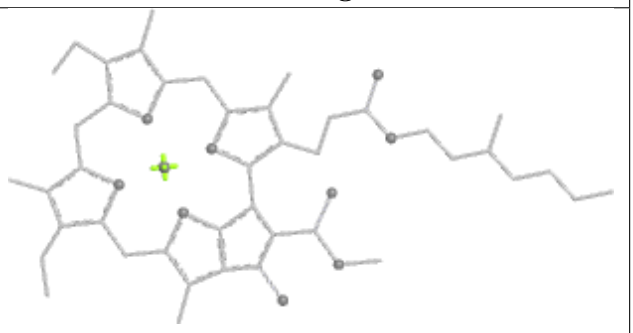
Bond lengths



Bond angles

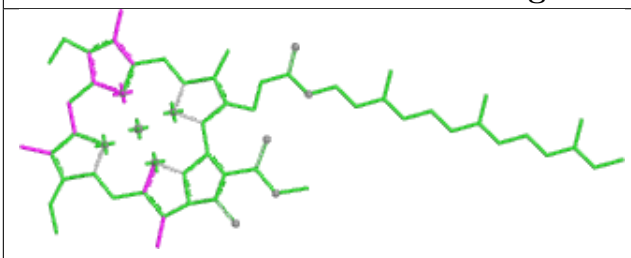


Torsions

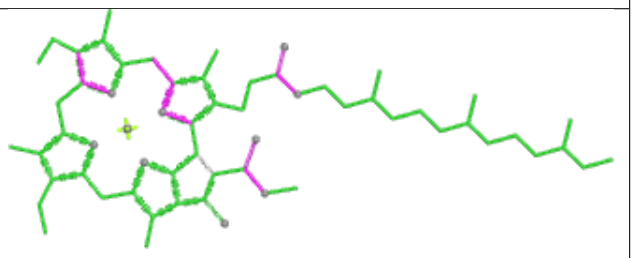


Rings

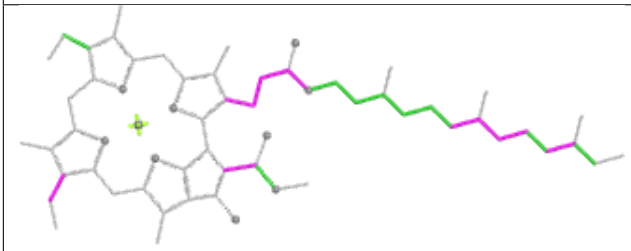
## Ligand CLA 1 303



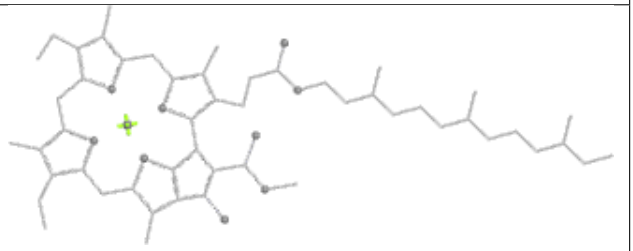
Bond lengths



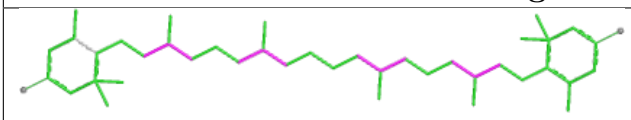
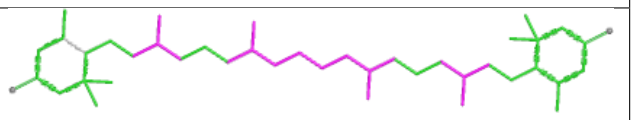
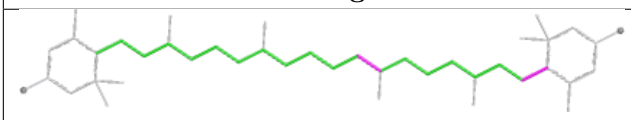
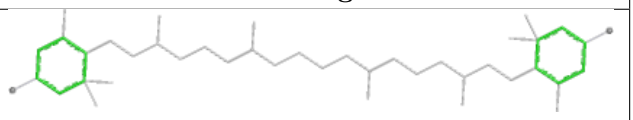
Bond angles

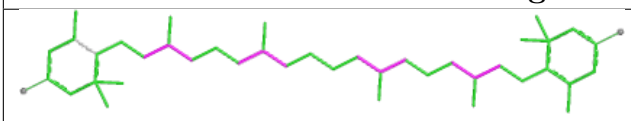
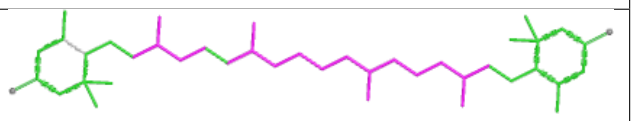
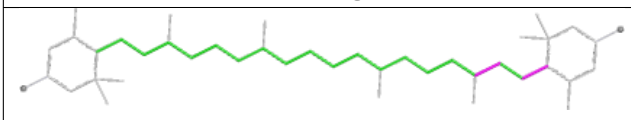
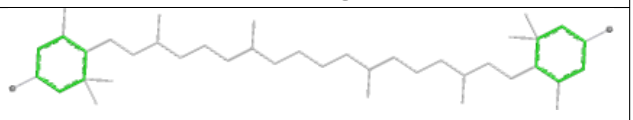


Torsions

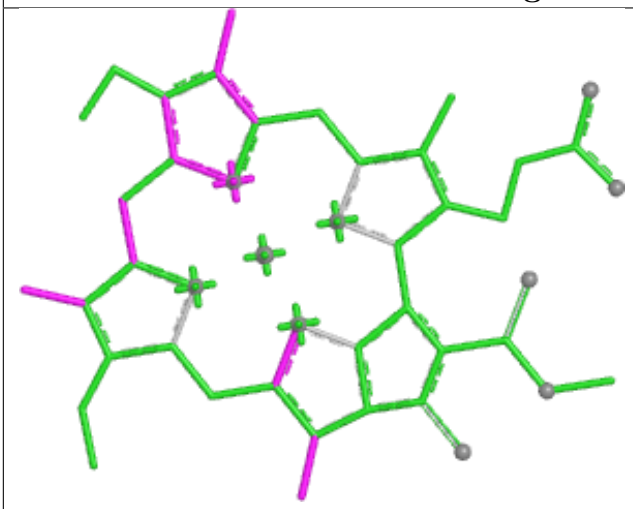


Rings

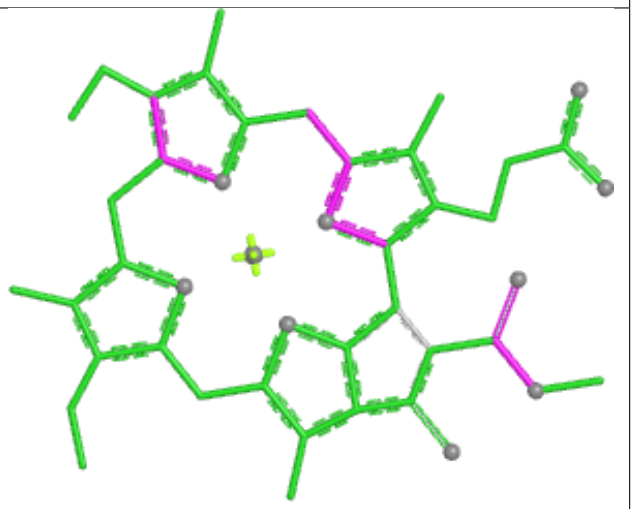
| Ligand LUT 1 317 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand LUT 2 616 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

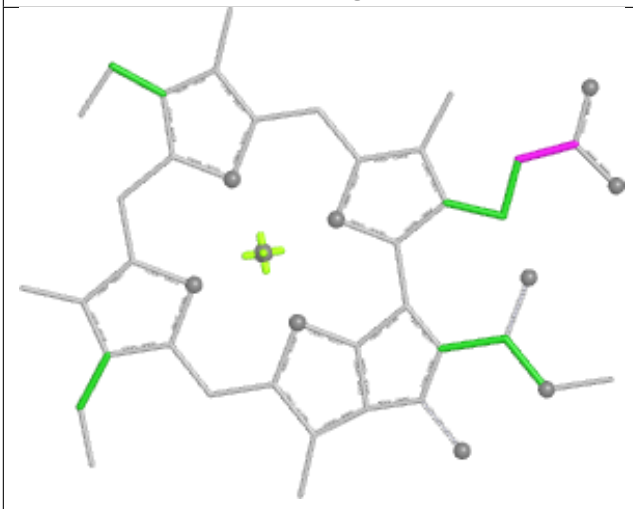
**Ligand CLA A 836**



**Bond lengths**



**Bond angles**

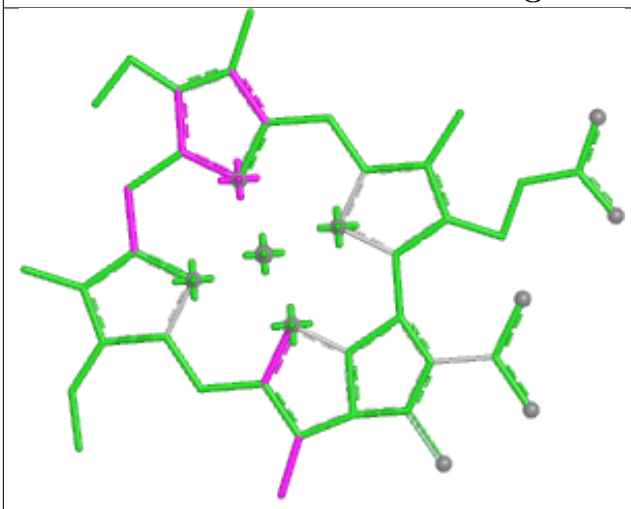


**Torsions**

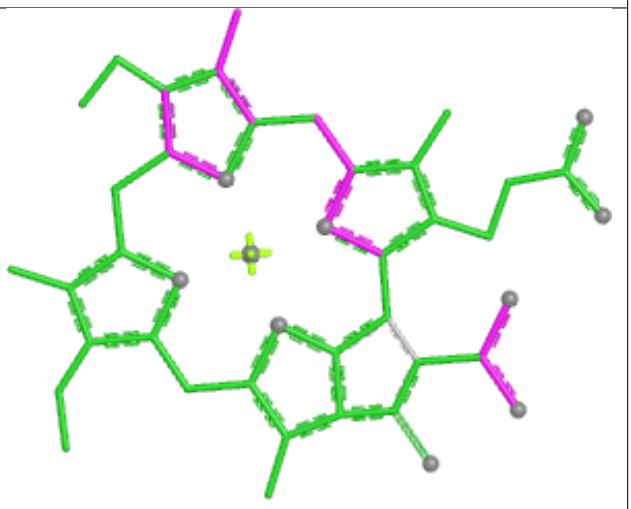


**Rings**

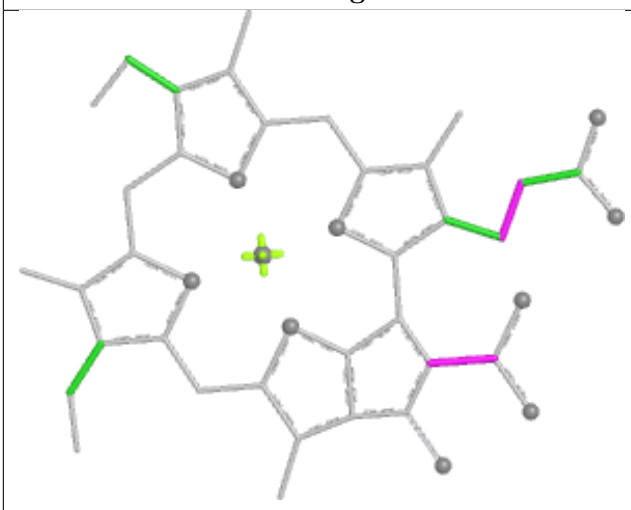
## Ligand CLA B 813



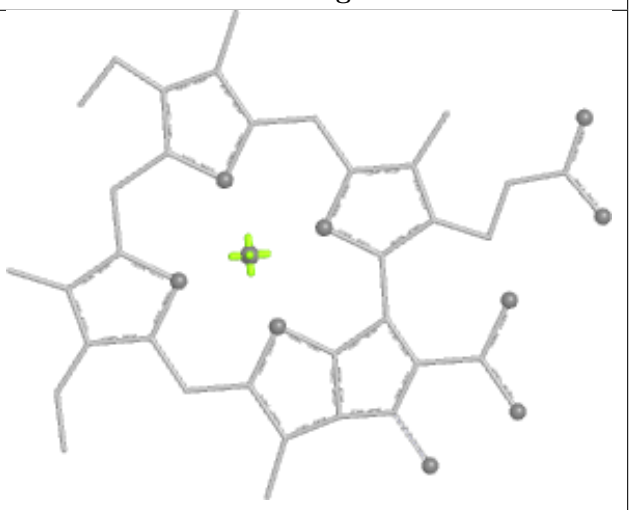
Bond lengths



Bond angles

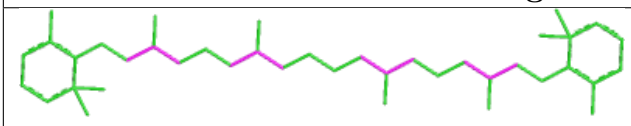


Torsions

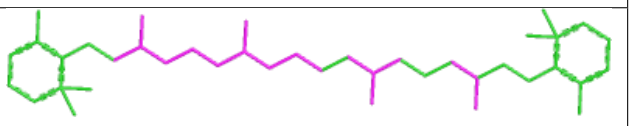


Rings

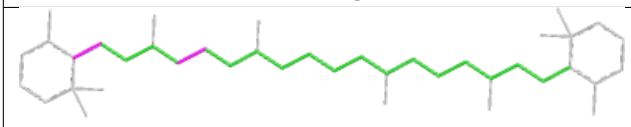
## Ligand BCR J 103



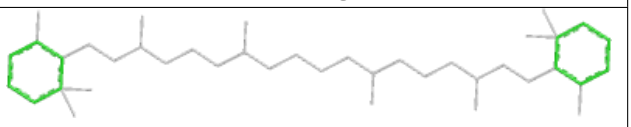
Bond lengths



Bond angles

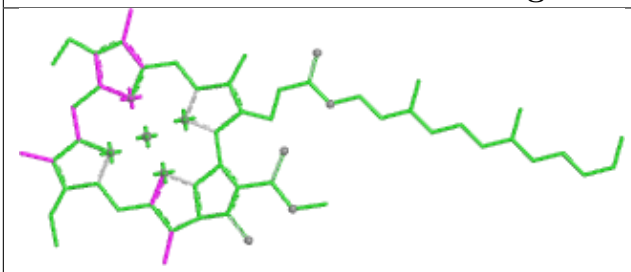


Torsions

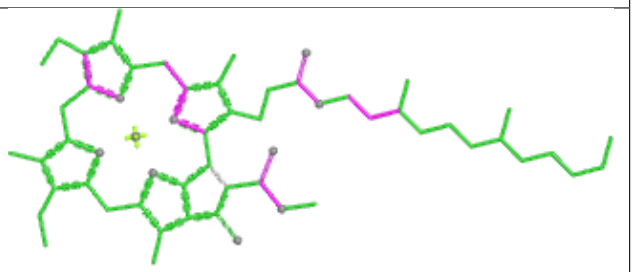


Rings

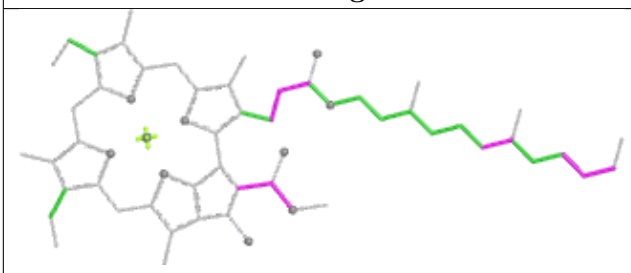
## Ligand CLA b 303



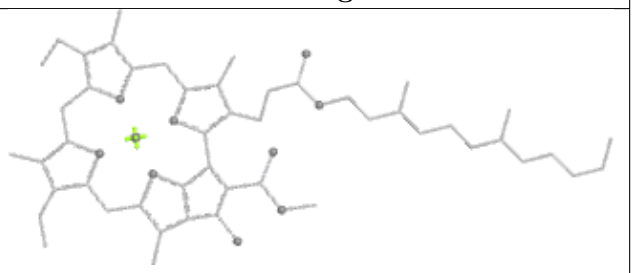
Bond lengths



Bond angles

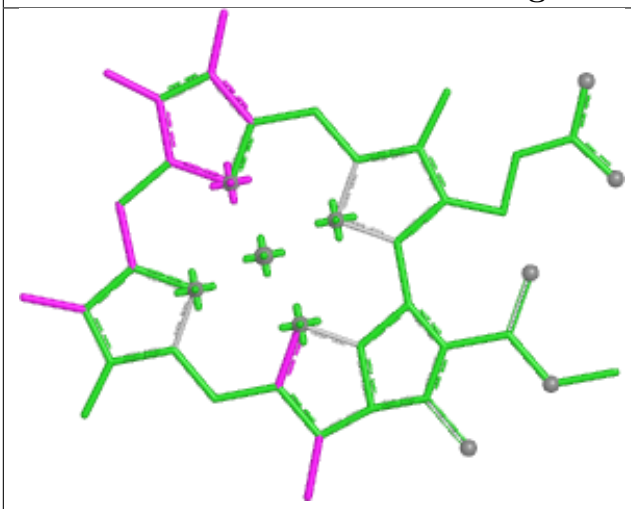


Torsions

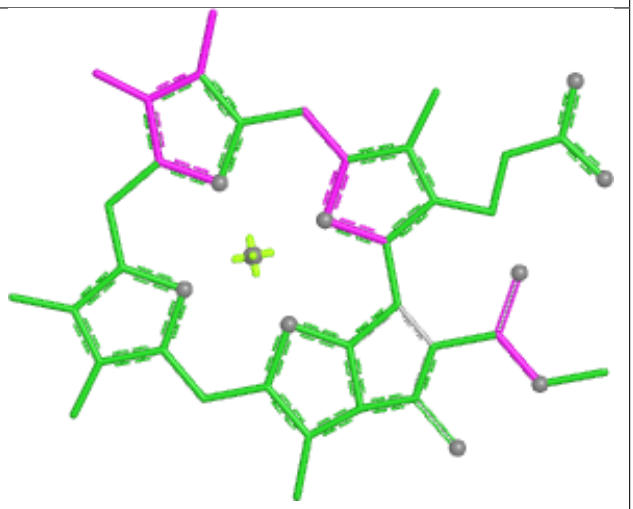


Rings

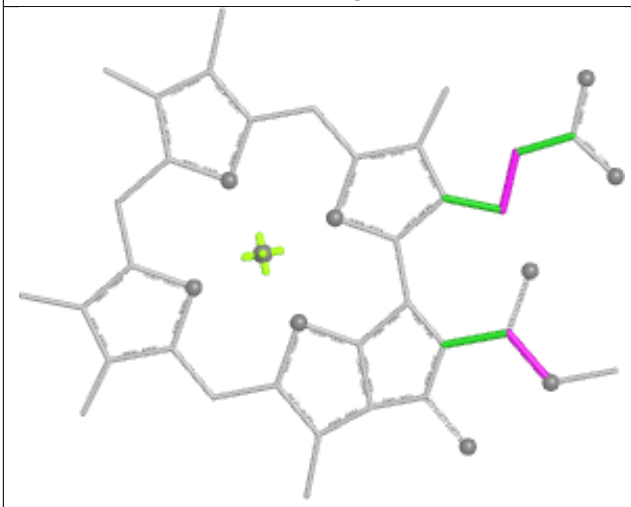
## Ligand CLA 1 316



Bond lengths



Bond angles

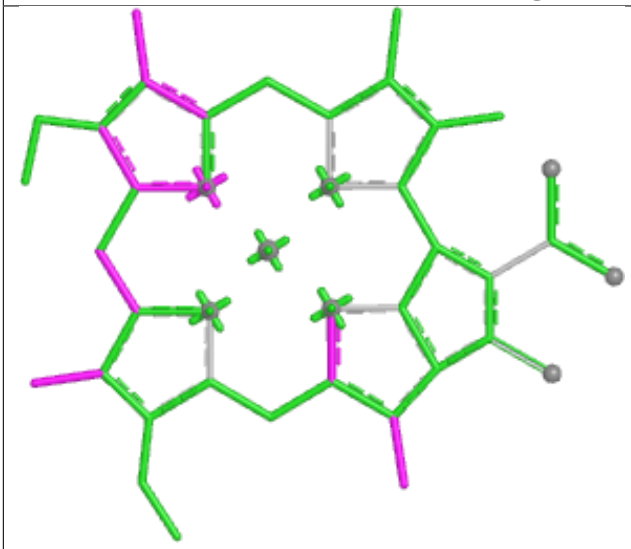


Torsions

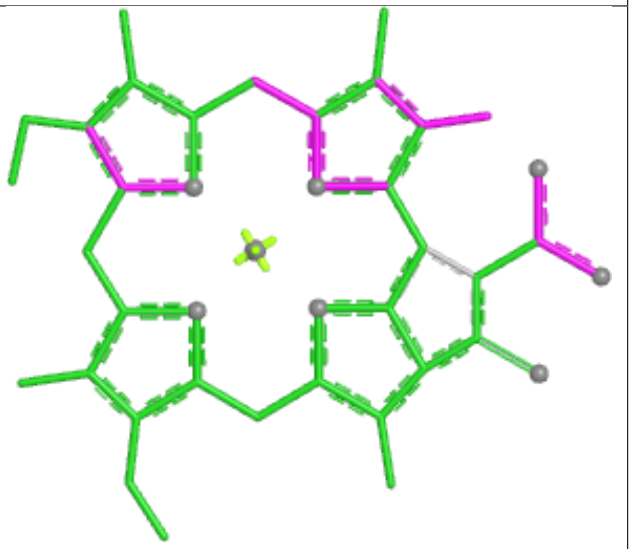


Rings

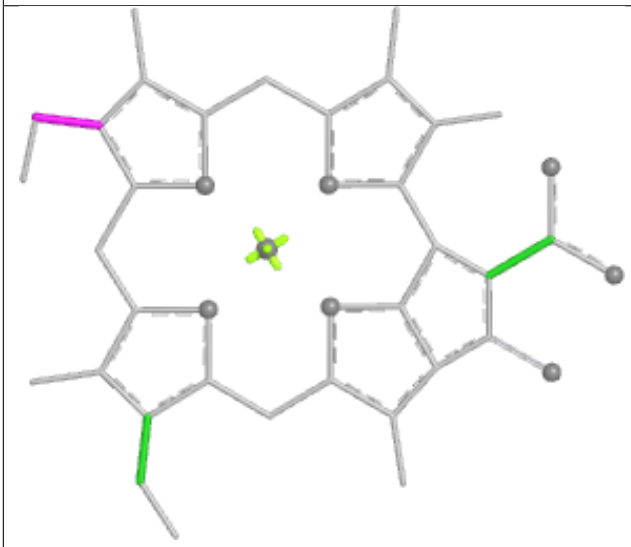
**Ligand CLA 3 413**



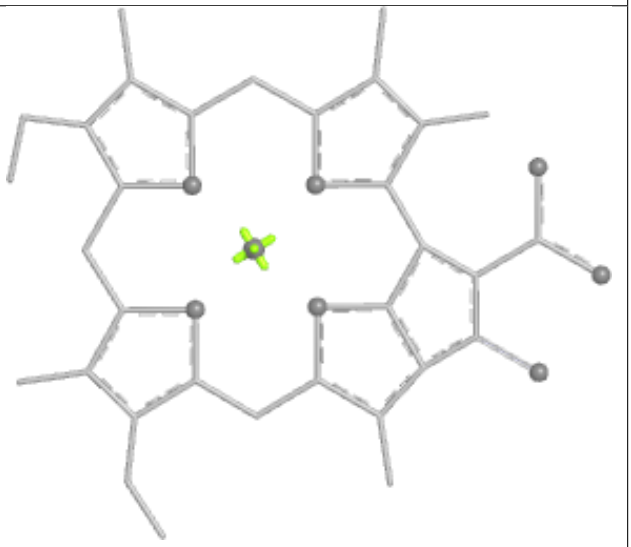
**Bond lengths**



**Bond angles**

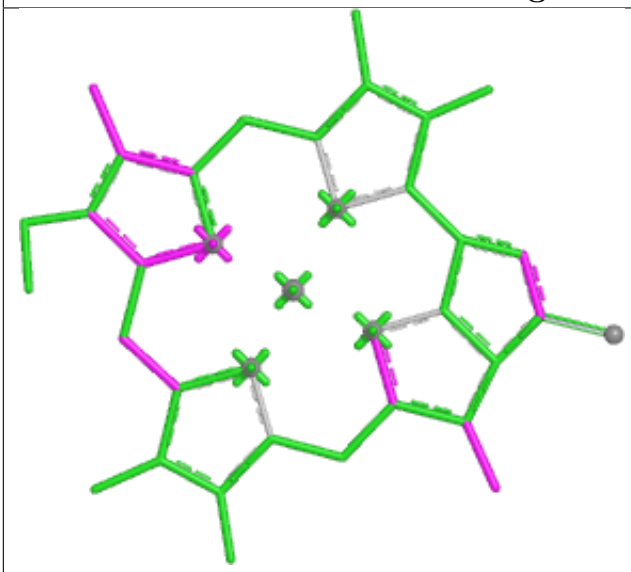


**Torsions**

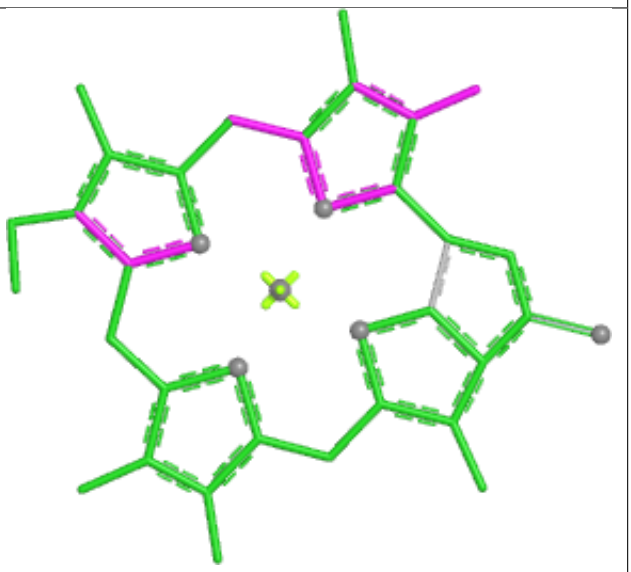


**Rings**

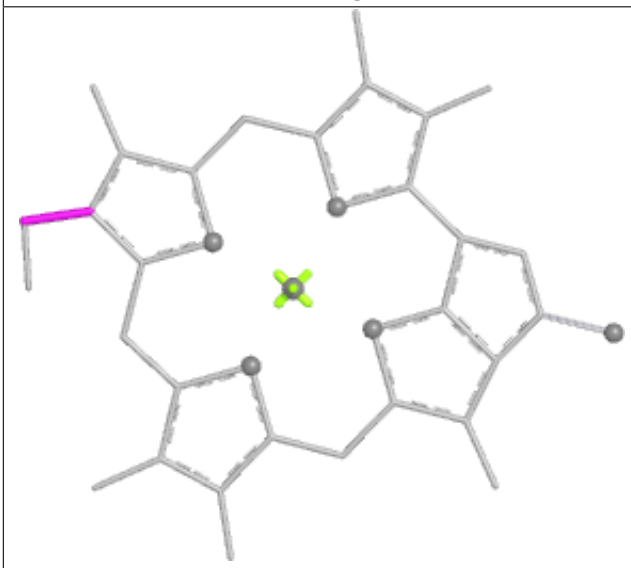
## Ligand CLA 3 414



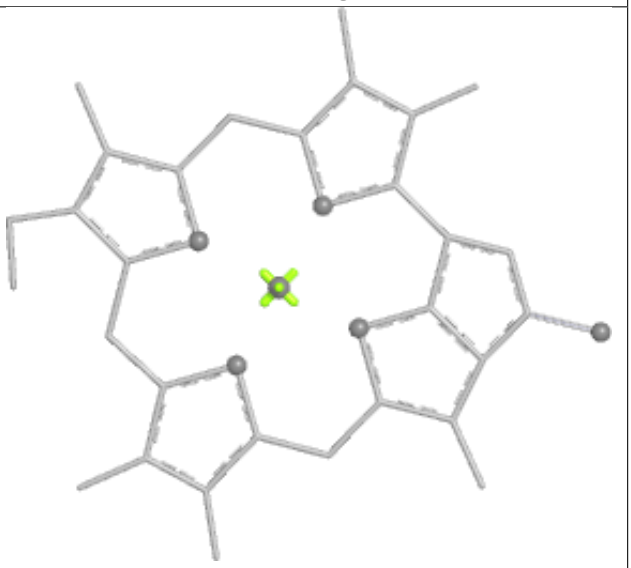
Bond lengths



Bond angles

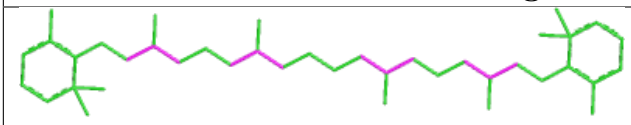


Torsions

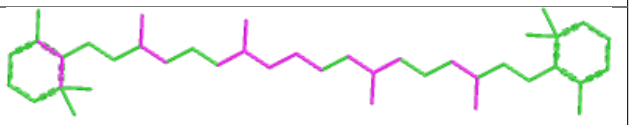


Rings

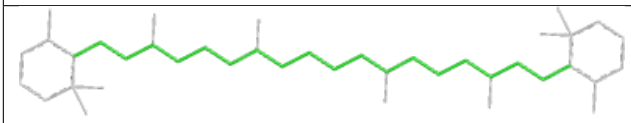
## Ligand BCR B 842



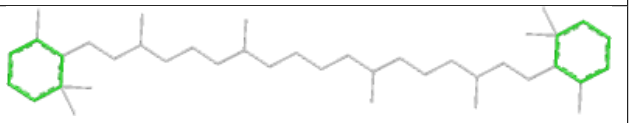
Bond lengths



Bond angles

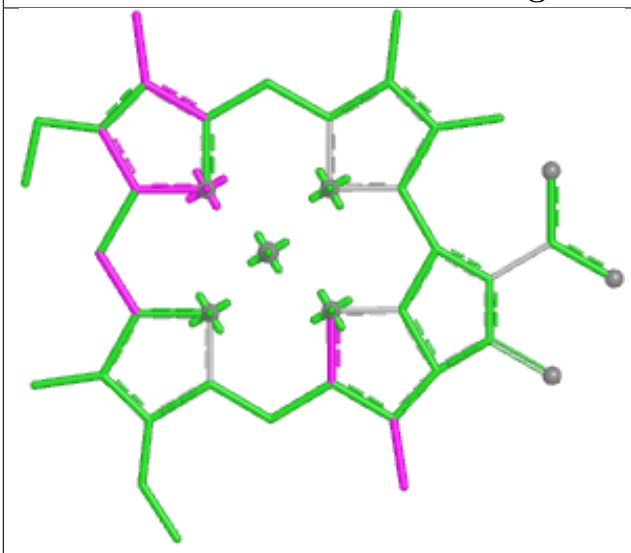


Torsions

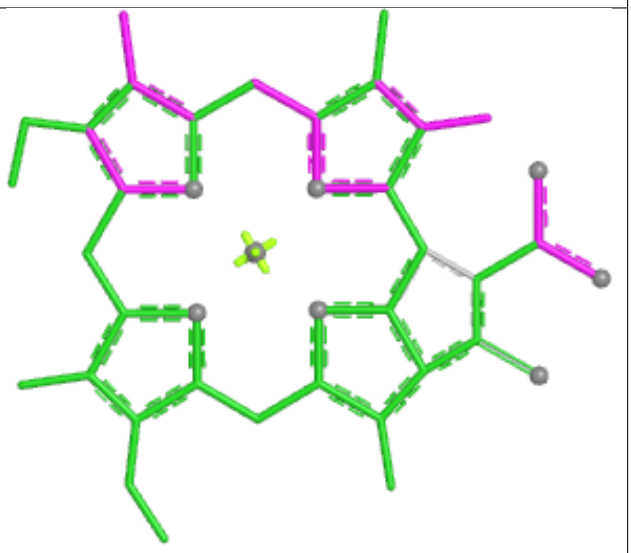


Rings

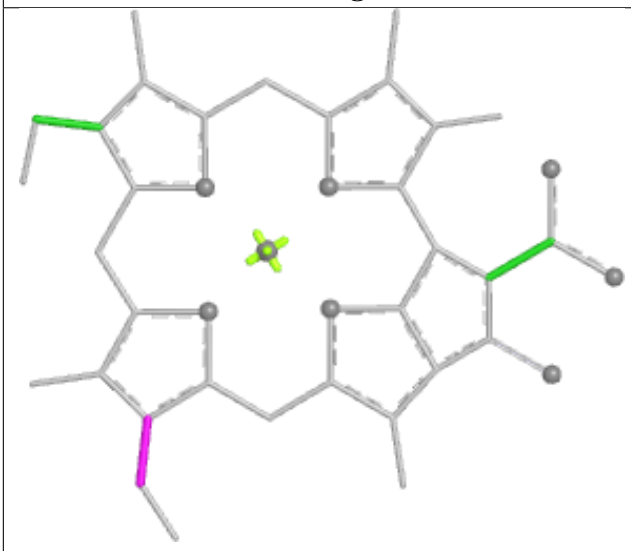
**Ligand CLA 3 401**



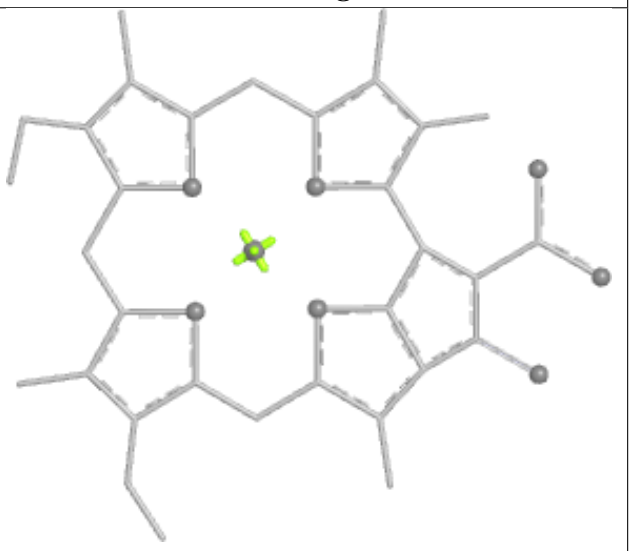
Bond lengths



Bond angles

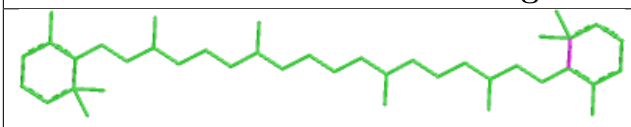


Torsions

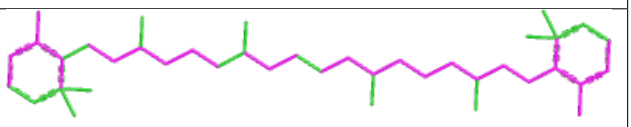


Rings

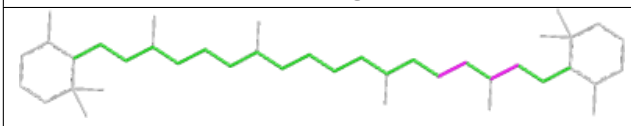
**Ligand BCR K 205**



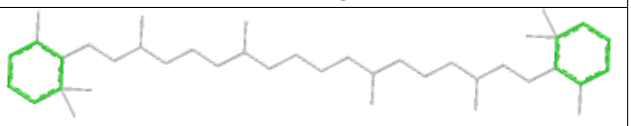
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

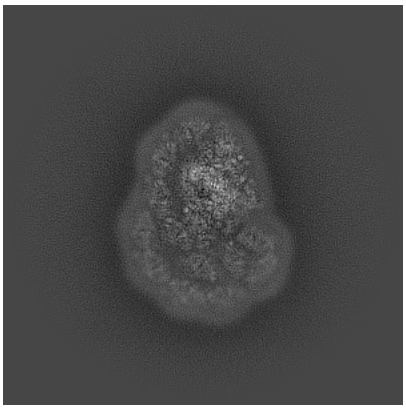
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33401. These allow visual inspection of the internal detail of the map and identification of artifacts.

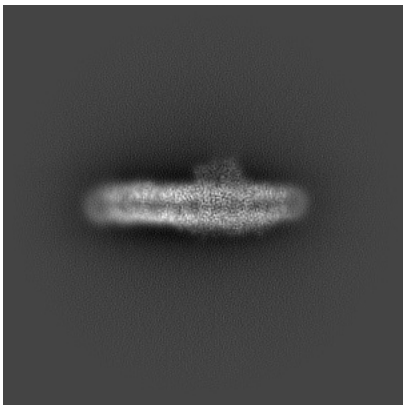
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

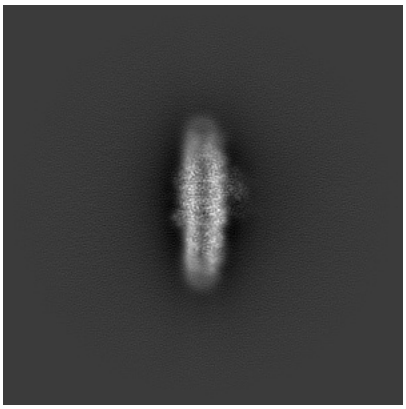
### 6.1.1 Primary map



X

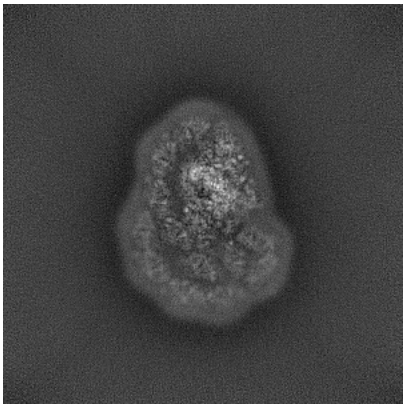


Y

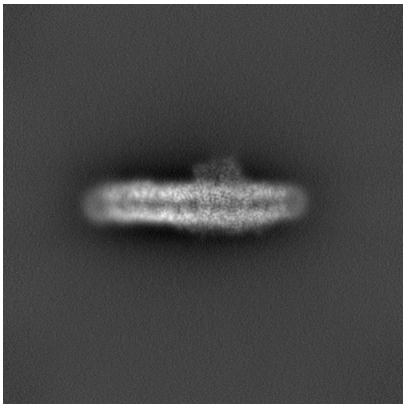


Z

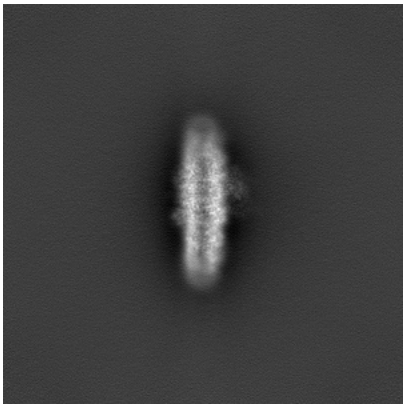
### 6.1.2 Raw map



X



Y

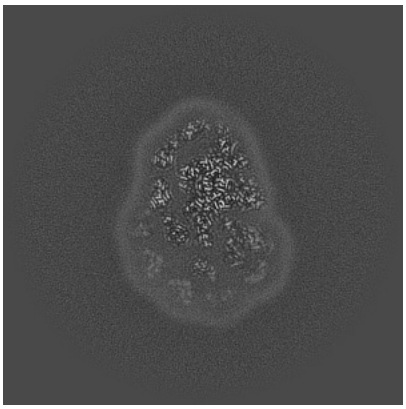


Z

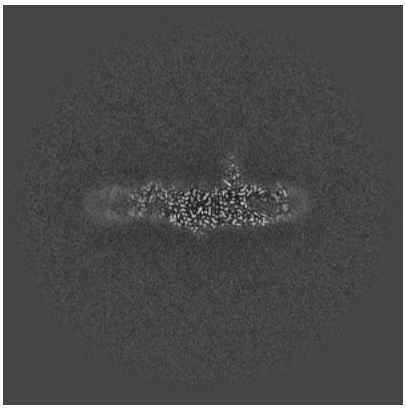
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

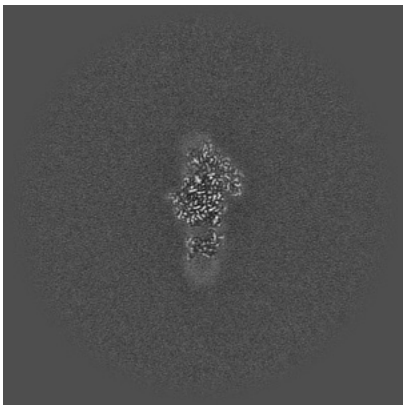
### 6.2.1 Primary map



X Index: 240

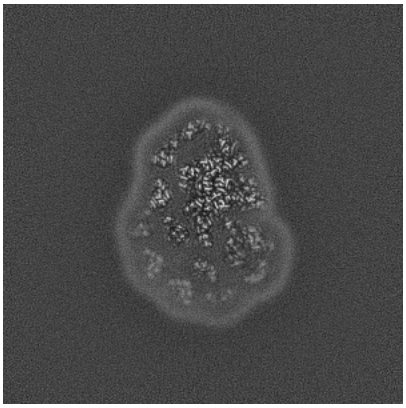


Y Index: 240

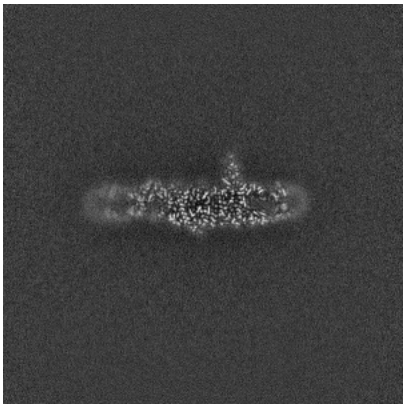


Z Index: 240

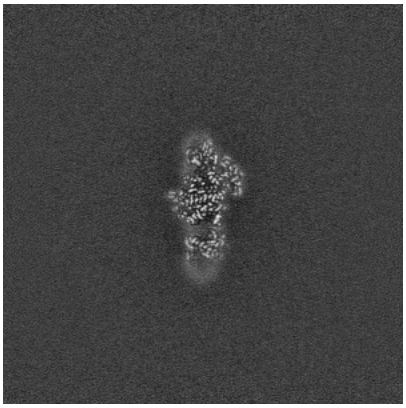
### 6.2.2 Raw map



X Index: 240



Y Index: 240

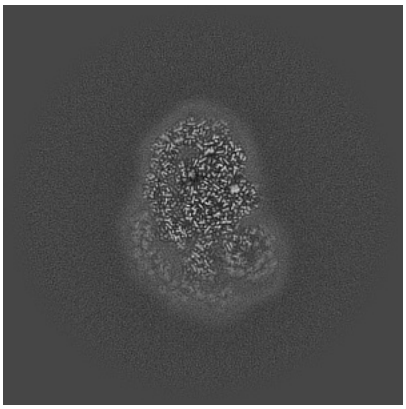


Z Index: 240

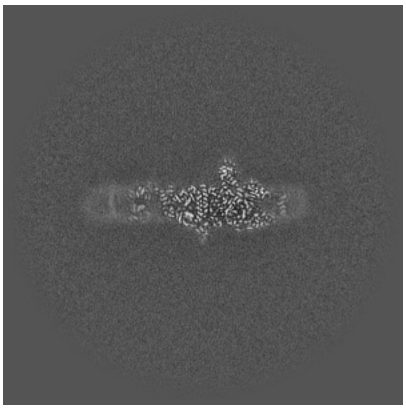
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

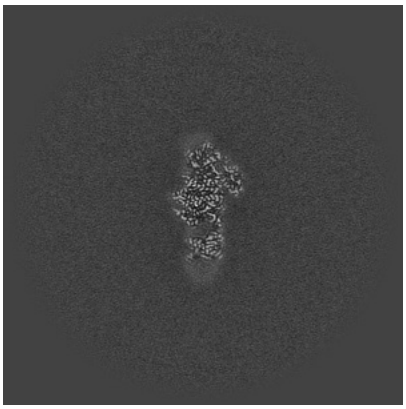
### 6.3.1 Primary map



X Index: 252

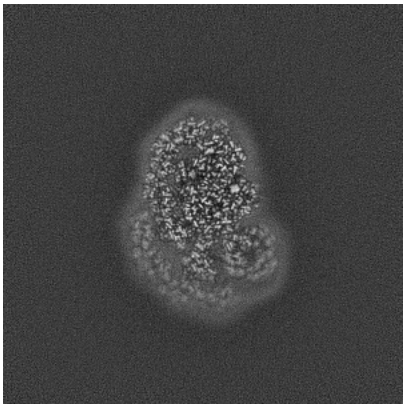


Y Index: 247

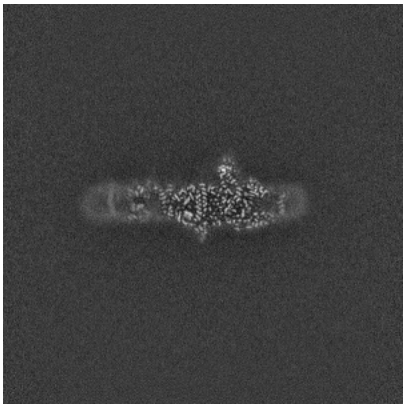


Z Index: 243

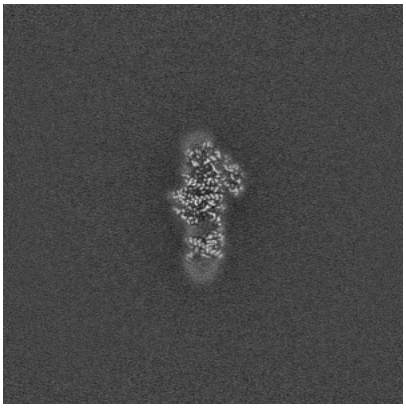
### 6.3.2 Raw map



X Index: 252



Y Index: 247

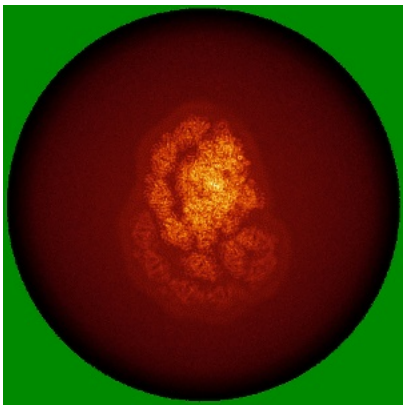


Z Index: 242

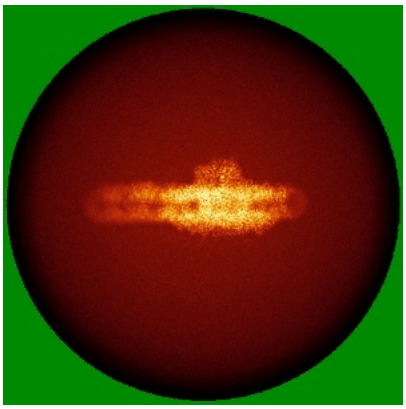
The images above show the largest variance slices of the map in three orthogonal directions.

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

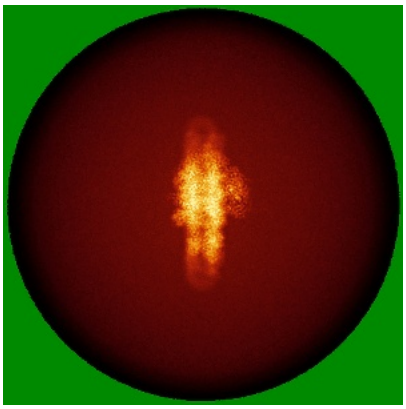
### 6.4.1 Primary map



X

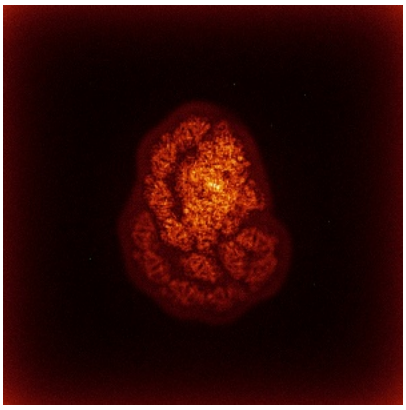


Y

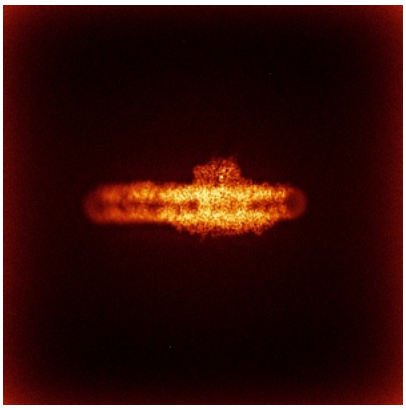


Z

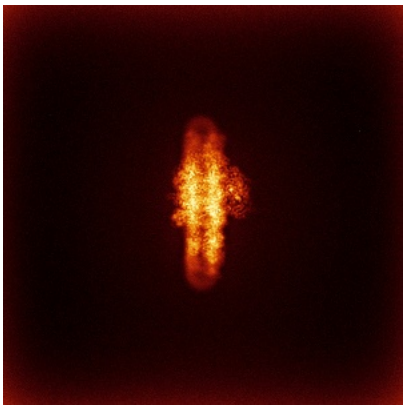
### 6.4.2 Raw map



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)

This section was not generated.

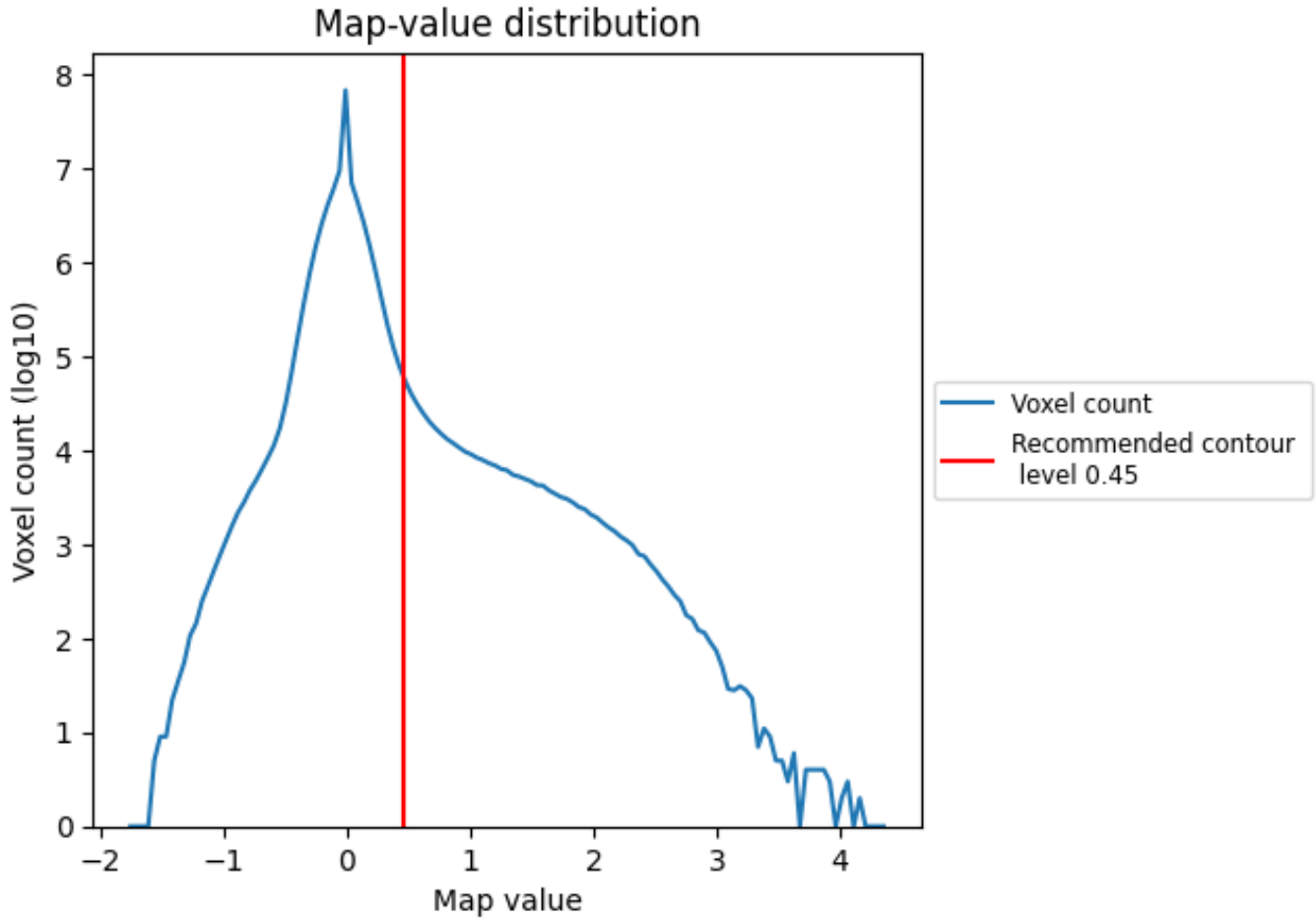
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

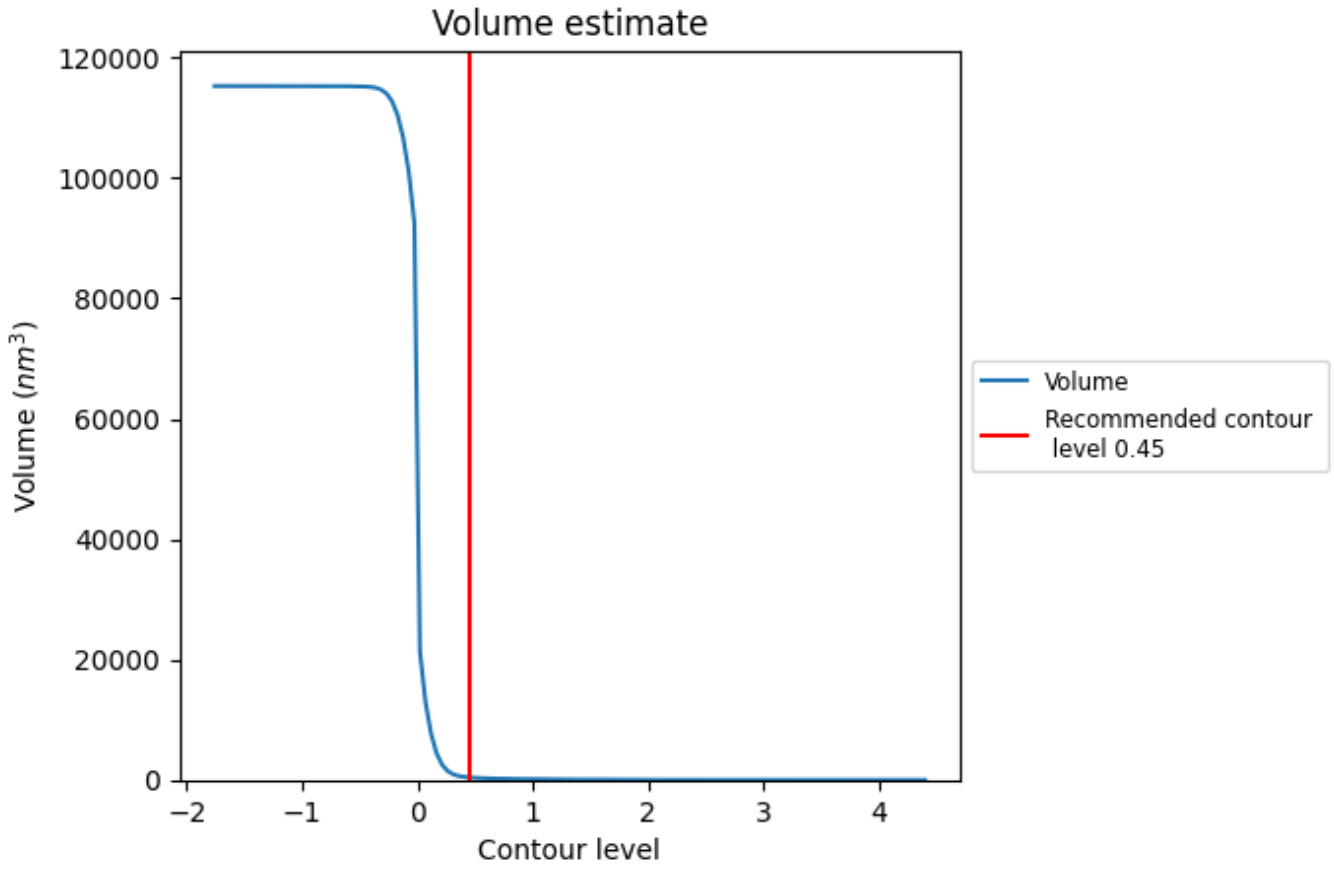
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

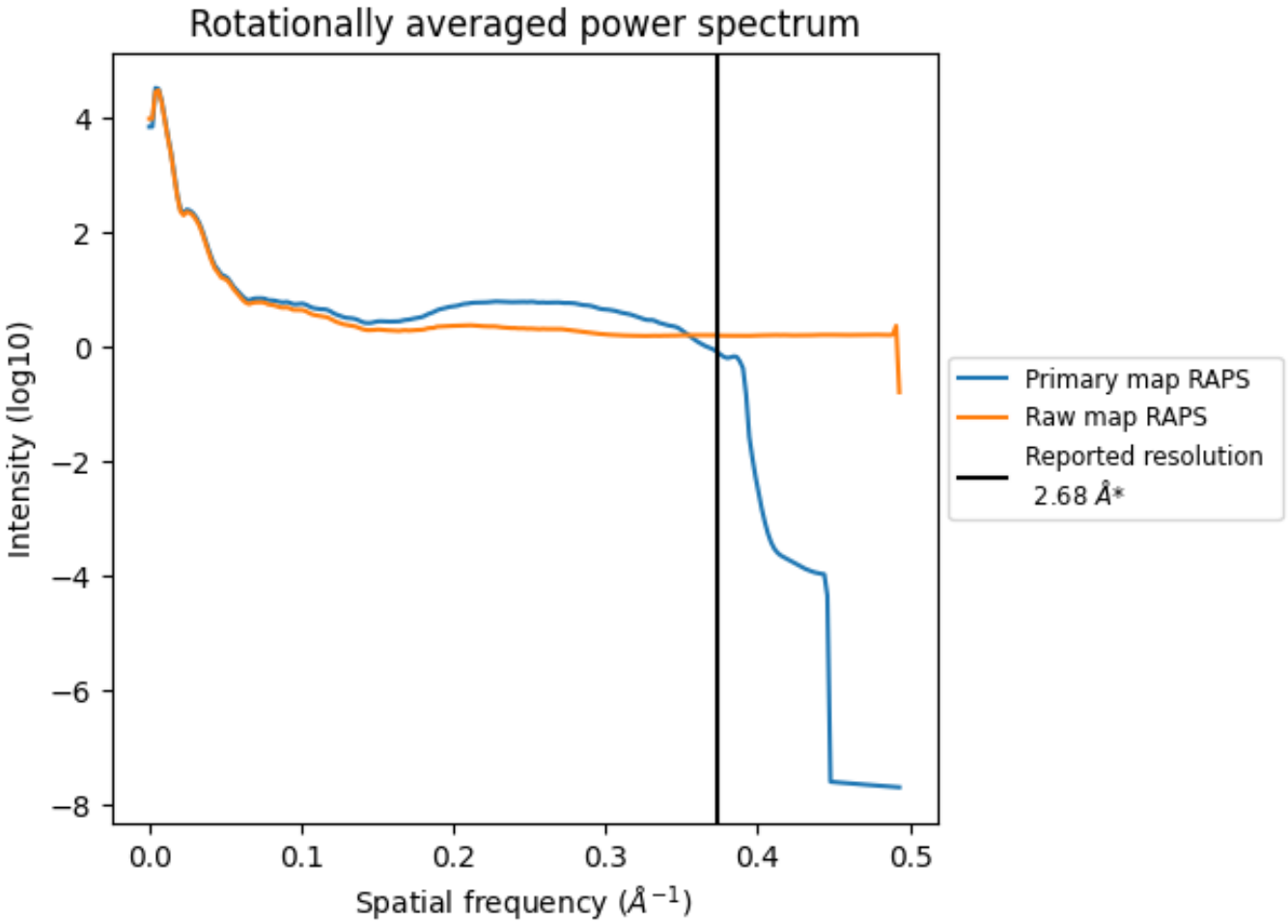
## 7.2 Volume estimate




The volume at the recommended contour level is 418 $nm^3$; this corresponds to an approximate mass of 378 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)

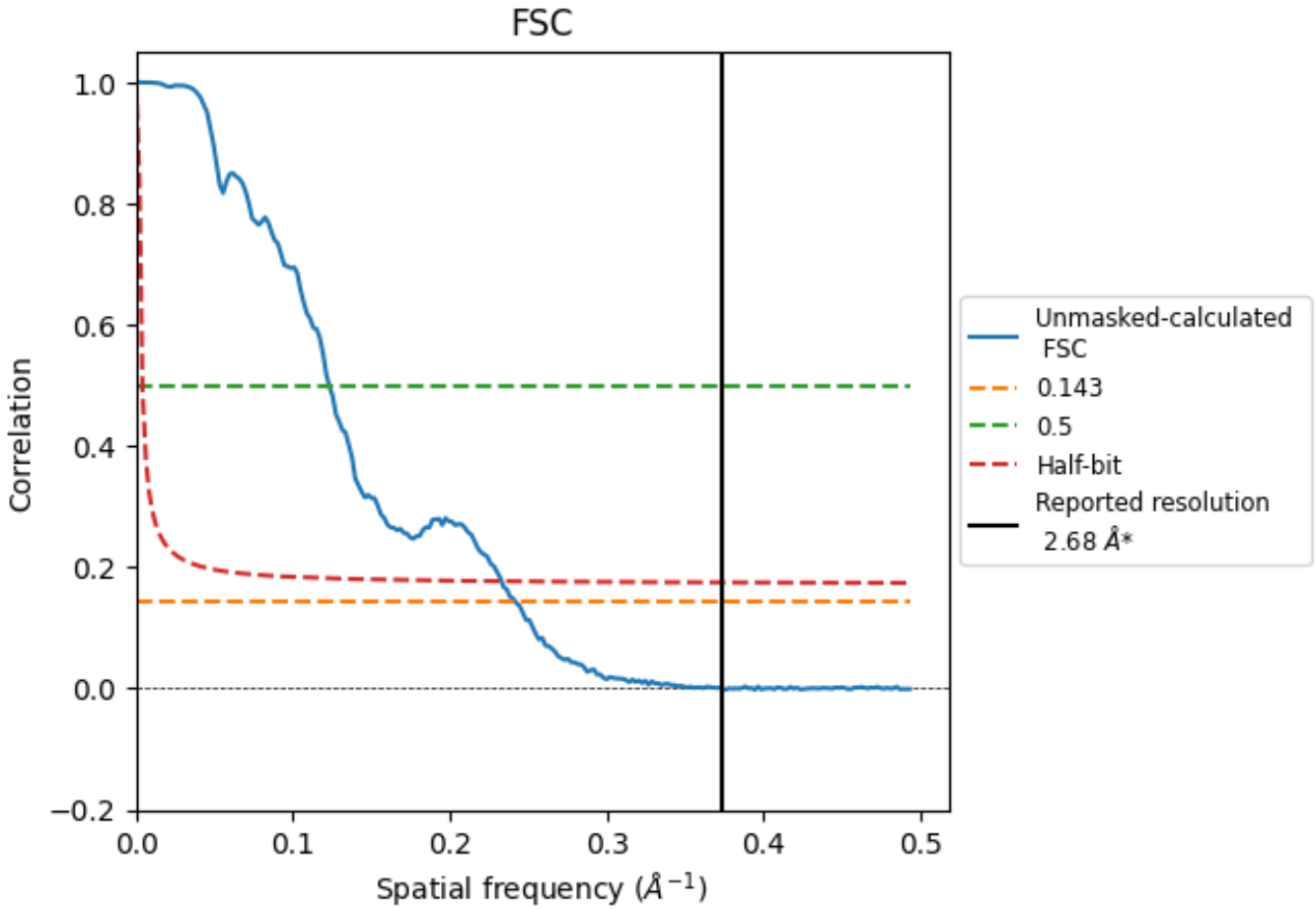



*Reported resolution corresponds to spatial frequency of 0.373 Å$^{-1}$

# 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 0.373 Å$^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.68 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 4.14 | 8.13 | 4.29 |

*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 4.14 differs from the reported value 2.68 by more than 10 %

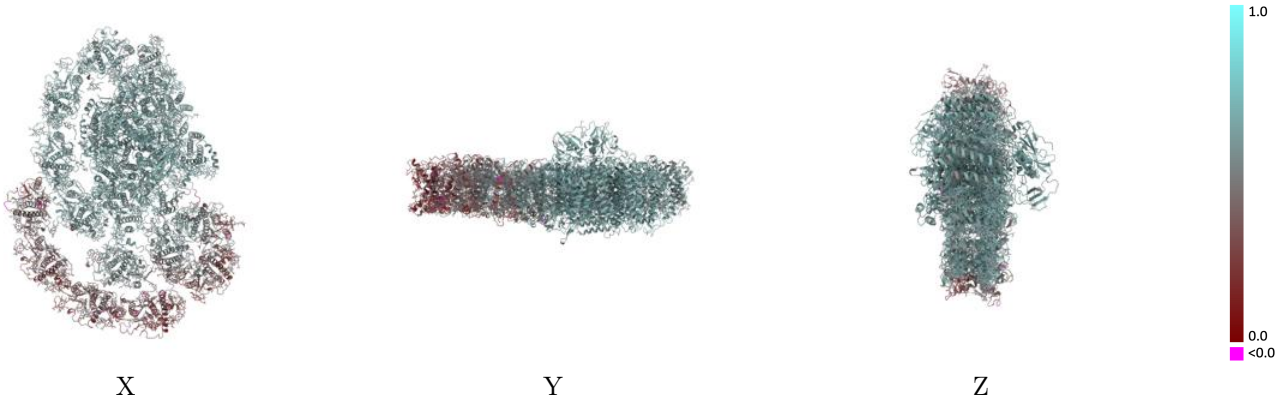
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33401 and PDB model 7XQP. Per-residue inclusion information can be found in section 3 on page 38.

## 9.1 Map-model overlay

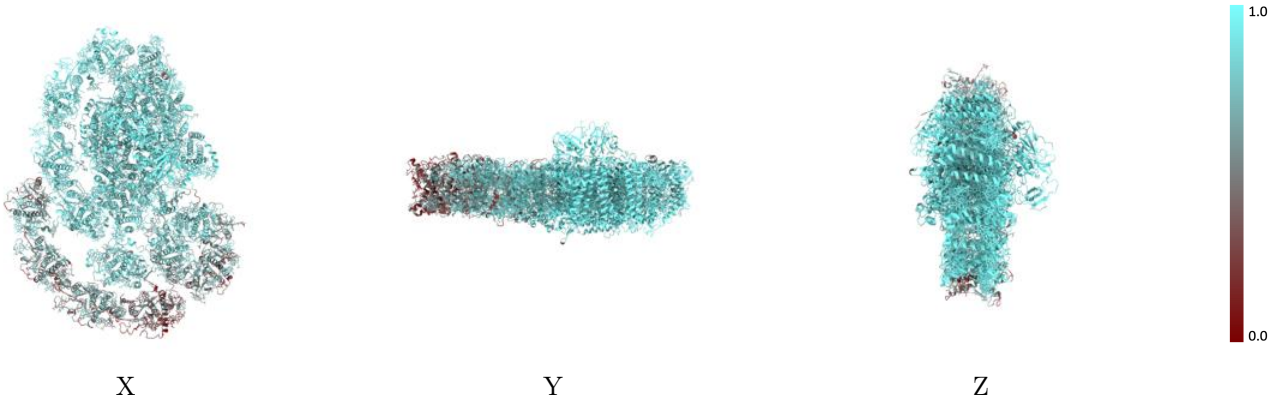
This section was not generated.

## 9.2 Q-score mapped to coordinate model



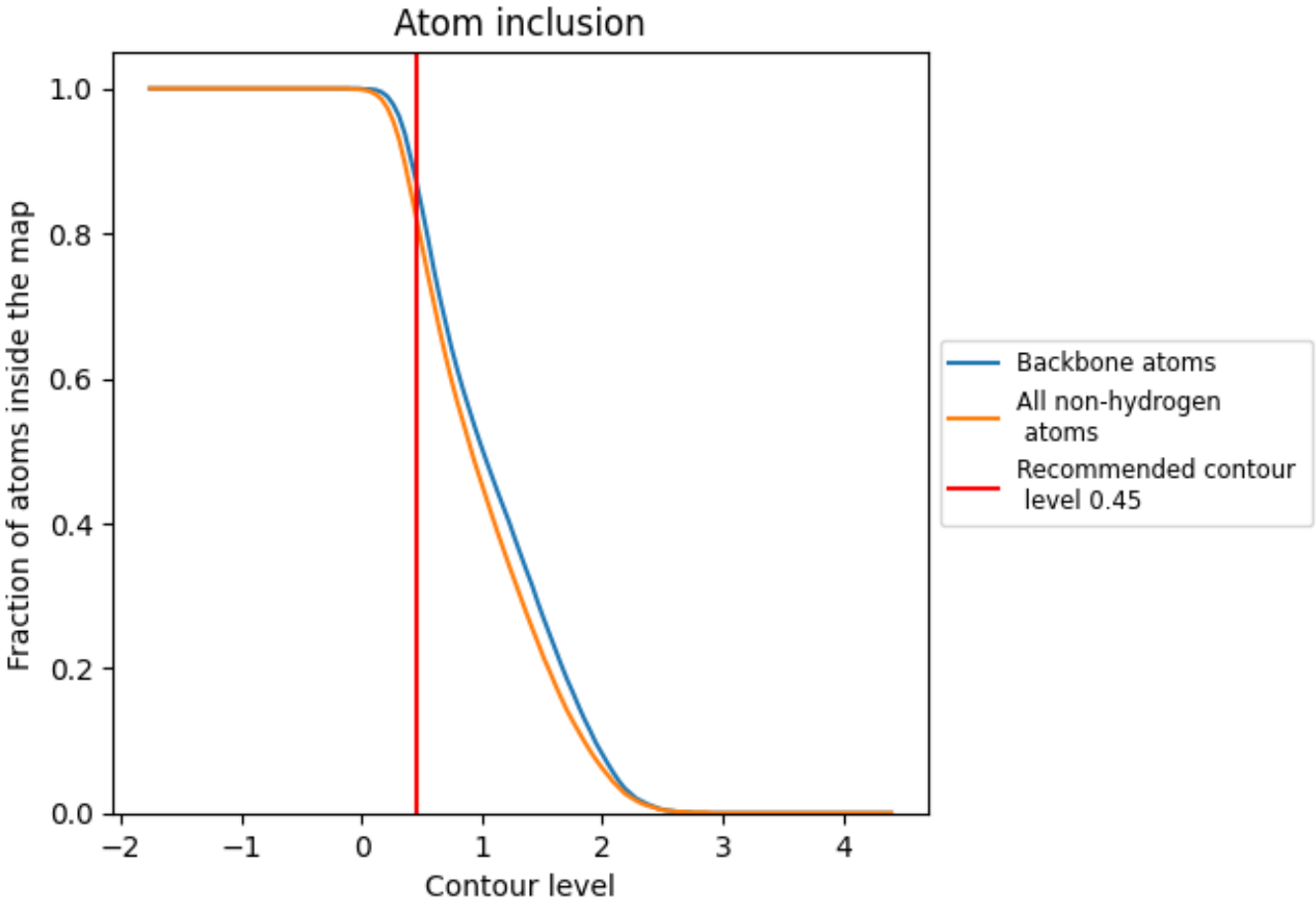

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.45).

## 9.4 Atom inclusion (i)




At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.45) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8260 | 0.5360 |
| 1 | 0.9160 | 0.5760 |
| 2 | 0.9220 | 0.5910 |
| 3 | 0.9350 | 0.6030 |
| 4 | 0.9200 | 0.5810 |
| 5 | 0.5830 | 0.3590 |
| 6 | 0.5300 | 0.3330 |
| 7 | 0.3390 | 0.2870 |
| 8 | 0.5420 | 0.3320 |
| 9 | 0.8250 | 0.5250 |
| A | 0.9620 | 0.6340 |
| B | 0.9610 | 0.6300 |
| C | 0.9730 | 0.6210 |
| D | 0.9470 | 0.6150 |
| E | 0.9410 | 0.6070 |
| F | 0.9220 | 0.6030 |
| G | 0.7980 | 0.5530 |
| H | 0.8880 | 0.5780 |
| I | 0.9470 | 0.6180 |
| J | 0.9350 | 0.6110 |
| K | 0.9400 | 0.6090 |
| L | 0.9430 | 0.6120 |
| M | 0.8980 | 0.5880 |
| O | 0.8320 | 0.5260 |
| a | 0.5470 | 0.3560 |
| b | 0.7680 | 0.4910 |
| c | 0.7450 | 0.4660 |

