# Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 05:05 am GMT

| | | |
|---|---|---|
| PDB ID | : | 6ZZX |
| EMDB ID | : | EMD-11588 |
| Title | : | Structure of low-light grown Chlorella ohadii Photosystem I |
| Authors | : | Caspy, I.; Nelson, N.; Nechushtai, R.; Neumann, E.; Shkolnisky, Y. |
| Deposited on | : | 2020-08-05 |
| Resolution | : | 2.70 Å(reported) |
| Based on initial model | : | 6IJO |

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:

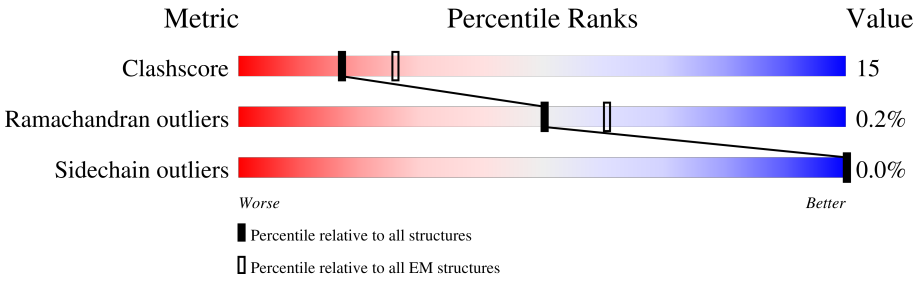
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 741 | 73% 27% |
| 2 | B | 731 | 78% 22% |
| 3 | C | 80 | 79% 21% |
| 4 | D | 143 | 80% 20% |
| 5 | E | 64 | 80% 20% |
| 6 | F | 165 | 84% 16% |
| 7 | G | 99 | 84% 16% |
| 8 | H | 94 | 5% 68% 32% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | J | 41 | 73% 27% |
| 10 | K | 86 | 87% 13% |
| 11 | L | 157 | 75% 25% |
| 12 | M | 31 | 68% 32% |
| 13 | I | 35 | 66% 34% |
| 14 | O | 87 | 34% 71% 26% |
| 15 | 1 | 192 | 74% 26% |
| 15 | a | 192 | 100% |
| 16 | 3 | 241 | 81% 19% |
| 17 | 4 | 207 | 81% 19% |
| 18 | 5 | 229 | 72% 28% |
| 19 | 6 | 231 | 77% 23% |
| 20 | 7 | 221 | 86% 14% |
| 21 | 8 | 219 | 78% 21% |
| 22 | 2 | 215 | 76% 24% |
| 23 | 9 | 183 | 80% 20% |

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 |
|---|---|---|---|---|---|---|---|
| 24 | CL0 | A | 1011 | X | - | - | - |
| 25 | CLA | 1 | 601 | X | - | - | - |
| 25 | CLA | 1 | 602 | X | - | - | - |
| 25 | CLA | 1 | 603 | X | - | - | - |
| 25 | CLA | 1 | 605 | X | - | - | - |
| 25 | CLA | 1 | 606 | X | - | - | - |
| 25 | CLA | 1 | 607 | X | - | - | - |
| 25 | CLA | 1 | 608 | X | - | - | - |
| 25 | CLA | 1 | 612 | X | - | - | - |
| 25 | CLA | 1 | 615 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 2 | 601 | X | - | - | - |
| 25 | CLA | 2 | 602 | X | - | - | - |
| 25 | CLA | 2 | 603 | X | - | - | - |
| 25 | CLA | 2 | 604 | X | - | - | - |
| 25 | CLA | 2 | 605 | X | - | - | - |
| 25 | CLA | 2 | 606 | X | - | - | - |
| 25 | CLA | 2 | 607 | X | - | - | - |
| 25 | CLA | 2 | 608 | X | - | - | - |
| 25 | CLA | 2 | 612 | X | - | - | - |
| 25 | CLA | 2 | 615 | X | - | - | - |
| 25 | CLA | 2 | 621 | X | - | - | - |
| 25 | CLA | 3 | 601 | X | - | - | - |
| 25 | CLA | 3 | 602 | X | - | - | - |
| 25 | CLA | 3 | 605 | X | - | - | - |
| 25 | CLA | 3 | 606 | X | - | - | - |
| 25 | CLA | 3 | 607 | X | - | - | - |
| 25 | CLA | 3 | 610 | X | - | - | - |
| 25 | CLA | 3 | 612 | X | - | - | - |
| 25 | CLA | 3 | 613 | X | - | - | - |
| 25 | CLA | 3 | 616 | X | - | - | - |
| 25 | CLA | 3 | 618 | X | - | - | - |
| 25 | CLA | 4 | 601 | X | - | - | - |
| 25 | CLA | 4 | 602 | X | - | - | - |
| 25 | CLA | 4 | 603 | X | - | - | - |
| 25 | CLA | 4 | 604 | X | - | - | - |
| 25 | CLA | 4 | 605 | X | - | - | - |
| 25 | CLA | 4 | 606 | X | - | - | - |
| 25 | CLA | 4 | 607 | X | - | - | - |
| 25 | CLA | 4 | 608 | X | - | - | - |
| 25 | CLA | 4 | 610 | X | - | - | - |
| 25 | CLA | 4 | 611 | X | - | - | - |
| 25 | CLA | 4 | 612 | X | - | - | - |
| 25 | CLA | 4 | 615 | X | - | - | - |
| 25 | CLA | 4 | 616 | X | - | - | - |
| 25 | CLA | 4 | 617 | X | - | - | - |
| 25 | CLA | 5 | 601 | X | - | - | - |
| 25 | CLA | 5 | 602 | X | - | - | - |
| 25 | CLA | 5 | 603 | X | - | - | - |
| 25 | CLA | 5 | 604 | X | - | - | - |
| 25 | CLA | 5 | 605 | X | - | - | - |
| 25 | CLA | 5 | 606 | X | - | - | - |
| 25 | CLA | 5 | 607 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 5 | 608 | X | - | - | - |
| 25 | CLA | 5 | 609 | X | - | - | - |
| 25 | CLA | 5 | 612 | X | - | - | - |
| 25 | CLA | 5 | 614 | X | - | - | - |
| 25 | CLA | 5 | 615 | X | - | - | - |
| 25 | CLA | 6 | 601 | X | - | - | - |
| 25 | CLA | 6 | 602 | X | - | - | - |
| 25 | CLA | 6 | 603 | X | - | - | - |
| 25 | CLA | 6 | 604 | X | - | - | - |
| 25 | CLA | 6 | 605 | X | - | - | - |
| 25 | CLA | 6 | 606 | X | - | - | - |
| 25 | CLA | 6 | 607 | X | - | - | - |
| 25 | CLA | 6 | 608 | X | - | - | - |
| 25 | CLA | 6 | 612 | X | - | - | - |
| 25 | CLA | 6 | 615 | X | - | - | - |
| 25 | CLA | 6 | 618 | X | - | - | - |
| 25 | CLA | 7 | 601 | X | - | - | - |
| 25 | CLA | 7 | 602 | X | - | - | - |
| 25 | CLA | 7 | 603 | X | - | - | - |
| 25 | CLA | 7 | 604 | X | - | - | - |
| 25 | CLA | 7 | 605 | X | - | - | - |
| 25 | CLA | 7 | 606 | X | - | - | - |
| 25 | CLA | 7 | 607 | X | - | - | - |
| 25 | CLA | 7 | 608 | X | - | - | - |
| 25 | CLA | 7 | 610 | X | - | - | - |
| 25 | CLA | 7 | 612 | X | - | - | - |
| 25 | CLA | 8 | 602 | X | - | - | - |
| 25 | CLA | 8 | 605 | X | - | - | - |
| 25 | CLA | 8 | 606 | X | - | - | - |
| 25 | CLA | 8 | 607 | X | - | - | - |
| 25 | CLA | 8 | 608 | X | - | - | - |
| 25 | CLA | 8 | 609 | X | - | - | - |
| 25 | CLA | 8 | 611 | X | - | - | - |
| 25 | CLA | 8 | 612 | X | - | - | - |
| 25 | CLA | 8 | 615 | X | - | - | - |
| 25 | CLA | 8 | 618 | X | - | - | - |
| 25 | CLA | 8 | 620 | X | - | - | - |
| 25 | CLA | 9 | 602 | X | - | - | - |
| 25 | CLA | 9 | 604 | X | - | - | - |
| 25 | CLA | 9 | 605 | X | - | - | - |
| 25 | CLA | 9 | 606 | X | - | - | - |
| 25 | CLA | 9 | 607 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 9 | 609 | X | - | - | - |
| 25 | CLA | 9 | 612 | X | - | - | - |
| 25 | CLA | A | 1012 | X | - | - | - |
| 25 | CLA | A | 1013 | X | - | - | - |
| 25 | CLA | A | 1101 | X | - | - | - |
| 25 | CLA | A | 1102 | X | - | - | - |
| 25 | CLA | A | 1103 | X | - | - | - |
| 25 | CLA | A | 1104 | X | - | - | - |
| 25 | CLA | A | 1105 | X | - | - | - |
| 25 | CLA | A | 1106 | X | - | - | - |
| 25 | CLA | A | 1107 | X | - | - | - |
| 25 | CLA | A | 1108 | X | - | - | - |
| 25 | CLA | A | 1109 | X | - | - | - |
| 25 | CLA | A | 1110 | X | - | - | - |
| 25 | CLA | A | 1111 | X | - | - | - |
| 25 | CLA | A | 1112 | X | - | - | - |
| 25 | CLA | A | 1113 | X | - | - | - |
| 25 | CLA | A | 1115 | X | - | - | - |
| 25 | CLA | A | 1116 | X | - | - | - |
| 25 | CLA | A | 1117 | X | - | - | - |
| 25 | CLA | A | 1118 | X | - | - | - |
| 25 | CLA | A | 1119 | X | - | - | - |
| 25 | CLA | A | 1120 | X | - | - | - |
| 25 | CLA | A | 1121 | X | - | - | - |
| 25 | CLA | A | 1122 | X | - | - | - |
| 25 | CLA | A | 1123 | X | - | - | - |
| 25 | CLA | A | 1124 | X | - | - | - |
| 25 | CLA | A | 1125 | X | - | - | - |
| 25 | CLA | A | 1126 | X | - | - | - |
| 25 | CLA | A | 1127 | X | - | - | - |
| 25 | CLA | A | 1128 | X | - | - | - |
| 25 | CLA | A | 1129 | X | - | - | - |
| 25 | CLA | A | 1130 | X | - | - | - |
| 25 | CLA | A | 1131 | X | - | - | - |
| 25 | CLA | A | 1132 | X | - | - | - |
| 25 | CLA | A | 1133 | X | - | - | - |
| 25 | CLA | A | 1134 | X | - | - | - |
| 25 | CLA | A | 1135 | X | - | - | - |
| 25 | CLA | A | 1136 | X | - | - | - |
| 25 | CLA | A | 1137 | X | - | - | - |
| 25 | CLA | A | 1138 | X | - | - | - |
| 25 | CLA | A | 1139 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | CLA | A | 1140 | X | - | - | - |
| 25 | CLA | A | 1141 | X | - | - | - |
| 25 | CLA | B | 1021 | X | - | - | - |
| 25 | CLA | B | 1022 | X | - | - | - |
| 25 | CLA | B | 1023 | X | - | - | - |
| 25 | CLA | B | 1201 | X | - | - | - |
| 25 | CLA | B | 1202 | X | - | - | - |
| 25 | CLA | B | 1203 | X | - | - | - |
| 25 | CLA | B | 1204 | X | - | - | - |
| 25 | CLA | B | 1205 | X | - | - | - |
| 25 | CLA | B | 1206 | X | - | - | - |
| 25 | CLA | B | 1207 | X | - | - | - |
| 25 | CLA | B | 1208 | X | - | - | - |
| 25 | CLA | B | 1209 | X | - | - | - |
| 25 | CLA | B | 1210 | X | - | - | - |
| 25 | CLA | B | 1211 | X | - | - | - |
| 25 | CLA | B | 1212 | X | - | - | - |
| 25 | CLA | B | 1213 | X | - | - | - |
| 25 | CLA | B | 1214 | X | - | - | - |
| 25 | CLA | B | 1215 | X | - | - | - |
| 25 | CLA | B | 1216 | X | - | - | - |
| 25 | CLA | B | 1217 | X | - | - | - |
| 25 | CLA | B | 1218 | X | - | - | - |
| 25 | CLA | B | 1219 | X | - | - | - |
| 25 | CLA | B | 1220 | X | - | - | - |
| 25 | CLA | B | 1221 | X | - | - | - |
| 25 | CLA | B | 1222 | X | - | - | - |
| 25 | CLA | B | 1223 | X | - | - | - |
| 25 | CLA | B | 1224 | X | - | - | - |
| 25 | CLA | B | 1225 | X | - | - | - |
| 25 | CLA | B | 1226 | X | - | - | - |
| 25 | CLA | B | 1227 | X | - | - | - |
| 25 | CLA | B | 1228 | X | - | - | - |
| 25 | CLA | B | 1229 | X | - | - | - |
| 25 | CLA | B | 1230 | X | - | - | - |
| 25 | CLA | B | 1231 | X | - | - | - |
| 25 | CLA | B | 1232 | X | - | - | - |
| 25 | CLA | B | 1235 | X | - | - | - |
| 25 | CLA | B | 1236 | X | - | - | - |
| 25 | CLA | B | 1237 | X | - | - | - |
| 25 | CLA | B | 1238 | X | - | - | - |
| 25 | CLA | B | 1239 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 25 | CLA | B | 1240 | X | - | - | - |
| 25 | CLA | F | 1301 | X | - | - | - |
| 25 | CLA | F | 1302 | X | - | - | - |
| 25 | CLA | G | 1601 | X | - | - | - |
| 25 | CLA | G | 1602 | X | - | - | - |
| 25 | CLA | G | 1603 | X | - | - | - |
| 25 | CLA | H | 1701 | X | - | - | - |
| 25 | CLA | H | 1702 | X | - | - | - |
| 25 | CLA | H | 1703 | X | - | - | - |
| 25 | CLA | J | 1901 | X | - | - | - |
| 25 | CLA | K | 1401 | X | - | - | - |
| 25 | CLA | K | 1402 | X | - | - | - |
| 25 | CLA | K | 1403 | X | - | - | - |
| 25 | CLA | K | 1404 | X | - | - | - |
| 25 | CLA | L | 1501 | X | - | - | - |
| 25 | CLA | L | 1502 | X | - | - | - |
| 25 | CLA | L | 1503 | X | - | - | - |
| 25 | CLA | L | 1504 | X | - | - | - |
| 25 | CLA | O | 1801 | X | - | - | - |
| 25 | CLA | O | 1802 | X | - | - | - |
| 25 | CLA | O | 1803 | X | - | - | - |
| 25 | CLA | a | 601 | X | - | - | - |
| 25 | CLA | a | 602 | X | - | - | - |
| 25 | CLA | a | 603 | X | - | - | - |
| 25 | CLA | a | 605 | X | - | - | - |
| 25 | CLA | a | 607 | X | - | - | - |
| 25 | CLA | a | 608 | X | - | - | - |
| 25 | CLA | a | 611 | X | - | - | - |
| 25 | CLA | a | 612 | X | - | - | - |
| 25 | CLA | a | 615 | X | - | - | - |
| 26 | CHL | 1 | 604 | X | - | - | - |
| 26 | CHL | 1 | 609 | X | - | - | - |
| 26 | CHL | 1 | 610 | X | - | - | - |
| 26 | CHL | 1 | 611 | X | - | - | - |
| 26 | CHL | 1 | 613 | X | - | - | - |
| 26 | CHL | 2 | 609 | X | - | - | - |
| 26 | CHL | 2 | 610 | X | - | - | - |
| 26 | CHL | 2 | 613 | X | - | - | - |
| 26 | CHL | 3 | 603 | X | - | - | - |
| 26 | CHL | 3 | 604 | X | - | - | - |
| 26 | CHL | 3 | 608 | X | - | - | - |
| 26 | CHL | 3 | 611 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 26 | CHL | 4 | 609 | X | - | - | - |
| 26 | CHL | 4 | 613 | X | - | - | - |
| 26 | CHL | 4 | 618 | X | - | - | - |
| 26 | CHL | 5 | 610 | X | - | - | - |
| 26 | CHL | 5 | 611 | X | - | - | - |
| 26 | CHL | 5 | 613 | X | - | - | - |
| 26 | CHL | 5 | 617 | X | - | - | - |
| 26 | CHL | 5 | 618 | X | - | - | - |
| 26 | CHL | 6 | 609 | X | - | - | - |
| 26 | CHL | 6 | 610 | X | - | - | - |
| 26 | CHL | 6 | 611 | X | - | - | - |
| 26 | CHL | 6 | 613 | X | - | - | - |
| 26 | CHL | 6 | 617 | X | - | - | - |
| 26 | CHL | 6 | 619 | X | - | - | - |
| 26 | CHL | 7 | 609 | X | - | - | - |
| 26 | CHL | 7 | 611 | X | - | - | - |
| 26 | CHL | 7 | 613 | X | - | - | - |
| 26 | CHL | 7 | 615 | X | - | - | - |
| 26 | CHL | 7 | 617 | X | - | - | - |
| 26 | CHL | 8 | 601 | X | - | - | - |
| 26 | CHL | 8 | 603 | X | - | - | - |
| 26 | CHL | 8 | 604 | X | - | - | - |
| 26 | CHL | 8 | 610 | X | - | - | - |
| 26 | CHL | 8 | 613 | X | - | - | - |
| 26 | CHL | 9 | 601 | X | - | - | - |
| 26 | CHL | 9 | 603 | X | - | - | - |
| 26 | CHL | 9 | 608 | X | - | - | - |
| 26 | CHL | 9 | 610 | X | - | - | - |
| 26 | CHL | 9 | 613 | X | - | - | - |
| 26 | CHL | A | 1114 | X | - | - | - |
| 26 | CHL | a | 604 | X | - | - | - |
| 26 | CHL | a | 606 | X | - | - | - |
| 26 | CHL | a | 609 | X | - | - | - |
| 26 | CHL | a | 610 | X | - | - | - |
| 26 | CHL | a | 613 | X | - | - | - |
| 39 | NEX | F | 4001 | X | - | - | - |
| 40 | RRX | 3 | 506 | X | - | - | - |
| 40 | RRX | J | 4002 | X | - | - | - |
| 43 | LUT | 2 | 507 | X | - | - | - |
| 43 | LUT | 4 | 501 | X | - | - | - |
| 43 | LUT | 7 | 501 | X | - | - | - |
| 46 | QTB | a | 504 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 50 | XAT | 2 | 501 | X | - | - | - |
| 50 | XAT | 7 | 502 | X | - | - | - |
| 50 | XAT | 9 | 504 | X | - | - | - |
| 50 | XAT | 9 | 507 | X | - | - | - |

# 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 56369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 741 | 5824 | 3815 | 988 | 1001 | 20 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 368 | ALA | SER | conflict | UNP W8SY74 |
| A | 437 | ILE | MET | conflict | UNP W8SY74 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 731 | 5796 | 3807 | 980 | 994 | 15 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | ? | - | THR | deletion | UNP W8SUA3 |
| B | 5 | LEU | - | insertion | UNP W8SUA3 |
| B | 241 | ALA | VAL | conflict | UNP W8SUA3 |
| B | 402 | ALA | GLU | conflict | UNP W8SUA3 |
| B | 403 | GLN | ALA | conflict | UNP W8SUA3 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 80 | 601 | 367 | 104 | 119 | 11 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1124 | 716 | 196 | 208 | 4 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 188 | ALA | VAL | conflict | UNP A0A2P6TKF8 |
| D | 320 | ILE | VAL | conflict | UNP A0A2P6TKF8 |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 5 | E | 64 | Total | C | N | O | 0 | 0 |
| | | | 509 | 323 | 91 | 95 | | |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 44 | GLN | THR | conflict | UNP A0A2P6U4S6 |
| E | 48 | LEU | MET | conflict | UNP A0A2P6U4S6 |
| E | 96 | VAL | GLU | conflict | UNP A0A2P6U4S6 |
| E | 97 | ALA | GLU | conflict | UNP A0A2P6U4S6 |
| E | 98 | ALA | VAL | conflict | UNP A0A2P6U4S6 |

- Molecule 6 is a protein called PSI-F.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1277 | 830 | 216 | 228 | 3 | | |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 346 | LEU | MET | conflict | UNP A0A2P6TPV8 |
| F | 348 | ASN | LYS | conflict | UNP A0A2P6TPV8 |
| F | 351 | ALA | GLU | conflict | UNP A0A2P6TPV8 |
| F | 352 | ASP | GLY | conflict | UNP A0A2P6TPV8 |
| F | 360 | LYS | GLN | conflict | UNP A0A2P6TPV8 |
| F | 364 | ALA | ASP | conflict | UNP A0A2P6TPV8 |
| F | 367 | GLU | ASN | conflict | UNP A0A2P6TPV8 |
| F | 430 | ALA | SER | conflict | UNP A0A2P6TPV8 |
| F | 431 | ALA | SER | conflict | UNP A0A2P6TPV8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 432 | THR | MET | conflict | UNP A0A2P6TPV8 |
| F | 433 | ALA | THR | conflict | UNP A0A2P6TPV8 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 727 | 466 | 127 | 130 | 4 | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 1229 | ALA | SER | conflict | UNP A0A2P6TZI8 |
| G | 1272 | LEU | MET | conflict | UNP A0A2P6TZI8 |
| G | 1285 | ILE | VAL | conflict | UNP A0A2P6TZI8 |
| G | 1313 | ILE | LEU | conflict | UNP A0A2P6TZI8 |
| G | 1317 | SER | HIS | conflict | UNP A0A2P6TZI8 |
| G | 1320 | GLY | GLN | conflict | UNP A0A2P6TZI8 |
| G | 1321 | LEU | VAL | conflict | UNP A0A2P6TZI8 |
| G | 1324 | ASN | VAL | conflict | UNP A0A2P6TZI8 |

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 729 | 457 | 132 | 139 | 1 | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| H | 92 | ILE | VAL | conflict | UNP A0A2P6TPU7 |
| H | 102 | GLY | LEU | conflict | UNP A0A2P6TPU7 |
| H | 105 | ALA | SER | conflict | UNP A0A2P6TPU7 |
| H | 106 | ALA | SER | conflict | UNP A0A2P6TPU7 |
| H | 109 | ARG | SER | conflict | UNP A0A2P6TPU7 |
| H | ? | - | ILE | deletion | UNP A0A2P6TPU7 |
| H | 113 | VAL | LYS | conflict | UNP A0A2P6TPU7 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 316 | 212 | 46 | 57 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | K | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 613 | 390 | 106 | 115 | 2 | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| K | 74 | ALA | GLU | conflict | UNP A0A2P6U0J1 |
| K | 103 | LEU | ILE | conflict | UNP A0A2P6U0J1 |
| K | 105 | CYS | VAL | conflict | UNP A0A2P6U0J1 |
| K | 107 | ILE | VAL | conflict | UNP A0A2P6U0J1 |
| K | 108 | VAL | ILE | conflict | UNP A0A2P6U0J1 |
| K | 112 | LYS | ARG | conflict | UNP A0A2P6U0J1 |
| K | 113 | SER | GLY | conflict | UNP A0A2P6U0J1 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1165 | 758 | 192 | 211 | 4 | | |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| L | 350 | TYR | PHE | conflict | UNP A0A2P6TC44 |
| L | 364 | ASP | ASN | conflict | UNP A0A2P6TC44 |
| L | ? | - | ALA | deletion | UNP A0A2P6TC44 |
| L | 421 | ASP | GLU | conflict | UNP A0A2P6TC44 |
| L | 443 | LEU | ILE | conflict | UNP A0A2P6TC44 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | M | 31 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 163 | 36 | 39 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | I | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 270 | 183 | 37 | 47 | 3 | | |

- Molecule 14 is a protein called Photosystem I subunit O.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | O | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 679 | 453 | 109 | 115 | 2 | | |

- 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 |
| | | | 1405 | 900 | 237 | 261 | 7 | | |
| 15 | a | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1405 | 900 | 237 | 261 | 7 | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1 | 166 | SER | LEU | conflict | UNP A0A2P6TT36 |
| 1 | 167 | LYS | GLU | conflict | UNP A0A2P6TT36 |
| 1 | 171 | THR | VAL | conflict | UNP A0A2P6TT36 |
| 1 | 194 | THR | ASN | conflict | UNP A0A2P6TT36 |
| 1 | 196 | ALA | GLN | conflict | UNP A0A2P6TT36 |
| 1 | 204 | SER | ALA | conflict | UNP A0A2P6TT36 |
| 1 | 210 | MET | LEU | conflict | UNP A0A2P6TT36 |
| a | 166 | SER | LEU | conflict | UNP A0A2P6TT36 |
| a | 167 | LYS | GLU | conflict | UNP A0A2P6TT36 |
| a | 171 | THR | VAL | conflict | UNP A0A2P6TT36 |
| a | 194 | THR | ASN | conflict | UNP A0A2P6TT36 |
| a | 196 | ALA | GLN | conflict | UNP A0A2P6TT36 |
| a | 204 | SER | ALA | conflict | UNP A0A2P6TT36 |
| a | 210 | MET | LEU | conflict | UNP A0A2P6TT36 |

- Molecule 16 is a protein called Glutathione reductase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | 3 | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1844 | 1194 | 302 | 337 | 11 | | |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 3 | 314 | CYS | GLY | conflict | UNP A0A2P6TMT4 |
| 3 | 329 | ILE | VAL | conflict | UNP A0A2P6TMT4 |
| 3 | 339 | THR | SER | conflict | UNP A0A2P6TMT4 |
| 3 | 359 | LYS | ASN | conflict | UNP A0A2P6TMT4 |
| 3 | 405 | GLY | ALA | conflict | UNP A0A2P6TMT4 |
| 3 | 429 | GLU | ALA | conflict | UNP A0A2P6TMT4 |
| 3 | 484 | THR | ARG | conflict | UNP A0A2P6TMT4 |
| 3 | 485 | ILE | ARG | conflict | UNP A0A2P6TMT4 |
| 3 | 486 | LEU | ARG | conflict | UNP A0A2P6TMT4 |
| 3 | 487 | LYS | ALA | conflict | UNP A0A2P6TMT4 |

- Molecule 17 is a protein called Lhca4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 4 | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1631 | 1056 | 277 | 294 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | 5 | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1786 | 1146 | 310 | 317 | 13 | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 5 | 32 | LYS | ASP | conflict | UNP A0A2P6U4K1 |
| 5 | 38 | VAL | ALA | conflict | UNP A0A2P6U4K1 |
| 5 | 40 | ALA | SER | conflict | UNP A0A2P6U4K1 |
| 5 | 42 | GLY | ALA | conflict | UNP A0A2P6U4K1 |
| 5 | 113 | SER | GLY | conflict | UNP A0A2P6U4K1 |
| 5 | 127 | ILE | LEU | conflict | UNP A0A2P6U4K1 |
| 5 | 195 | VAL | ILE | conflict | UNP A0A2P6U4K1 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | 6 | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1787 | 1168 | 295 | 314 | 10 | | |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 6 | 83 | CYS | ALA | conflict | UNP A0A2P6TPR7 |
| 6 | 94 | LEU | MET | conflict | UNP A0A2P6TPR7 |
| 6 | 196 | ILE | VAL | conflict | UNP A0A2P6TPR7 |
| 6 | 201 | ALA | GLY | conflict | UNP A0A2P6TPR7 |
| 6 | 250 | GLN | ASN | conflict | UNP A0A2P6TPR7 |

- Molecule 20 is a protein called Lhca7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | 7 | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1698 | 1090 | 294 | 308 | 6 | | |

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 8 | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1669 | 1073 | 285 | 305 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 8 | 103 | GLU | ASP | conflict | UNP A0A2P6TZ50 |

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | 2 | 215 | Total | C | N | O | S | 0 | 0 |
| | | | 1666 | 1074 | 277 | 309 | 6 | | |

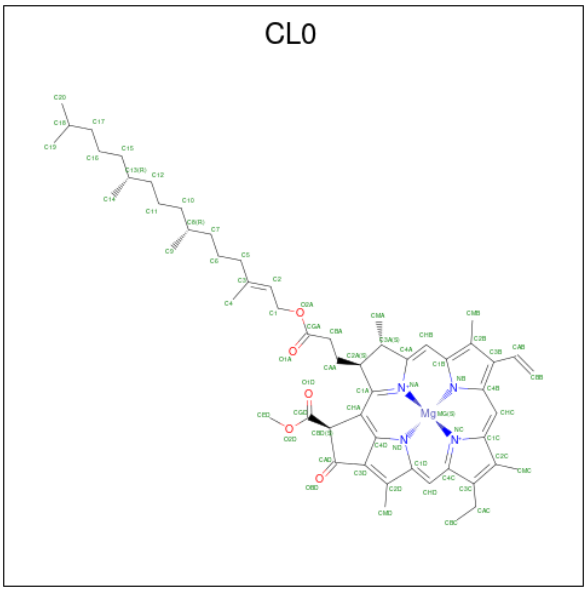
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 2 | 64 | ASP | GLU | conflict | UNP A0A2P6TMX4 |
| 2 | 97 | PRO | ASN | conflict | UNP A0A2P6TMX4 |

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

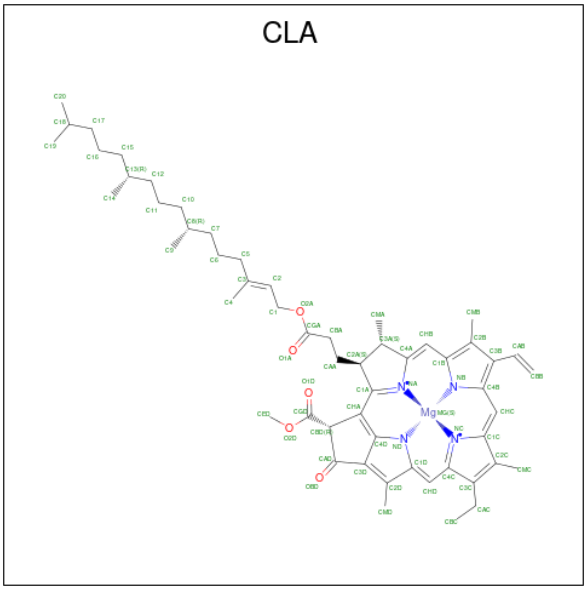
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | 9 | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1406 | 909 | 237 | 254 | 6 | | |

- Molecule 24 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 24 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 2532 | 2112 | 42 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 2583 | 2164 | 41 | 168 | 210 | |
| 25 | F | 1 | Total | C | Mg | N | O | 0 |
| | | | 105 | 85 | 2 | 8 | 10 | |
| 25 | F | 1 | Total | C | Mg | N | O | 0 |
| | | | 105 | 85 | 2 | 8 | 10 | |
| 25 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 155 | 125 | 3 | 12 | 15 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 155 | 125 | 3 | 12 | 15 | |
| 25 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 155 | 125 | 3 | 12 | 15 | |
| 25 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 156 | 126 | 3 | 12 | 15 | |
| 25 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 156 | 126 | 3 | 12 | 15 | |
| 25 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 156 | 126 | 3 | 12 | 15 | |
| 25 | J | 1 | Total | C | Mg | N | O | 0 |
| | | | 42 | 34 | 1 | 4 | 3 | |
| 25 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 200 | 160 | 4 | 16 | 20 | |
| 25 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 200 | 160 | 4 | 16 | 20 | |
| 25 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 200 | 160 | 4 | 16 | 20 | |
| 25 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 200 | 160 | 4 | 16 | 20 | |
| 25 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 205 | 165 | 4 | 16 | 20 | |
| 25 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 205 | 165 | 4 | 16 | 20 | |
| 25 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 205 | 165 | 4 | 16 | 20 | |
| 25 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 205 | 165 | 4 | 16 | 20 | |
| 25 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 134 | 108 | 3 | 12 | 11 | |
| 25 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 134 | 108 | 3 | 12 | 11 | |
| 25 | O | 1 | Total | C | Mg | N | O | 0 |
| | | | 134 | 108 | 3 | 12 | 11 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 528 | 438 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 496 | 406 | 9 | 36 | 45 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 576 | 476 | 10 | 40 | 50 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 768 | 628 | 14 | 56 | 70 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 642 | 522 | 12 | 48 | 60 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 624 | 514 | 11 | 44 | 55 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 566 | 466 | 10 | 40 | 50 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 573 | 463 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |

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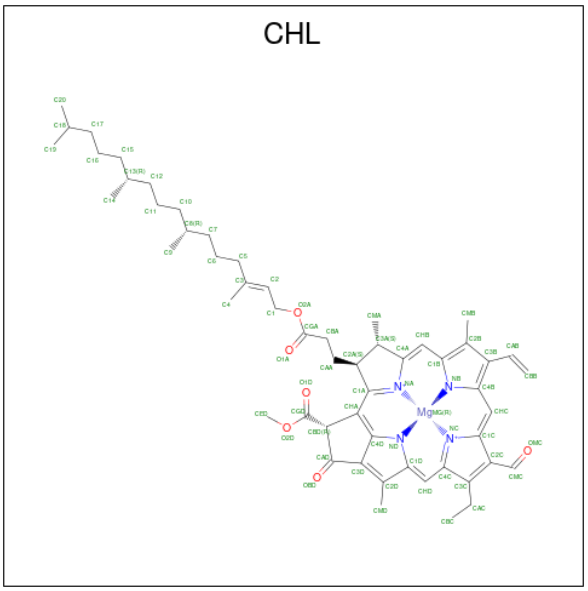
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 615 | 505 | 11 | 44 | 55 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |
| 25 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 379 | 309 | 7 | 28 | 35 | |

- Molecule 26 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 26 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 26 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 284 | 229 | 5 | 20 | 30 | |
| 26 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 284 | 229 | 5 | 20 | 30 | |
| 26 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 284 | 229 | 5 | 20 | 30 | |
| 26 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 284 | 229 | 5 | 20 | 30 | |
| 26 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 284 | 229 | 5 | 20 | 30 | |
| 26 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 264 | 209 | 5 | 20 | 30 | |
| 26 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 264 | 209 | 5 | 20 | 30 | |
| 26 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 264 | 209 | 5 | 20 | 30 | |
| 26 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 264 | 209 | 5 | 20 | 30 | |
| 26 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 264 | 209 | 5 | 20 | 30 | |
| 26 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 236 | 194 | 4 | 16 | 22 | |
| 26 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 236 | 194 | 4 | 16 | 22 | |
| 26 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 236 | 194 | 4 | 16 | 22 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 26 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 236 | 194 | 4 | 16 | 22 | |
| 26 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 174 | 141 | 3 | 12 | 18 | |
| 26 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 174 | 141 | 3 | 12 | 18 | |
| 26 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 174 | 141 | 3 | 12 | 18 | |
| 26 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 271 | 216 | 5 | 20 | 30 | |
| 26 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 271 | 216 | 5 | 20 | 30 | |
| 26 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 271 | 216 | 5 | 20 | 30 | |
| 26 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 271 | 216 | 5 | 20 | 30 | |
| 26 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 271 | 216 | 5 | 20 | 30 | |
| 26 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 333 | 269 | 6 | 24 | 34 | |
| 26 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 333 | 269 | 6 | 24 | 34 | |
| 26 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 333 | 269 | 6 | 24 | 34 | |
| 26 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 333 | 269 | 6 | 24 | 34 | |
| 26 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 333 | 269 | 6 | 24 | 34 | |
| 26 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 333 | 269 | 6 | 24 | 34 | |
| 26 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |

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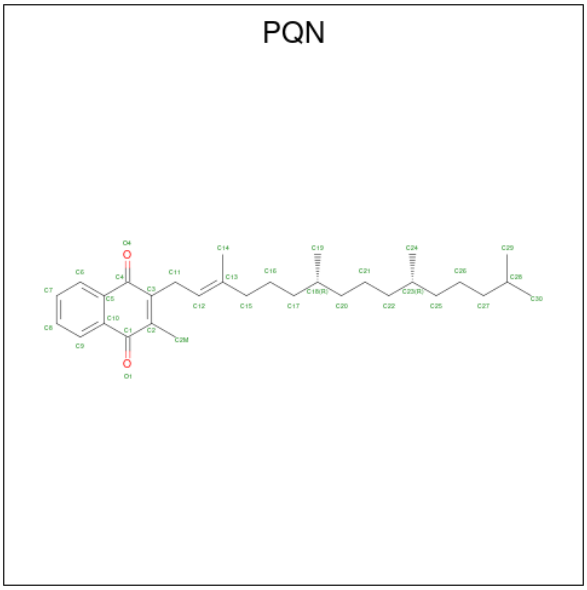
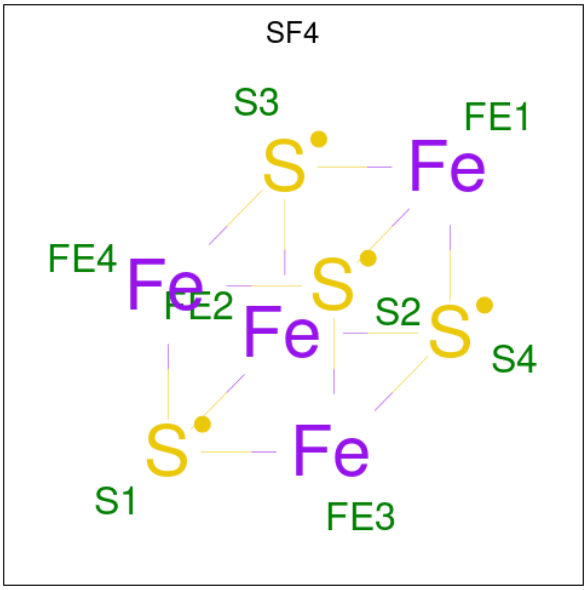
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 26 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 296 | 241 | 5 | 20 | 30 | |
| 26 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 165 | 132 | 3 | 12 | 18 | |
| 26 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 165 | 132 | 3 | 12 | 18 | |
| 26 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 165 | 132 | 3 | 12 | 18 | |
| 26 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 273 | 220 | 5 | 20 | 28 | |
| 26 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 273 | 220 | 5 | 20 | 28 | |
| 26 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 273 | 220 | 5 | 20 | 28 | |
| 26 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 273 | 220 | 5 | 20 | 28 | |
| 26 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 273 | 220 | 5 | 20 | 28 | |

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



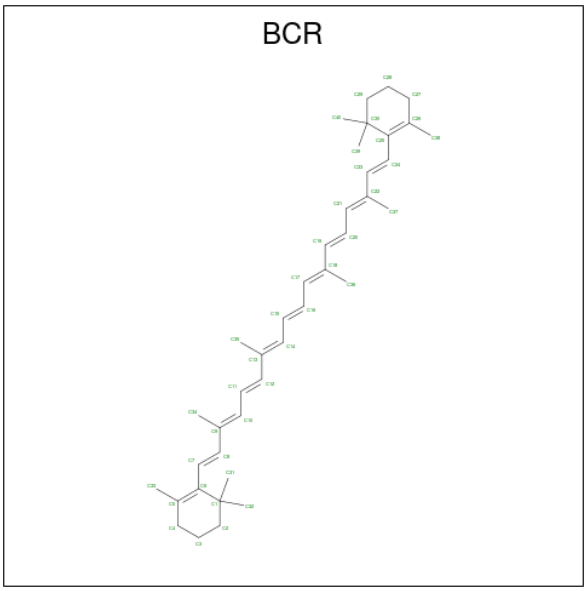
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 27 | A | 1 | Total C O<br>33 31 2 | 0 |
| 27 | B | 1 | Total C O<br>33 31 2 | 0 |

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 28 | A | 1 | Total Fe S<br>8 4 4 | 0 |
| 28 | C | 1 | Total Fe S<br>16 8 8 | 0 |
| 28 | C | 1 | Total Fe S<br>16 8 8 | 0 |

- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 29 | A | 1 | Total C<br>200 200 | 0 |
| 29 | A | 1 | Total C<br>200 200 | 0 |
| 29 | A | 1 | Total C<br>200 200 | 0 |
| 29 | A | 1 | Total C<br>200 200 | 0 |
| 29 | A | 1 | Total C<br>200 200 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | B | 1 | Total C<br>280 280 | 0 |
| 29 | G | 1 | Total C<br>40 40 | 0 |
| 29 | H | 1 | Total C<br>40 40 | 0 |

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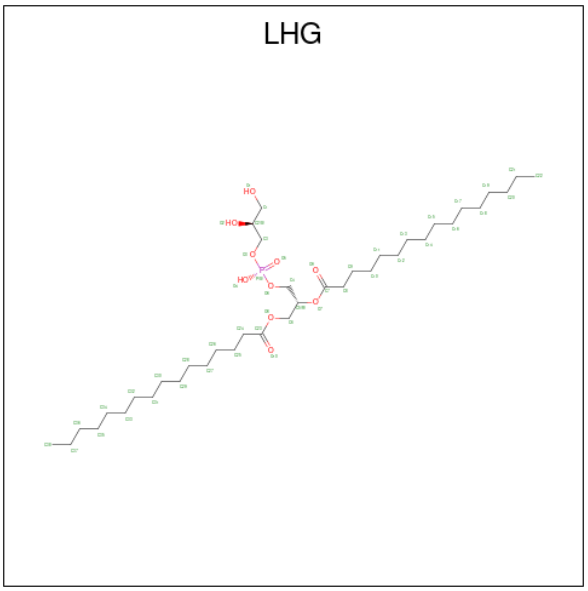
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 29 | J | 1 | Total C<br>40 40 | 0 |
| 29 | K | 1 | Total C<br>80 80 | 0 |
| 29 | K | 1 | Total C<br>80 80 | 0 |
| 29 | L | 1 | Total C<br>120 120 | 0 |
| 29 | L | 1 | Total C<br>120 120 | 0 |
| 29 | L | 1 | Total C<br>120 120 | 0 |
| 29 | I | 1 | Total C<br>40 40 | 0 |
| 29 | O | 1 | Total C<br>40 40 | 0 |
| 29 | 3 | 1 | Total C<br>120 120 | 0 |
| 29 | 3 | 1 | Total C<br>120 120 | 0 |
| 29 | 3 | 1 | Total C<br>120 120 | 0 |
| 29 | 4 | 1 | Total C<br>40 40 | 0 |
| 29 | 5 | 1 | Total C<br>80 80 | 0 |
| 29 | 5 | 1 | Total C<br>80 80 | 0 |
| 29 | 6 | 1 | Total C<br>80 80 | 0 |
| 29 | 6 | 1 | Total C<br>80 80 | 0 |
| 29 | 7 | 1 | Total C<br>40 40 | 0 |
| 29 | 8 | 1 | Total C<br>40 40 | 0 |

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 30 | A | 1 | Total<br>144 | C<br>111 | O<br>30 | P<br>3 | 0 |
| 30 | A | 1 | Total<br>144 | C<br>111 | O<br>30 | P<br>3 | 0 |
| 30 | A | 1 | Total<br>144 | C<br>111 | O<br>30 | P<br>3 | 0 |
| 30 | B | 1 | Total<br>98 | C<br>76 | O<br>20 | P<br>2 | 0 |
| 30 | B | 1 | Total<br>98 | C<br>76 | O<br>20 | P<br>2 | 0 |
| 30 | F | 1 | Total<br>79 | C<br>57 | O<br>20 | P<br>2 | 0 |
| 30 | F | 1 | Total<br>79 | C<br>57 | O<br>20 | P<br>2 | 0 |
| 30 | 1 | 1 | Total<br>84 | C<br>62 | O<br>20 | P<br>2 | 0 |
| 30 | 1 | 1 | Total<br>84 | C<br>62 | O<br>20 | P<br>2 | 0 |
| 30 | a | 1 | Total<br>35 | C<br>24 | O<br>10 | P<br>1 | 0 |
| 30 | 3 | 1 | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0 |
| 30 | 4 | 1 | Total<br>81 | C<br>59 | O<br>20 | P<br>2 | 0 |
| 30 | 4 | 1 | Total<br>81 | C<br>59 | O<br>20 | P<br>2 | 0 |
| 30 | 5 | 1 | Total<br>49 | C<br>38 | O<br>10 | P<br>1 | 0 |

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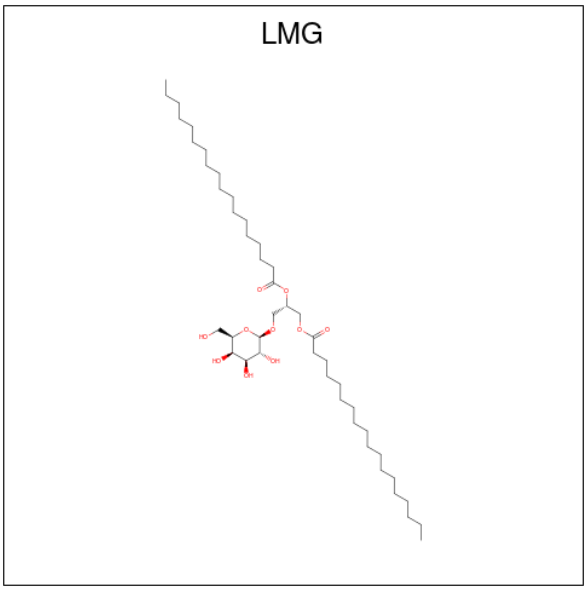
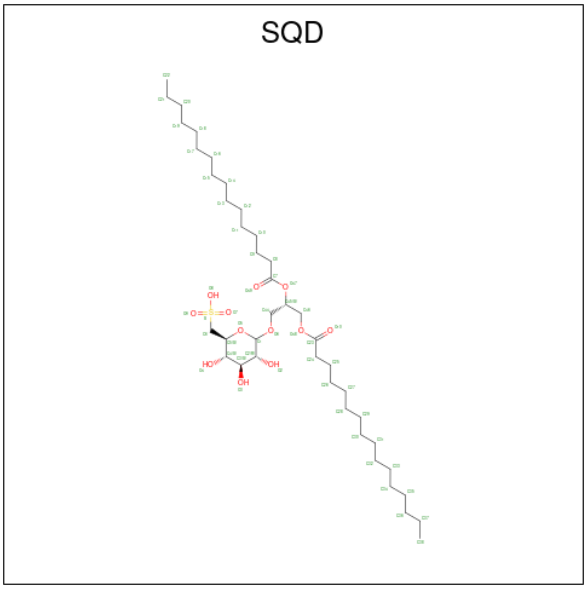
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 30 | 6 | 1 | Total | C | O | P | 0 |
| | | | 86 | 64 | 20 | 2 | |
| 30 | 6 | 1 | Total | C | O | P | 0 |
| | | | 86 | 64 | 20 | 2 | |
| 30 | 7 | 1 | Total | C | O | P | 0 |
| | | | 108 | 75 | 30 | 3 | |
| 30 | 7 | 1 | Total | C | O | P | 0 |
| | | | 108 | 75 | 30 | 3 | |
| 30 | 7 | 1 | Total | C | O | P | 0 |
| | | | 108 | 75 | 30 | 3 | |
| 30 | 8 | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 30 | 2 | 1 | Total | C | O | P | 0 |
| | | | 98 | 76 | 20 | 2 | |
| 30 | 2 | 1 | Total | C | O | P | 0 |
| | | | 98 | 76 | 20 | 2 | |
| 30 | 9 | 1 | Total | C | O | P | 0 |
| | | | 82 | 60 | 20 | 2 | |
| 30 | 9 | 1 | Total | C | O | P | 0 |
| | | | 82 | 60 | 20 | 2 | |

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



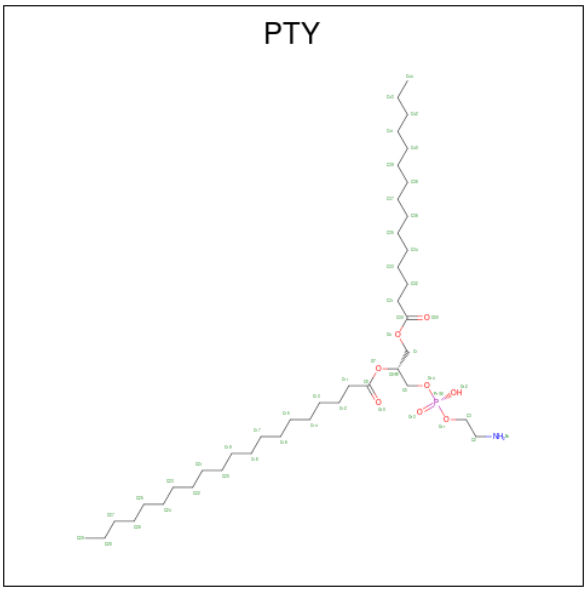

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 31 | A | 1 | Total | C | O | 0 |
| | | | 42 | 32 | 10 | |

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



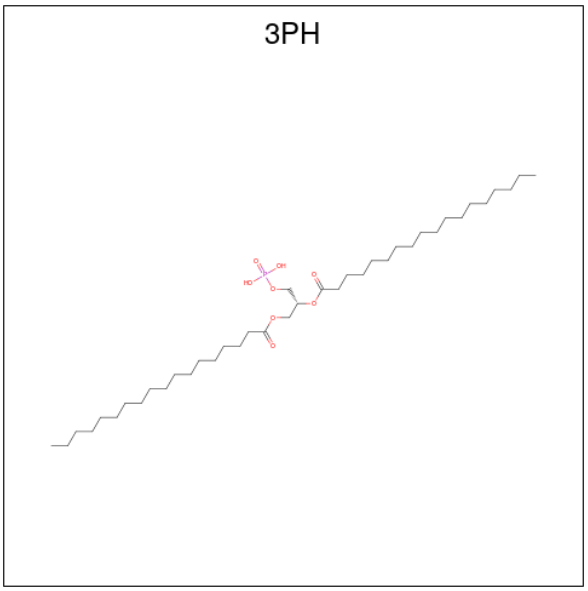

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 32 | A | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | G | 1 | Total | C | O | S | 0 |
| | | | 46 | 33 | 12 | 1 | |
| 32 | H | 1 | Total | C | O | S | 0 |
| | | | 45 | 32 | 12 | 1 | |
| 32 | I | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |
| 32 | 7 | 1 | Total | C | O | S | 0 |
| | | | 39 | 26 | 12 | 1 | |

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



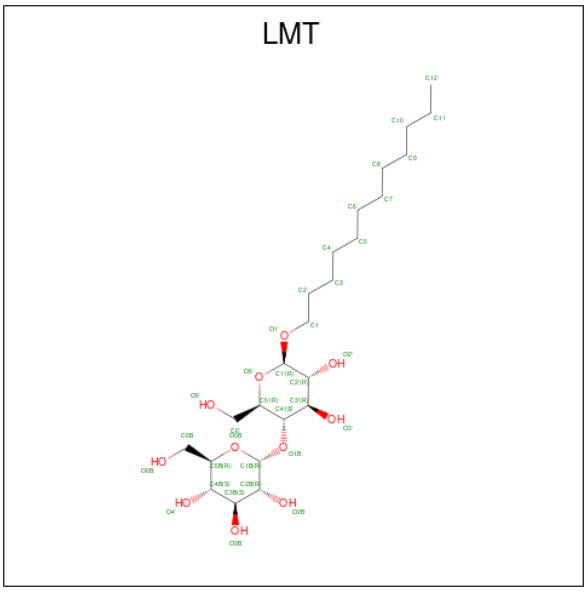

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 33 | A | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 33 | B | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 33 | G | 1 | Total | C | N | O | P | 0 |
| | | | 56 | 36 | 2 | 16 | 2 | |
| 33 | G | 1 | Total | C | N | O | P | 0 |
| | | | 56 | 36 | 2 | 16 | 2 | |
| 33 | J | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 33 | a | 1 | Total | C | N | O | P | 0 |
| | | | 76 | 56 | 2 | 16 | 2 | |
| 33 | a | 1 | Total | C | N | O | P | 0 |
| | | | 76 | 56 | 2 | 16 | 2 | |
| 33 | 3 | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 33 | 5 | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 33 | 7 | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 33 | 9 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 34 | A | 1 | Total | C | O | P | 0 |
| | | | 33 | 24 | 8 | 1 | |

- Molecule 35 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 35 | A | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 35 | B | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |

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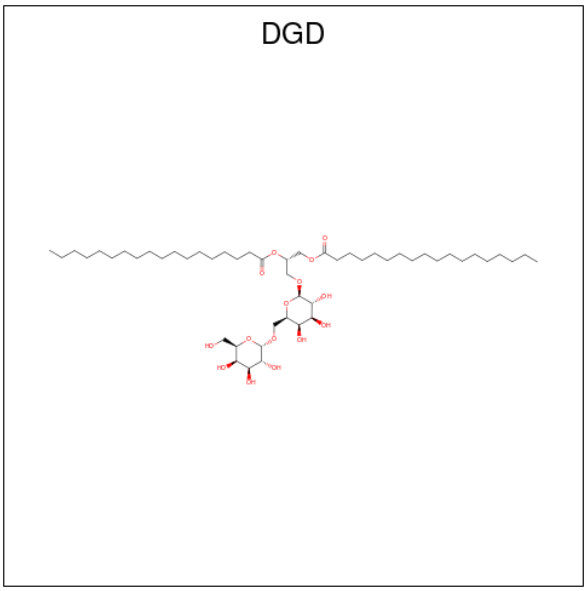
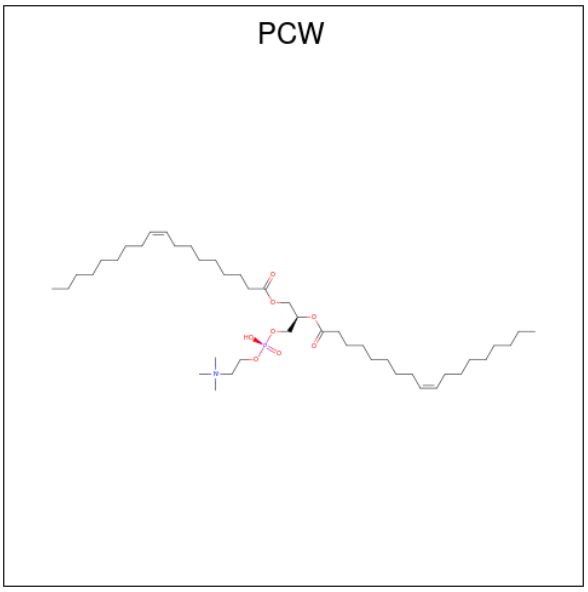
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 35 | 1 | 1 | Total C O<br>35 24 11 | 0 |
| 35 | 2 | 1 | Total C O<br>35 24 11 | 0 |

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



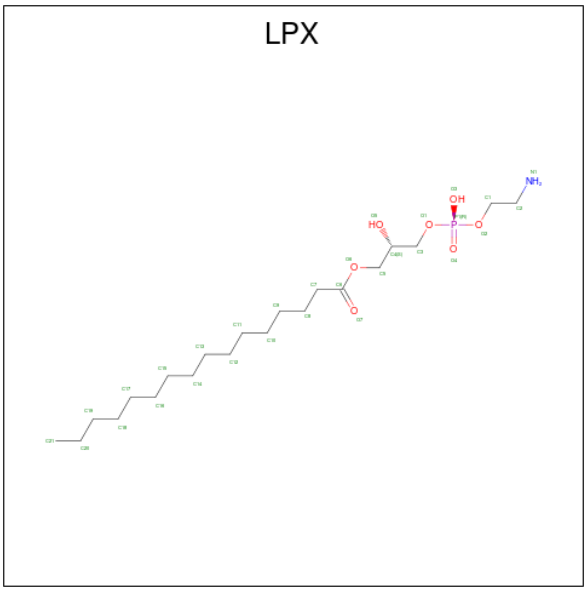

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 36 | B | 1 | Total C O<br>66 51 15 | 0 |
| 36 | 7 | 1 | Total C O<br>50 35 15 | 0 |
| 36 | 8 | 1 | Total C O<br>105 75 30 | 0 |
| 36 | 8 | 1 | Total C O<br>105 75 30 | 0 |

- Molecule 37 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



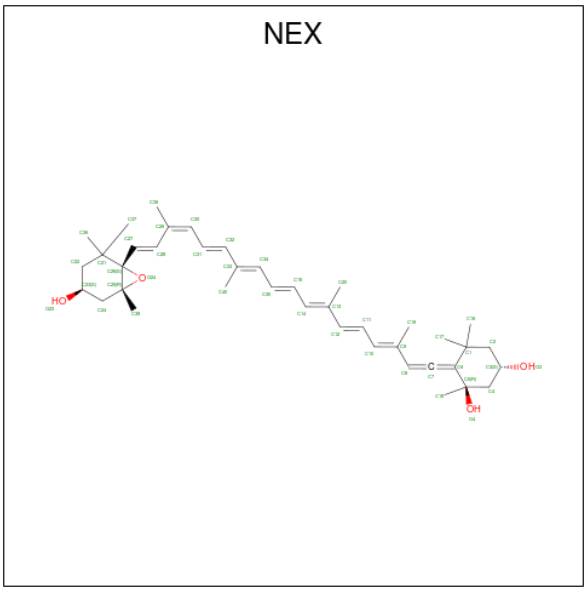

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | B | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 37 | K | 1 | Total | C | N | O | P | 0 |
| | | | 77 | 57 | 2 | 16 | 2 | |
| 37 | K | 1 | Total | C | N | O | P | 0 |
| | | | 77 | 57 | 2 | 16 | 2 | |
| 37 | 6 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |

- Molecule 38 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: $C_{21}H_{44}NO_7P$).



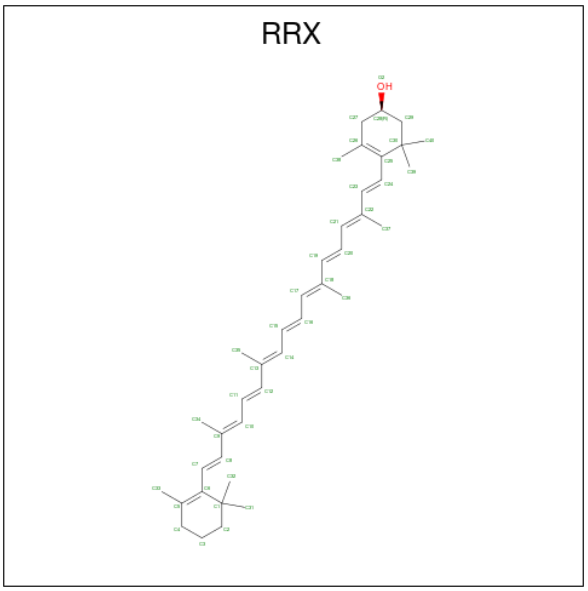
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 38 | F | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 21 | 1 | 7 | 1 | |

- Molecule 39 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 (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



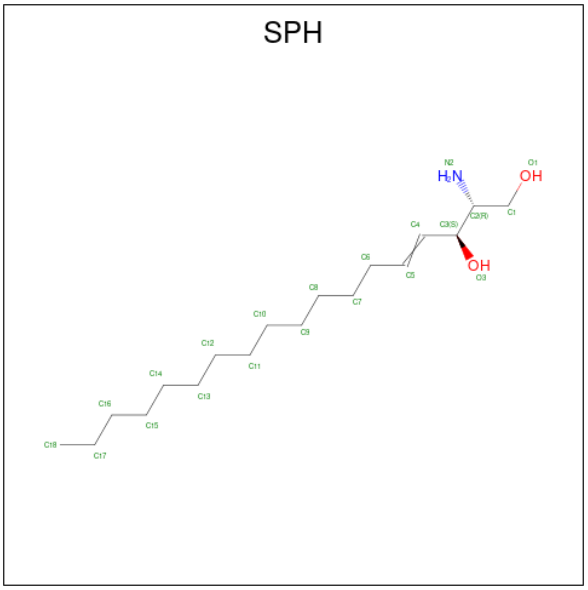

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 39 | F | 1 | Total | C | O | 0 |
| | | | 44 | 40 | 4 | |

- Molecule 40 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 40 | J | 1 | Total C O<br>41 40 1 | 0 |
| 40 | 3 | 1 | Total C O<br>41 40 1 | 0 |

- Molecule 41 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 41 | J | 1 | Total C N O<br>21 18 1 2 | 0 |
| 41 | 4 | 1 | Total C N O<br>21 18 1 2 | 0 |

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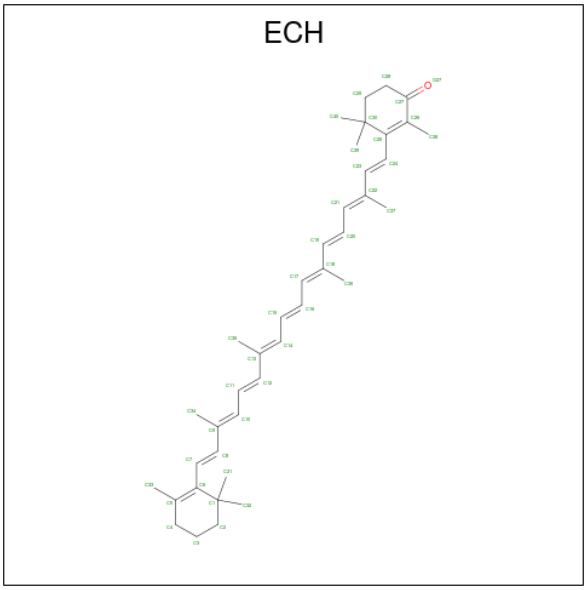
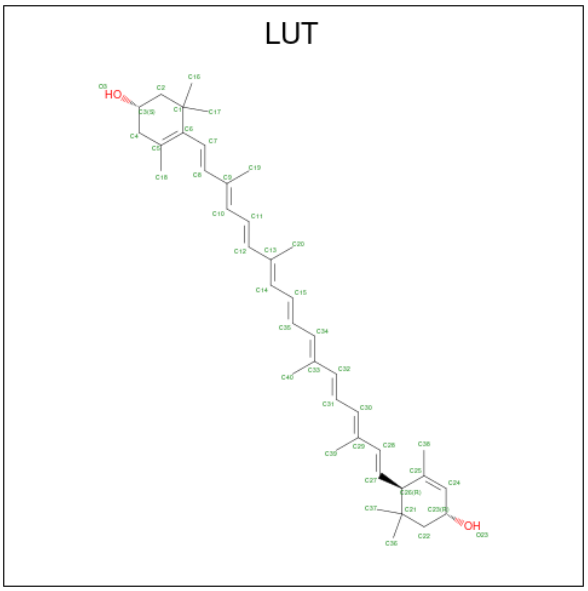
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 41 | 6 | 1 | Total | C | N | O | 0 |
| | | | 21 | 18 | 1 | 2 | |
| 41 | 9 | 1 | Total | C | N | O | 0 |
| | | | 21 | 18 | 1 | 2 | |

- Molecule 42 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 42 | M | 1 | Total | C | O | 0 |
| | | | 41 | 40 | 1 | |

- Molecule 43 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 43 | 1 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | 1 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | a | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 43 | a | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 43 | a | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 43 | 3 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | 3 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | 4 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | 4 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | 5 | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 43 | 5 | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 43 | 5 | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 43 | 6 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 43 | 6 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |

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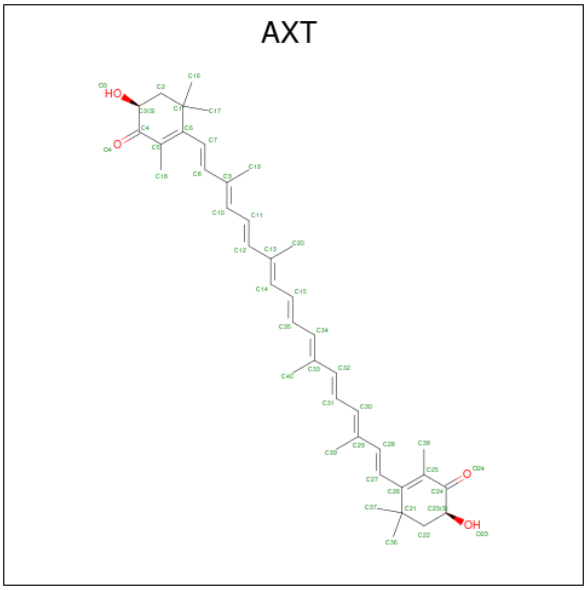
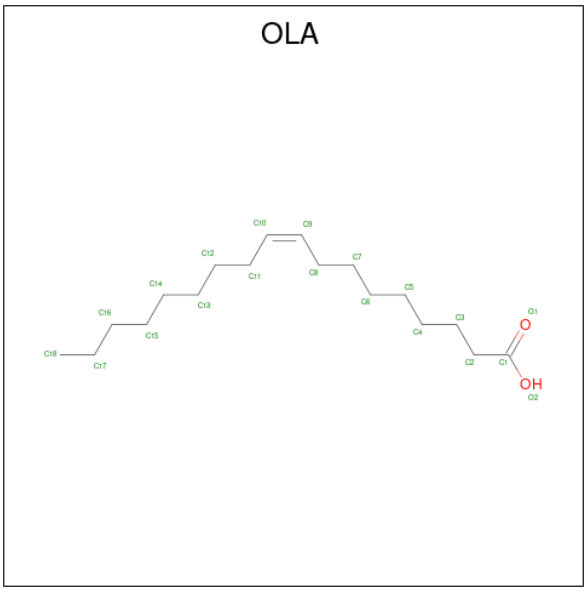
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 43 | 7 | 1 | Total C O<br>42 40 2 | 0 |
| 43 | 8 | 1 | Total C O<br>84 80 4 | 0 |
| 43 | 8 | 1 | Total C O<br>84 80 4 | 0 |
| 43 | 2 | 1 | Total C O<br>84 80 4 | 0 |
| 43 | 2 | 1 | Total C O<br>84 80 4 | 0 |
| 43 | 9 | 1 | Total C O<br>84 80 4 | 0 |
| 43 | 9 | 1 | Total C O<br>84 80 4 | 0 |

- Molecule 44 is ASTAXANTHIN (three-letter code: AXT) (formula: $C_{40}H_{52}O_4$).



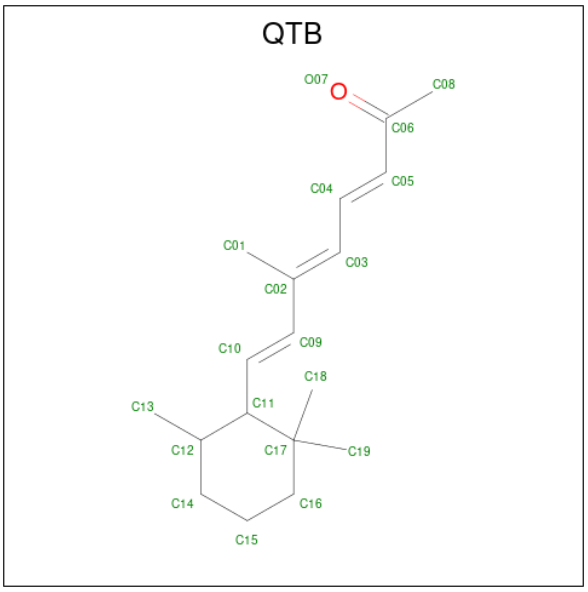

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 44 | 1 | 1 | Total C O<br>43 40 3 | 0 |
| 44 | 7 | 1 | Total C O<br>43 40 3 | 0 |

- Molecule 45 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



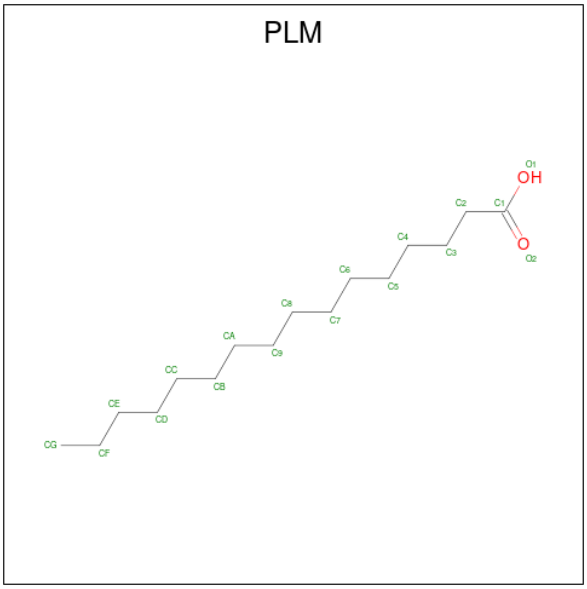

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 45 | 1 | 1 | Total | C | O | 0 |
| | | | 20 | 18 | 2 | |
| 45 | a | 1 | Total | C | O | 0 |
| | | | 20 | 18 | 2 | |
| 45 | 8 | 1 | Total | C | O | 0 |
| | | | 40 | 36 | 4 | |
| 45 | 8 | 1 | Total | C | O | 0 |
| | | | 40 | 36 | 4 | |

- Molecule 46 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7 -trien-2-one (three-letter code: QTB) (formula: $C_{18}H_{28}O$).



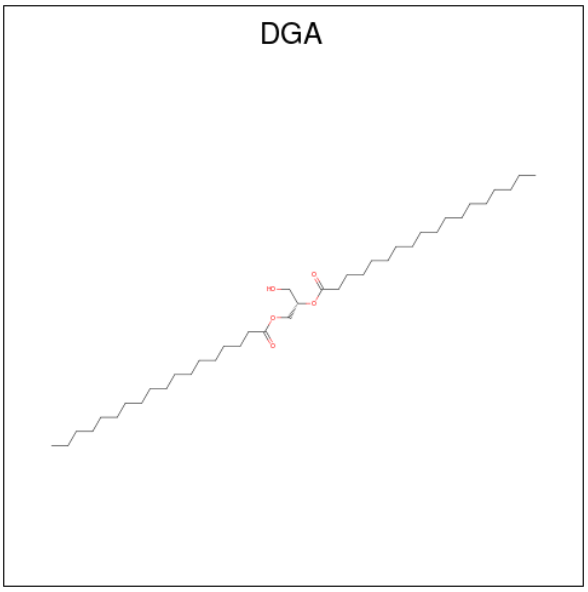
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 46 | a | 1 | Total C O<br>19 18 1 | 0 |

- Molecule 47 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



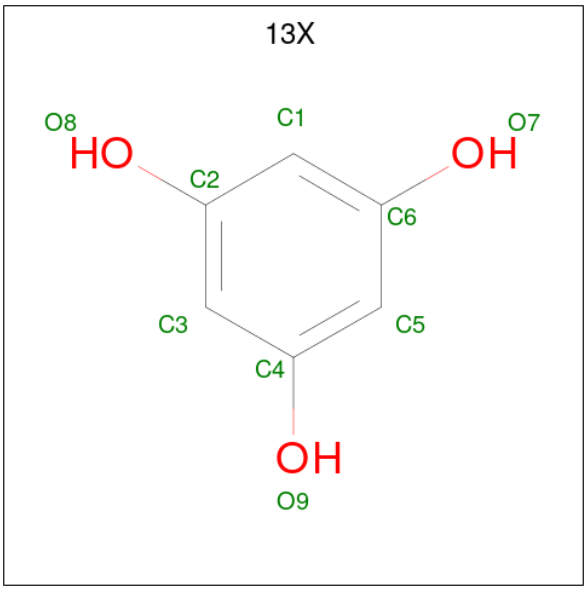

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 47 | a | 1 | Total C O<br>17 16 1 | 0 |
| 47 | 4 | 1 | Total C O<br>35 32 3 | 0 |
| 47 | 4 | 1 | Total C O<br>35 32 3 | 0 |
| 47 | 5 | 1 | Total C O<br>18 16 2 | 0 |
| 47 | 6 | 1 | Total C O<br>18 16 2 | 0 |
| 47 | 8 | 1 | Total C O<br>35 32 3 | 0 |
| 47 | 8 | 1 | Total C O<br>35 32 3 | 0 |

- Molecule 48 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



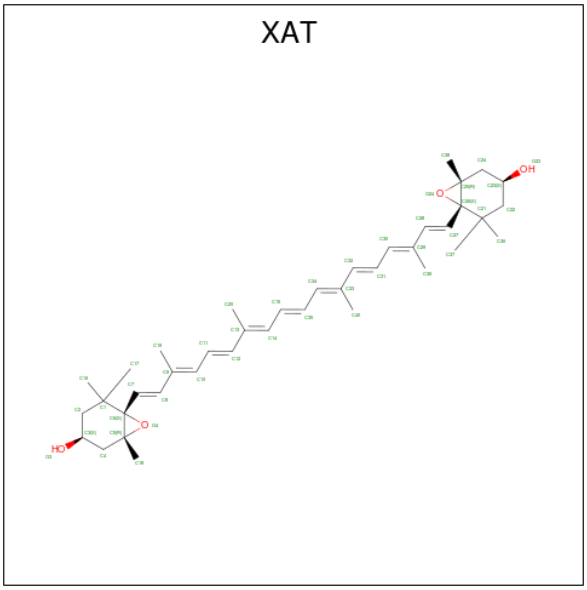

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 48 | 3 | 1 | Total C O<br>24 19 5 | 0 |
| 48 | 5 | 1 | Total C O<br>23 18 5 | 0 |
| 48 | 8 | 1 | Total C O<br>40 35 5 | 0 |
| 48 | 2 | 1 | Total C O<br>37 32 5 | 0 |

- Molecule 49 is benzene-1,3,5-triol (three-letter code: 13X) (formula: $C_6H_6O_3$).



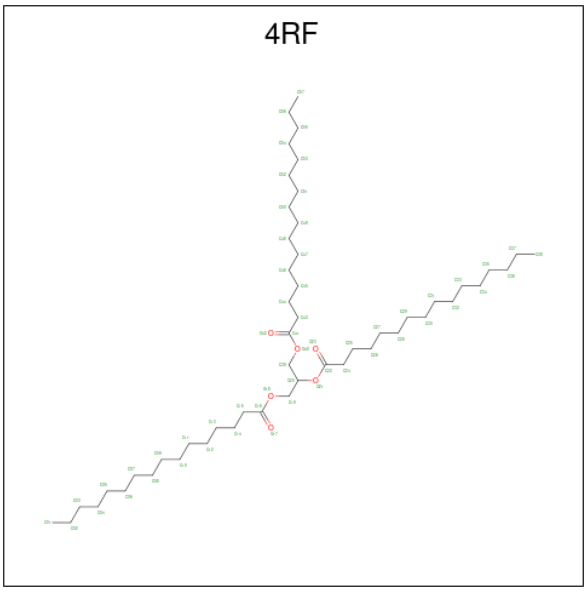
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 49 | 6 | 1 | Total C O<br>9 6 3 | 0 |

- Molecule 50 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 (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



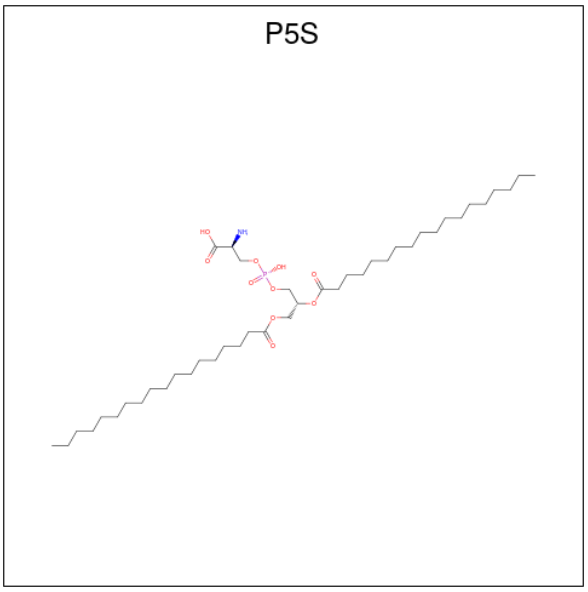

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 50 | 7 | 1 | Total C O<br>44 40 4 | 0 |
| 50 | 2 | 1 | Total C O<br>44 40 4 | 0 |
| 50 | 9 | 1 | Total C O<br>88 80 8 | 0 |
| 50 | 9 | 1 | Total C O<br>88 80 8 | 0 |

- Molecule 51 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: $C_{51}H_{98}O_6$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 51 | 7 | 1 | Total | C | O | 0 |
| | | | 37 | 31 | 6 | |

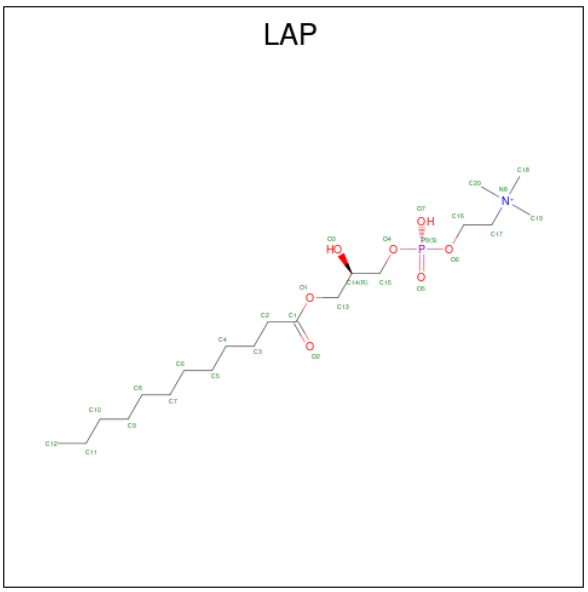
- Molecule 52 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 52 | 8 | 1 | Total | C | N | O | P | 0 |
| | | | 37 | 25 | 1 | 10 | 1 | |

- Molecule 53 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (three-letter code: LAP) (formula:

$C_{20}H_{43}NO_7P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 53 | 8 | 1 | Total | C | N | O | P | 0 |
| | | | 29 | 20 | 1 | 7 | 1 | |

- Molecule 54 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 54 | A | 20 | Total | O | 0 |
| | | | 21 | 21 | |
| 54 | A | 1 | Total | O | 0 |
| | | | 21 | 21 | |
| 54 | B | 2 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 2 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 5 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 6 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 4 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 3 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 1 | Total | O | 0 |
| | | | 24 | 24 | |
| 54 | B | 1 | Total | O | 0 |
| | | | 24 | 24 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 54 | C | 1 | Total O<br>2 2 | 0 |
| 54 | C | 1 | Total O<br>2 2 | 0 |
| 54 | D | 1 | Total O<br>2 2 | 0 |
| 54 | D | 1 | Total O<br>2 2 | 0 |
| 54 | E | 1 | Total O<br>1 1 | 0 |
| 54 | F | 1 | Total O<br>3 3 | 0 |
| 54 | F | 1 | Total O<br>3 3 | 0 |
| 54 | F | 1 | Total O<br>3 3 | 0 |
| 54 | G | 1 | Total O<br>3 3 | 0 |
| 54 | G | 2 | Total O<br>3 3 | 0 |
| 54 | H | 1 | Total O<br>1 1 | 0 |
| 54 | J | 1 | Total O<br>1 1 | 0 |
| 54 | K | 3 | Total O<br>3 3 | 0 |
| 54 | L | 1 | Total O<br>2 2 | 0 |
| 54 | L | 1 | Total O<br>2 2 | 0 |
| 54 | M | 1 | Total O<br>1 1 | 0 |
| 54 | 1 | 5 | Total O<br>5 5 | 0 |
| 54 | a | 1 | Total O<br>1 1 | 0 |
| 54 | 3 | 4 | Total O<br>5 5 | 0 |
| 54 | 3 | 1 | Total O<br>5 5 | 0 |
| 54 | 4 | 3 | Total O<br>4 4 | 0 |

*Continued on next page...*

*Continued from previous page...*

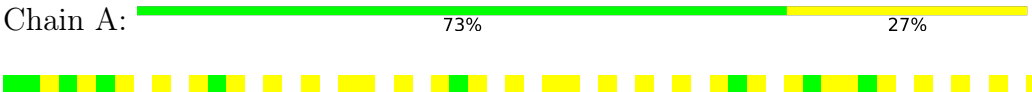
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 54 | 4 | 1 | Total O<br>4 4 | 0 |
| 54 | 5 | 3 | Total O<br>3 3 | 0 |
| 54 | 6 | 7 | Total O<br>7 7 | 0 |
| 54 | 7 | 2 | Total O<br>2 2 | 0 |
| 54 | 8 | 1 | Total O<br>2 2 | 0 |
| 54 | 8 | 1 | Total O<br>2 2 | 0 |
| 54 | 2 | 4 | Total O<br>4 4 | 0 |
| 54 | 9 | 1 | Total O<br>2 2 | 0 |
| 54 | 9 | 1 | Total O<br>2 2 | 0 |

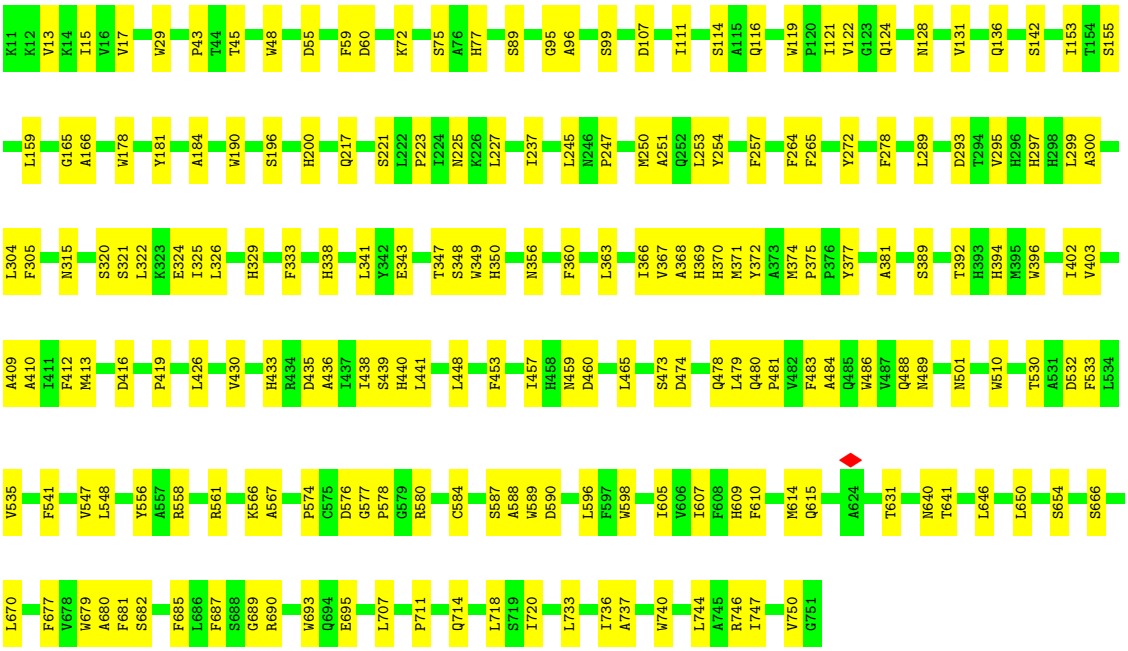
# 3 Residue-property plots (i)

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

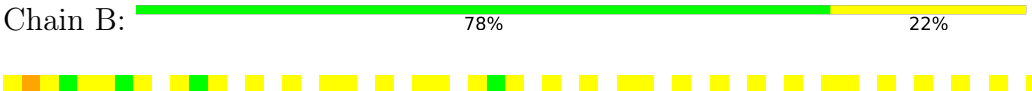
Chain A:

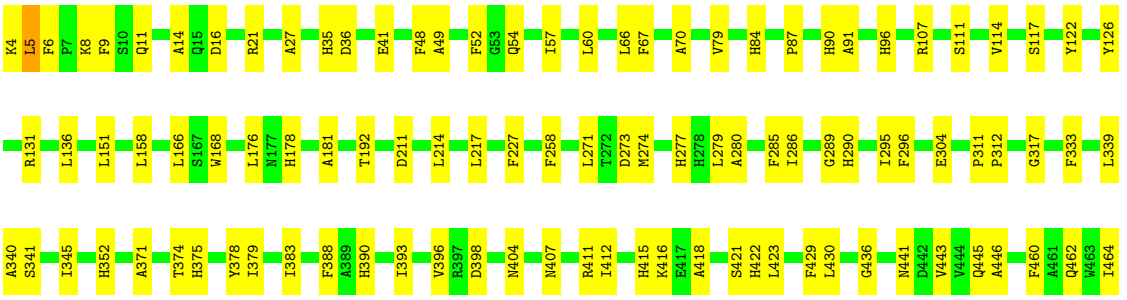


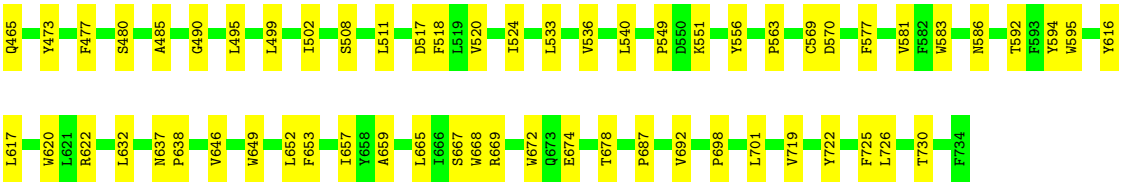



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

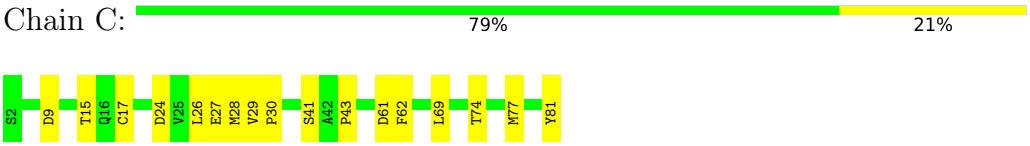
Chain B:



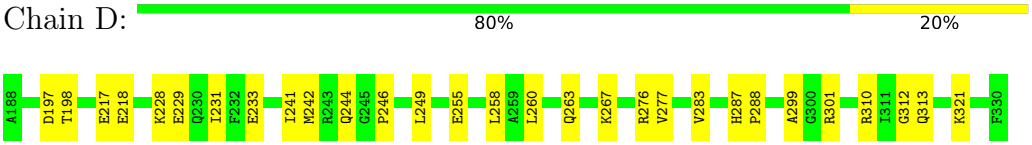





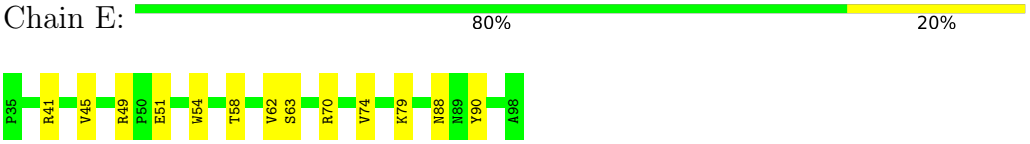

• Molecule 3: Photosystem I iron-sulfur center



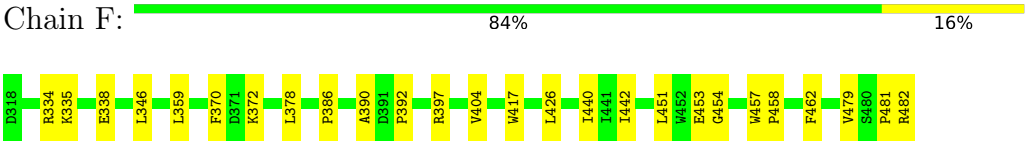

• Molecule 4: Photosystem I reaction center subunit chloroplastic



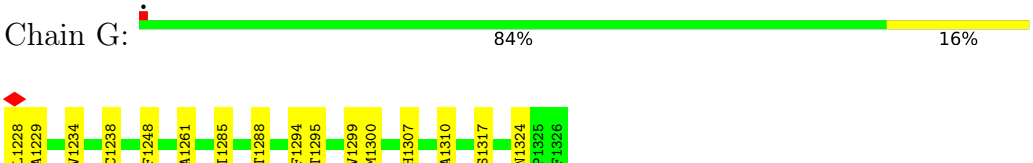

• Molecule 5: Photosystem I reaction center subunit IV



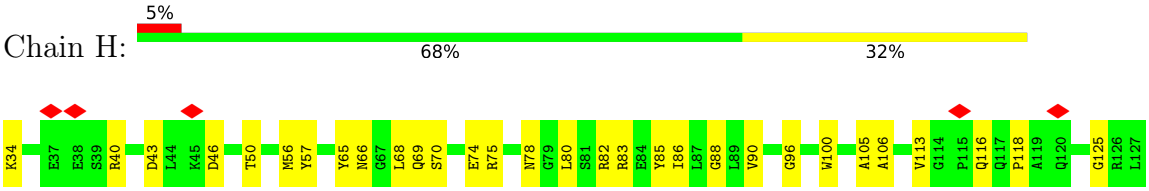

• Molecule 6: PSI-F




• Molecule 7: Photosystem I reaction center subunit chloroplastic

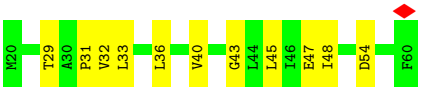



• Molecule 8: Photosystem I reaction center subunit VI-chloroplastic-like



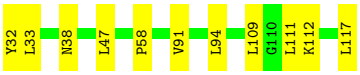
• Molecule 9: Photosystem I reaction center subunit IX

Chain J:



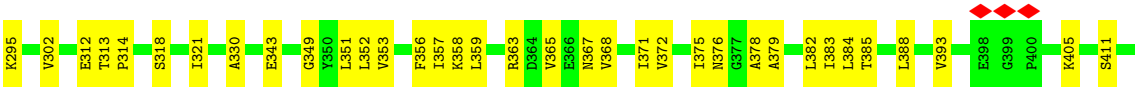

• Molecule 10: Photosystem I reaction center subunit chloroplastic

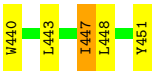
Chain K:




• Molecule 11: Photosystem I reaction center subunit XI

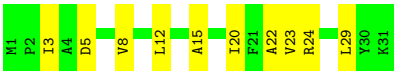
Chain L:



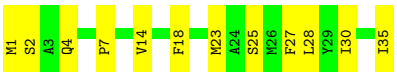

• Molecule 12: Photosystem I reaction center subunit XII

Chain M:



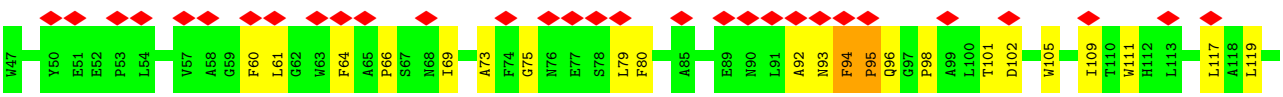

• Molecule 13: Photosystem I reaction center subunit VIII

Chain I:



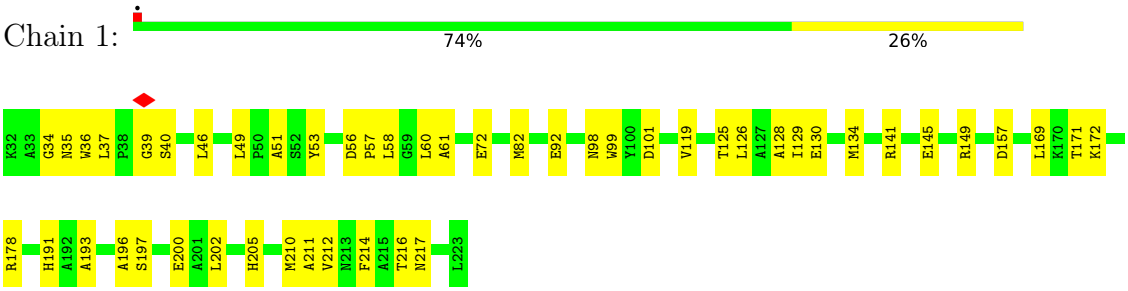

• Molecule 14: Photosystem I subunit O

Chain O:



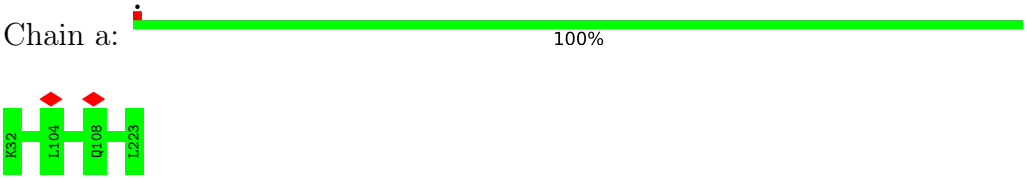
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



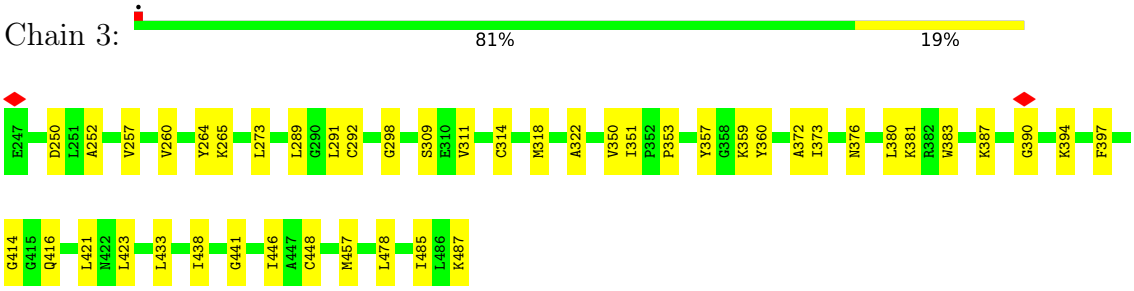

• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain a:



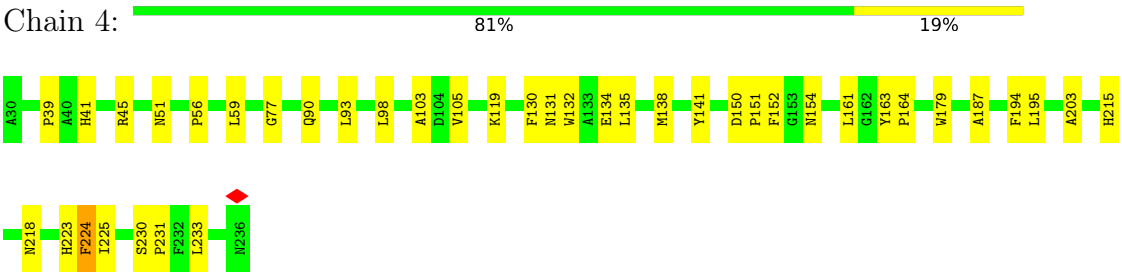

• Molecule 16: Glutathione reductase

Chain 3:



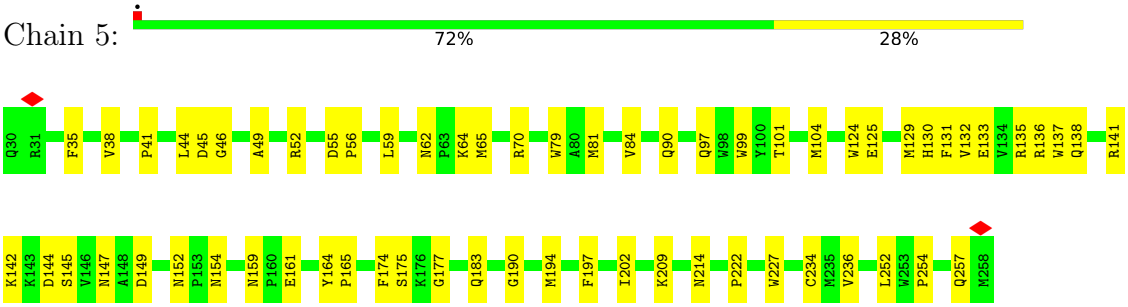

• Molecule 17: Lhca4

Chain 4:



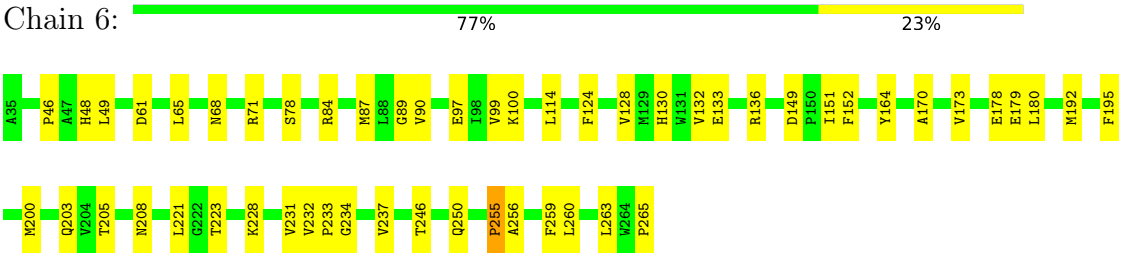

• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



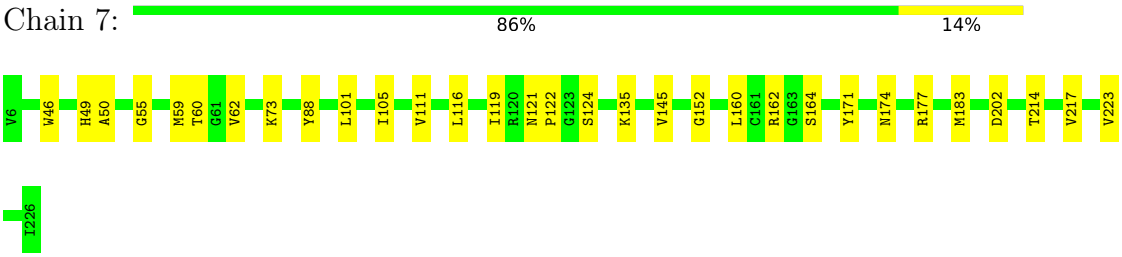
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



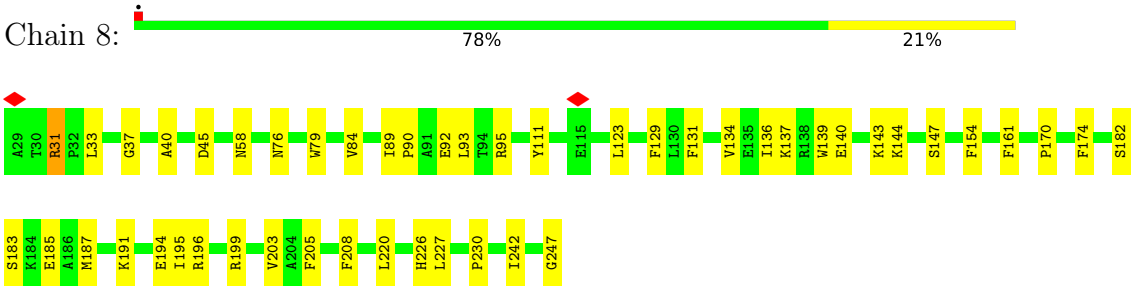

• Molecule 20: Lhca7

Chain 7:



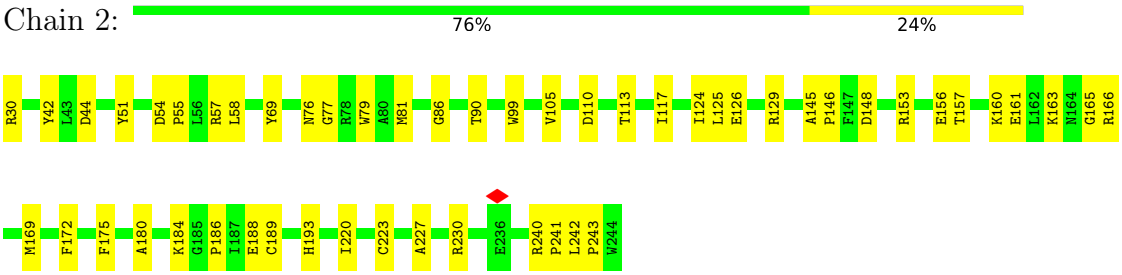

• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



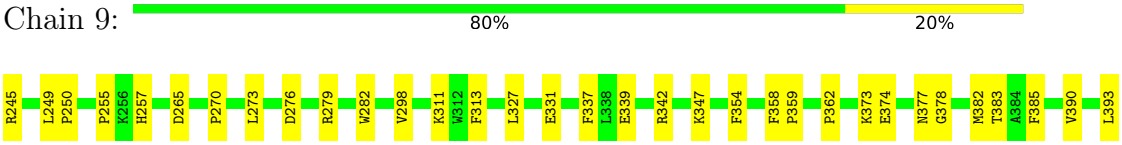

• Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain 2:




• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain 9:



L394
T395
R396
M414
P423
G427

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 185138 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 49.05 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.091 | Depositor |
| Minimum map value | -0.046 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.0112 | Depositor |
| Map size (Å) | 394.56, 394.56, 394.56 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.82199997, 0.82199997, 0.82199997 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, QTB, SF4, AXT, LPX, OLA, PLM, LHG, XAT, LUT, CL0, DGD, BCR, LMT, LMG, CLA, 13X, 3PH, NEX, 4RF, PTY, SQD, LAP, DGA, P5S, ECH, RRX, CHL, SPH, PCW

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 | 0.27 | 0/6022 | 0.47 | 0/8215 |
| 2 | B | 0.27 | 0/6006 | 0.48 | 1/8205 (0.0%) |
| 3 | C | 0.26 | 0/611 | 0.53 | 0/828 |
| 4 | D | 0.27 | 0/1150 | 0.52 | 0/1551 |
| 5 | E | 0.28 | 0/520 | 0.55 | 0/705 |
| 6 | F | 0.26 | 0/1309 | 0.47 | 0/1771 |
| 7 | G | 0.25 | 0/743 | 0.46 | 0/1007 |
| 8 | H | 0.27 | 0/744 | 0.54 | 0/1000 |
| 9 | J | 0.27 | 0/322 | 0.51 | 0/439 |
| 10 | K | 0.26 | 0/622 | 0.46 | 0/844 |
| 11 | L | 0.28 | 0/1195 | 0.51 | 0/1635 |
| 12 | M | 0.28 | 0/244 | 0.41 | 0/330 |
| 13 | I | 0.27 | 0/276 | 0.48 | 0/373 |
| 14 | O | 0.27 | 0/703 | 0.52 | 0/956 |
| 15 | 1 | 0.27 | 0/1443 | 0.48 | 0/1960 |
| 15 | a | 0.27 | 0/1443 | 0.47 | 0/1960 |
| 16 | 3 | 0.27 | 0/1896 | 0.46 | 0/2573 |
| 17 | 4 | 0.26 | 0/1681 | 0.44 | 0/2285 |
| 18 | 5 | 0.26 | 0/1842 | 0.45 | 0/2505 |
| 19 | 6 | 0.27 | 0/1845 | 0.48 | 0/2515 |
| 20 | 7 | 0.28 | 0/1748 | 0.49 | 0/2372 |
| 21 | 8 | 0.28 | 0/1717 | 0.48 | 0/2330 |
| 22 | 2 | 0.26 | 0/1708 | 0.47 | 0/2318 |
| 23 | 9 | 0.26 | 0/1444 | 0.45 | 0/1957 |
| All | All | 0.27 | 0/37234 | 0.48 | 1/50634 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 5 | LEU | CA-CB-CG | 5.50 | 127.94 | 115.30 |

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 | 5824 | 0 | 5675 | 174 | 0 |
| 2 | B | 5796 | 0 | 5576 | 146 | 0 |
| 3 | C | 601 | 0 | 576 | 13 | 0 |
| 4 | D | 1124 | 0 | 1129 | 20 | 0 |
| 5 | E | 509 | 0 | 507 | 8 | 0 |
| 6 | F | 1277 | 0 | 1296 | 19 | 0 |
| 7 | G | 727 | 0 | 724 | 15 | 0 |
| 8 | H | 729 | 0 | 705 | 26 | 0 |
| 9 | J | 316 | 0 | 332 | 9 | 0 |
| 10 | K | 613 | 0 | 639 | 11 | 0 |
| 11 | L | 1165 | 0 | 1181 | 39 | 0 |
| 12 | M | 239 | 0 | 255 | 11 | 0 |
| 13 | I | 270 | 0 | 287 | 12 | 0 |
| 14 | O | 679 | 0 | 661 | 24 | 0 |
| 15 | 1 | 1405 | 0 | 1370 | 46 | 0 |
| 15 | a | 1405 | 0 | 1370 | 0 | 0 |
| 16 | 3 | 1844 | 0 | 1805 | 39 | 0 |
| 17 | 4 | 1631 | 0 | 1575 | 34 | 0 |
| 18 | 5 | 1786 | 0 | 1736 | 53 | 0 |
| 19 | 6 | 1787 | 0 | 1760 | 45 | 0 |
| 20 | 7 | 1698 | 0 | 1640 | 30 | 0 |
| 21 | 8 | 1669 | 0 | 1619 | 53 | 0 |
| 22 | 2 | 1666 | 0 | 1657 | 50 | 0 |
| 23 | 9 | 1406 | 0 | 1385 | 35 | 0 |
| 24 | A | 65 | 0 | 72 | 6 | 0 |
| 25 | 1 | 528 | 0 | 523 | 52 | 0 |
| 25 | 2 | 615 | 0 | 568 | 44 | 0 |
| 25 | 3 | 576 | 0 | 555 | 37 | 0 |
| 25 | 4 | 768 | 0 | 685 | 46 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 25 | 5 | 642 | 0 | 564 | 38 | 0 |
| 25 | 6 | 624 | 0 | 591 | 34 | 0 |
| 25 | 7 | 566 | 0 | 525 | 39 | 0 |
| 25 | 8 | 573 | 0 | 480 | 42 | 0 |
| 25 | 9 | 379 | 0 | 338 | 29 | 0 |
| 25 | A | 2532 | 0 | 2566 | 221 | 0 |
| 25 | B | 2583 | 0 | 2685 | 203 | 0 |
| 25 | F | 105 | 0 | 88 | 8 | 0 |
| 25 | G | 155 | 0 | 130 | 9 | 0 |
| 25 | H | 156 | 0 | 130 | 8 | 0 |
| 25 | J | 42 | 0 | 30 | 1 | 0 |
| 25 | K | 200 | 0 | 161 | 12 | 0 |
| 25 | L | 205 | 0 | 168 | 16 | 0 |
| 25 | O | 134 | 0 | 95 | 5 | 0 |
| 25 | a | 496 | 0 | 443 | 0 | 0 |
| 26 | 1 | 284 | 0 | 248 | 31 | 0 |
| 26 | 2 | 165 | 0 | 137 | 7 | 0 |
| 26 | 3 | 236 | 0 | 223 | 21 | 0 |
| 26 | 4 | 174 | 0 | 154 | 15 | 0 |
| 26 | 5 | 271 | 0 | 217 | 18 | 0 |
| 26 | 6 | 333 | 0 | 284 | 25 | 0 |
| 26 | 7 | 296 | 0 | 267 | 24 | 0 |
| 26 | 8 | 296 | 0 | 265 | 19 | 0 |
| 26 | 9 | 273 | 0 | 233 | 26 | 0 |
| 26 | A | 66 | 0 | 69 | 9 | 0 |
| 26 | a | 264 | 0 | 205 | 0 | 0 |
| 27 | A | 33 | 0 | 46 | 7 | 0 |
| 27 | B | 33 | 0 | 46 | 5 | 0 |
| 28 | A | 8 | 0 | 0 | 0 | 0 |
| 28 | C | 16 | 0 | 0 | 1 | 0 |
| 29 | 3 | 120 | 0 | 158 | 12 | 0 |
| 29 | 4 | 40 | 0 | 53 | 8 | 0 |
| 29 | 5 | 80 | 0 | 103 | 10 | 0 |
| 29 | 6 | 80 | 0 | 106 | 8 | 0 |
| 29 | 7 | 40 | 0 | 52 | 9 | 0 |
| 29 | 8 | 40 | 0 | 53 | 3 | 0 |
| 29 | A | 200 | 0 | 264 | 24 | 0 |
| 29 | B | 280 | 0 | 371 | 34 | 0 |
| 29 | G | 40 | 0 | 53 | 5 | 0 |
| 29 | H | 40 | 0 | 53 | 4 | 0 |
| 29 | I | 40 | 0 | 52 | 2 | 0 |
| 29 | J | 40 | 0 | 53 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 29 | K | 80 | 0 | 106 | 8 | 0 |
| 29 | L | 120 | 0 | 159 | 6 | 0 |
| 29 | O | 40 | 0 | 52 | 1 | 0 |
| 30 | 1 | 84 | 0 | 114 | 6 | 0 |
| 30 | 2 | 98 | 0 | 148 | 11 | 0 |
| 30 | 3 | 49 | 0 | 74 | 1 | 0 |
| 30 | 4 | 81 | 0 | 108 | 4 | 0 |
| 30 | 5 | 49 | 0 | 74 | 2 | 0 |
| 30 | 6 | 86 | 0 | 118 | 6 | 0 |
| 30 | 7 | 108 | 0 | 126 | 3 | 0 |
| 30 | 8 | 37 | 0 | 44 | 1 | 0 |
| 30 | 9 | 82 | 0 | 110 | 7 | 0 |
| 30 | A | 144 | 0 | 213 | 11 | 0 |
| 30 | B | 98 | 0 | 148 | 7 | 0 |
| 30 | F | 79 | 0 | 101 | 4 | 0 |
| 30 | a | 35 | 0 | 40 | 0 | 0 |
| 31 | A | 42 | 0 | 54 | 0 | 0 |
| 32 | 7 | 39 | 0 | 41 | 1 | 0 |
| 32 | A | 54 | 0 | 77 | 8 | 0 |
| 32 | G | 46 | 0 | 55 | 4 | 0 |
| 32 | H | 45 | 0 | 53 | 3 | 0 |
| 32 | I | 54 | 0 | 77 | 5 | 0 |
| 33 | 3 | 38 | 0 | 49 | 3 | 0 |
| 33 | 5 | 38 | 0 | 49 | 3 | 0 |
| 33 | 7 | 33 | 0 | 39 | 0 | 0 |
| 33 | 9 | 48 | 0 | 72 | 3 | 0 |
| 33 | A | 34 | 0 | 41 | 4 | 0 |
| 33 | B | 42 | 0 | 60 | 4 | 0 |
| 33 | G | 56 | 0 | 62 | 2 | 0 |
| 33 | J | 28 | 0 | 29 | 2 | 0 |
| 33 | a | 76 | 0 | 98 | 0 | 0 |
| 34 | A | 33 | 0 | 39 | 3 | 0 |
| 35 | 1 | 35 | 0 | 46 | 5 | 0 |
| 35 | 2 | 35 | 0 | 45 | 5 | 0 |
| 35 | A | 35 | 0 | 45 | 1 | 0 |
| 35 | B | 35 | 0 | 45 | 2 | 0 |
| 36 | 7 | 50 | 0 | 58 | 3 | 0 |
| 36 | 8 | 105 | 0 | 126 | 8 | 0 |
| 36 | B | 66 | 0 | 96 | 4 | 0 |
| 37 | 6 | 36 | 0 | 44 | 4 | 0 |
| 37 | B | 39 | 0 | 50 | 1 | 0 |
| 37 | K | 77 | 0 | 99 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 38 | F | 30 | 0 | 43 | 2 | 0 |
| 39 | F | 44 | 0 | 54 | 5 | 0 |
| 40 | 3 | 41 | 0 | 56 | 1 | 0 |
| 40 | J | 41 | 0 | 56 | 2 | 0 |
| 41 | 4 | 21 | 0 | 37 | 0 | 0 |
| 41 | 6 | 21 | 0 | 37 | 1 | 0 |
| 41 | 9 | 21 | 0 | 37 | 2 | 0 |
| 41 | J | 21 | 0 | 37 | 1 | 0 |
| 42 | M | 41 | 0 | 54 | 5 | 0 |
| 43 | 1 | 84 | 0 | 110 | 7 | 0 |
| 43 | 2 | 84 | 0 | 110 | 11 | 0 |
| 43 | 3 | 84 | 0 | 110 | 7 | 0 |
| 43 | 4 | 84 | 0 | 110 | 10 | 0 |
| 43 | 5 | 126 | 0 | 165 | 13 | 0 |
| 43 | 6 | 84 | 0 | 110 | 10 | 0 |
| 43 | 7 | 42 | 0 | 55 | 5 | 0 |
| 43 | 8 | 84 | 0 | 110 | 11 | 0 |
| 43 | 9 | 84 | 0 | 110 | 17 | 0 |
| 43 | a | 126 | 0 | 165 | 0 | 0 |
| 44 | 1 | 43 | 0 | 52 | 3 | 0 |
| 44 | 7 | 43 | 0 | 52 | 10 | 0 |
| 45 | 1 | 20 | 0 | 33 | 2 | 0 |
| 45 | 8 | 40 | 0 | 66 | 1 | 0 |
| 45 | a | 20 | 0 | 33 | 0 | 0 |
| 46 | a | 19 | 0 | 0 | 0 | 0 |
| 47 | 4 | 35 | 0 | 62 | 3 | 0 |
| 47 | 5 | 18 | 0 | 31 | 3 | 0 |
| 47 | 6 | 18 | 0 | 31 | 1 | 0 |
| 47 | 8 | 35 | 0 | 62 | 6 | 0 |
| 47 | a | 17 | 0 | 31 | 0 | 0 |
| 48 | 2 | 37 | 0 | 56 | 6 | 0 |
| 48 | 3 | 24 | 0 | 30 | 3 | 0 |
| 48 | 5 | 23 | 0 | 28 | 3 | 0 |
| 48 | 8 | 40 | 0 | 65 | 5 | 0 |
| 49 | 6 | 9 | 0 | 6 | 0 | 0 |
| 50 | 2 | 44 | 0 | 56 | 2 | 0 |
| 50 | 7 | 44 | 0 | 56 | 3 | 0 |
| 50 | 9 | 88 | 0 | 112 | 8 | 0 |
| 51 | 7 | 37 | 0 | 49 | 6 | 0 |
| 52 | 8 | 37 | 0 | 40 | 2 | 0 |
| 53 | 8 | 29 | 0 | 42 | 5 | 0 |
| 54 | 1 | 5 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 54 | 2 | 4 | 0 | 0 | 0 | 0 |
| 54 | 3 | 5 | 0 | 0 | 0 | 0 |
| 54 | 4 | 4 | 0 | 0 | 0 | 0 |
| 54 | 5 | 3 | 0 | 0 | 0 | 0 |
| 54 | 6 | 7 | 0 | 0 | 0 | 0 |
| 54 | 7 | 2 | 0 | 0 | 0 | 0 |
| 54 | 8 | 2 | 0 | 0 | 0 | 0 |
| 54 | 9 | 2 | 0 | 0 | 0 | 0 |
| 54 | A | 21 | 0 | 0 | 1 | 0 |
| 54 | B | 24 | 0 | 0 | 0 | 0 |
| 54 | C | 2 | 0 | 0 | 0 | 0 |
| 54 | D | 2 | 0 | 0 | 0 | 0 |
| 54 | E | 1 | 0 | 0 | 0 | 0 |
| 54 | F | 3 | 0 | 0 | 0 | 0 |
| 54 | G | 3 | 0 | 0 | 0 | 0 |
| 54 | H | 1 | 0 | 0 | 0 | 0 |
| 54 | J | 1 | 0 | 0 | 0 | 0 |
| 54 | K | 3 | 0 | 0 | 0 | 0 |
| 54 | L | 2 | 0 | 0 | 0 | 0 |
| 54 | M | 1 | 0 | 0 | 0 | 0 |
| 54 | a | 1 | 0 | 0 | 0 | 0 |
| All | All | 56369 | 0 | 56465 | 1650 | 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 15.

All (1650) 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) |
|---|---|---|---|
| 11:L:295:LYS:N | 14:O:133:TYR:HH | 1.63 | 0.94 |
| 50:9:504:XAT:H32 | 50:9:507:XAT:H10 | 1.50 | 0.94 |
| 1:A:396:TRP:CD1 | 25:A:1126:CLA:HAB | 2.04 | 0.92 |
| 18:5:161:GLU:OE2 | 18:5:183:GLN:NE2 | 2.05 | 0.89 |
| 11:L:356:PHE:HB2 | 11:L:372:VAL:HG13 | 1.55 | 0.89 |
| 25:B:1218:CLA:HMD2 | 29:B:4001:BCR:HC7 | 1.56 | 0.88 |
| 1:A:389:SER:HB3 | 25:A:1126:CLA:HMA1 | 1.55 | 0.87 |
| 18:5:129:MET:HG3 | 25:5:612:CLA:HMC3 | 1.58 | 0.85 |
| 11:L:357:ILE:HG13 | 11:L:372:VAL:HG11 | 1.56 | 0.85 |
| 25:B:1220:CLA:HAB | 25:B:1227:CLA:HMD2 | 1.58 | 0.84 |
| 29:J:4001:BCR:H16C | 40:J:4002:RRX:H32 | 1.58 | 0.83 |
| 25:A:1131:CLA:HBB1 | 25:A:1132:CLA:H2 | 1.59 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:O:66:PRO:HA | 14:O:69:ILE:HG22 | 1.60 | 0.82 |
| 25:A:1129:CLA:HMA2 | 11:L:313:THR:HG21 | 1.62 | 0.82 |
| 2:B:285:PHE:HE1 | 25:B:1216:CLA:HAB | 1.43 | 0.82 |
| 11:L:353:VAL:HG13 | 11:L:376:ASN:HD22 | 1.46 | 0.81 |
| 43:4:501:LUT:H30 | 25:4:601:CLA:H71 | 1.63 | 0.80 |
| 11:L:451:TYR:H | 25:L:1504:CLA:HAB | 1.46 | 0.80 |
| 25:A:1110:CLA:H2 | 16:3:289:LEU:HD23 | 1.62 | 0.80 |
| 29:H:4001:BCR:H24C | 11:L:440:TRP:HE1 | 1.45 | 0.80 |
| 21:8:33:LEU:HD11 | 21:8:40:ALA:HB2 | 1.63 | 0.80 |
| 25:K:1403:CLA:HBA2 | 37:K:5002:PCW:H321 | 1.64 | 0.79 |
| 25:4:608:CLA:H2 | 26:4:609:CHL:H102 | 1.66 | 0.77 |
| 1:A:333:PHE:HB2 | 30:A:5001:LHG:HC41 | 1.66 | 0.77 |
| 25:5:612:CLA:H111 | 26:6:619:CHL:H43 | 1.67 | 0.76 |
| 22:2:184:LYS:HB3 | 22:2:188:GLU:HB3 | 1.66 | 0.76 |
| 1:A:489:ASN:HB3 | 14:O:101:THR:HG21 | 1.68 | 0.76 |
| 1:A:396:TRP:HD1 | 25:A:1126:CLA:HAB | 1.45 | 0.76 |
| 11:L:349:GLY:O | 11:L:376:ASN:ND2 | 2.18 | 0.76 |
| 29:7:503:BCR:H21C | 26:7:613:CHL:H2 | 1.66 | 0.76 |
| 29:6:503:BCR:H19C | 26:6:613:CHL:HBA2 | 1.67 | 0.75 |
| 19:6:65:LEU:HD23 | 20:7:160:LEU:HD21 | 1.68 | 0.75 |
| 14:O:60:PHE:O | 14:O:64:PHE:HB2 | 1.86 | 0.74 |
| 25:4:603:CLA:H2 | 25:4:608:CLA:HMD1 | 1.69 | 0.74 |
| 26:4:618:CHL:HBD | 26:4:618:CHL:HBA1 | 1.70 | 0.73 |
| 29:L:4001:BCR:H10C | 13:I:23:MET:HG2 | 1.69 | 0.73 |
| 25:A:1109:CLA:H102 | 25:A:1101:CLA:HBB2 | 1.71 | 0.73 |
| 25:B:1219:CLA:HBA1 | 35:B:5006:LMT:H12 | 1.70 | 0.73 |
| 25:B:1220:CLA:H72 | 29:B:4004:BCR:H10C | 1.69 | 0.73 |
| 11:L:357:ILE:HA | 11:L:372:VAL:HG21 | 1.71 | 0.73 |
| 2:B:16:ASP:HB3 | 2:B:21:ARG:HB2 | 1.70 | 0.72 |
| 21:8:139:TRP:HE1 | 36:8:803:DGD:HO3D | 1.33 | 0.72 |
| 29:A:4001:BCR:H362 | 29:A:4002:BCR:H21C | 1.71 | 0.72 |
| 2:B:111:SER:O | 8:H:116:GLN:NE2 | 2.22 | 0.72 |
| 8:H:68:LEU:HG | 25:H:1701:CLA:HAC1 | 1.70 | 0.72 |
| 43:2:507:LUT:H193 | 25:2:601:CLA:HBC1 | 1.71 | 0.72 |
| 25:2:603:CLA:HBD | 25:2:603:CLA:HBA1 | 1.72 | 0.72 |
| 25:6:603:CLA:H93 | 30:6:801:LHG:H322 | 1.71 | 0.72 |
| 44:7:504:AXT:H27 | 21:8:242:ILE:HG21 | 1.71 | 0.72 |
| 1:A:293:ASP:HB3 | 25:A:1116:CLA:HMA1 | 1.71 | 0.72 |
| 27:A:2001:PQN:H142 | 29:B:4006:BCR:H271 | 1.72 | 0.72 |
| 21:8:139:TRP:NE1 | 36:8:803:DGD:O3D | 2.23 | 0.71 |
| 25:2:604:CLA:H71 | 25:2:605:CLA:HMA1 | 1.71 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:670:LEU:HB3 | 25:A:1012:CLA:H71 | 1.73 | 0.71 |
| 26:6:613:CHL:HMB1 | 26:6:613:CHL:HBB1 | 1.72 | 0.71 |
| 4:D:312:GLY:N | 5:E:51:GLU:OE2 | 2.23 | 0.71 |
| 19:6:87:MET:SD | 25:6:601:CLA:HAB | 2.31 | 0.71 |
| 17:4:223:HIS:O | 17:4:225:ILE:N | 2.21 | 0.71 |
| 2:B:217:LEU:HD11 | 23:9:423:PRO:HA | 1.72 | 0.71 |
| 20:7:119:ILE:HA | 51:7:807:4RF:H52 | 1.73 | 0.71 |
| 25:B:1219:CLA:HBB1 | 25:B:1219:CLA:HMB1 | 1.72 | 0.71 |
| 43:3:502:LUT:H32 | 26:3:604:CHL:HBB1 | 1.73 | 0.70 |
| 25:A:1101:CLA:HBB1 | 25:A:1101:CLA:HHC | 1.73 | 0.70 |
| 1:A:369:HIS:HA | 1:A:372:TYR:CE1 | 2.26 | 0.70 |
| 19:6:200:MET:HG3 | 25:6:603:CLA:HAC2 | 1.73 | 0.70 |
| 43:2:502:LUT:H12 | 25:2:604:CLA:HAB | 1.72 | 0.70 |
| 25:B:1220:CLA:HBB2 | 25:B:1240:CLA:H52 | 1.74 | 0.70 |
| 25:4:605:CLA:HHC | 25:4:605:CLA:HBB1 | 1.71 | 0.70 |
| 26:4:609:CHL:H11 | 30:4:801:LHG:H182 | 1.74 | 0.70 |
| 20:7:121:ASN:ND2 | 21:8:37:GLY:O | 2.25 | 0.70 |
| 25:8:605:CLA:HHC | 25:8:605:CLA:HBB1 | 1.72 | 0.70 |
| 25:4:610:CLA:HBA1 | 25:4:612:CLA:HBC3 | 1.73 | 0.70 |
| 26:5:618:CHL:HED1 | 30:6:801:LHG:H311 | 1.72 | 0.70 |
| 25:B:1206:CLA:HBB1 | 25:B:1206:CLA:HMB1 | 1.73 | 0.70 |
| 13:I:25:SER:HB3 | 32:I:5001:SQD:H81 | 1.74 | 0.70 |
| 29:5:504:BCR:H373 | 26:6:619:CHL:H12 | 1.73 | 0.70 |
| 16:3:457:MET:HG3 | 16:3:485:ILE:HG13 | 1.73 | 0.70 |
| 29:3:504:BCR:HC7 | 26:3:611:CHL:HMB2 | 1.73 | 0.69 |
| 36:7:806:DGD:HA61 | 36:7:806:DGD:HB71 | 1.72 | 0.69 |
| 25:B:1209:CLA:H12 | 23:9:273:LEU:HD22 | 1.74 | 0.69 |
| 29:5:504:BCR:H383 | 26:5:610:CHL:H11 | 1.74 | 0.69 |
| 35:2:804:LMT:H5B | 35:2:804:LMT:H6D | 1.73 | 0.69 |
| 25:2:604:CLA:HMB1 | 25:2:604:CLA:HBB1 | 1.74 | 0.69 |
| 1:A:119:TRP:HE1 | 32:A:5005:SQD:H3 | 1.58 | 0.69 |
| 1:A:598:TRP:CH2 | 25:B:1022:CLA:HAB | 2.28 | 0.69 |
| 25:A:1102:CLA:HBB1 | 25:A:1102:CLA:HMB1 | 1.74 | 0.69 |
| 25:1:615:CLA:HBB1 | 25:1:615:CLA:HMB1 | 1.74 | 0.69 |
| 30:4:801:LHG:H122 | 30:4:801:LHG:H291 | 1.74 | 0.69 |
| 25:1:602:CLA:HBB1 | 25:1:602:CLA:HHC | 1.74 | 0.69 |
| 25:B:1222:CLA:H52 | 25:B:1231:CLA:HBB2 | 1.73 | 0.69 |
| 25:L:1504:CLA:HBB1 | 25:L:1504:CLA:HHC | 1.75 | 0.69 |
| 1:A:576:ASP:OD2 | 1:A:580:ARG:NH2 | 2.25 | 0.68 |
| 25:A:1012:CLA:HAB | 2:B:583:TRP:CH2 | 2.28 | 0.68 |
| 25:A:1105:CLA:HBC1 | 32:A:5005:SQD:H361 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:5:81:MET:SD | 25:5:601:CLA:HAB | 2.33 | 0.68 |
| 25:8:606:CLA:HMA2 | 26:8:613:CHL:HBC3 | 1.75 | 0.68 |
| 26:6:609:CHL:H12 | 30:6:801:LHG:H141 | 1.75 | 0.68 |
| 7:G:1307:HIS:CD2 | 29:G:4001:BCR:H352 | 2.28 | 0.68 |
| 26:5:613:CHL:HBB1 | 26:5:613:CHL:HMB1 | 1.74 | 0.68 |
| 25:8:606:CLA:HBD | 52:8:805:P5S:H3 | 1.74 | 0.68 |
| 18:5:159:ASN:HB3 | 18:5:165:PRO:HA | 1.76 | 0.68 |
| 30:B:5001:LHG:H301 | 30:B:5001:LHG:H161 | 1.76 | 0.68 |
| 32:H:5001:SQD:H261 | 25:2:605:CLA:H43 | 1.76 | 0.68 |
| 25:B:1202:CLA:HHC | 25:B:1202:CLA:HBB1 | 1.74 | 0.68 |
| 29:3:503:BCR:H271 | 25:3:613:CLA:H71 | 1.76 | 0.67 |
| 13:I:1:MET:O | 13:I:4:GLN:NE2 | 2.27 | 0.67 |
| 2:B:722:TYR:HB2 | 25:B:1021:CLA:HED3 | 1.75 | 0.67 |
| 2:B:388:PHE:HZ | 25:B:1222:CLA:HAB | 1.59 | 0.67 |
| 1:A:707:LEU:HD13 | 39:F:4001:NEX:H383 | 1.77 | 0.67 |
| 38:F:5003:LPX:H4 | 25:F:1301:CLA:HBA2 | 1.75 | 0.67 |
| 43:9:502:LUT:H32 | 25:9:604:CLA:HAB | 1.77 | 0.67 |
| 25:B:1209:CLA:HHC | 25:B:1209:CLA:HBB1 | 1.77 | 0.67 |
| 25:F:1302:CLA:HBD | 51:7:807:4RF:H5 | 1.76 | 0.67 |
| 43:8:502:LUT:H32 | 26:8:604:CHL:HBB1 | 1.77 | 0.67 |
| 23:9:394:LEU:HD12 | 26:9:603:CHL:HMD1 | 1.77 | 0.67 |
| 25:7:610:CLA:H13 | 30:7:803:LHG:H302 | 1.77 | 0.66 |
| 1:A:483:PHE:HB3 | 25:A:1135:CLA:H2 | 1.75 | 0.66 |
| 25:A:1138:CLA:H111 | 25:A:1138:CLA:HAB | 1.77 | 0.66 |
| 15:1:82:MET:SD | 25:1:601:CLA:HAB | 2.35 | 0.66 |
| 25:B:1023:CLA:H13 | 29:B:4007:BCR:H16C | 1.77 | 0.66 |
| 25:5:602:CLA:HHC | 25:5:602:CLA:HBB1 | 1.76 | 0.66 |
| 16:3:318:MET:SD | 25:3:601:CLA:HAB | 2.35 | 0.66 |
| 26:1:610:CHL:HMB1 | 26:1:610:CHL:HBB1 | 1.78 | 0.66 |
| 17:4:93:LEU:HG | 17:4:98:LEU:HB2 | 1.76 | 0.66 |
| 19:6:136:ARG:NH2 | 25:6:612:CLA:O1D | 2.29 | 0.66 |
| 25:L:1503:CLA:HMB1 | 25:L:1503:CLA:HBB1 | 1.78 | 0.66 |
| 50:9:507:XAT:H32 | 25:9:606:CLA:HBA2 | 1.78 | 0.66 |
| 25:B:1204:CLA:HED2 | 13:I:7:PRO:HB3 | 1.77 | 0.66 |
| 18:5:49:ALA:O | 18:5:70:ARG:NH2 | 2.28 | 0.65 |
| 43:3:502:LUT:H32 | 26:3:604:CHL:CBB | 2.26 | 0.65 |
| 2:B:398:ASP:OD2 | 4:D:321:LYS:NZ | 2.28 | 0.65 |
| 25:B:1208:CLA:H2 | 25:B:1209:CLA:HMD2 | 1.77 | 0.65 |
| 21:8:31:ARG:NH2 | 21:8:45:ASP:O | 2.29 | 0.65 |
| 25:8:606:CLA:HMB1 | 25:8:606:CLA:HBB1 | 1.77 | 0.65 |
| 20:7:49:HIS:CE1 | 51:7:807:4RF:H51 | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:9:610:CHL:OBD | 33:9:803:PTY:N1 | 2.29 | 0.65 |
| 26:9:601:CHL:HMB1 | 26:9:601:CHL:HBB1 | 1.79 | 0.65 |
| 29:A:4005:BCR:H24C | 25:B:1230:CLA:HMC2 | 1.78 | 0.65 |
| 16:3:350:VAL:HG13 | 16:3:351:ILE:HG13 | 1.78 | 0.65 |
| 26:6:619:CHL:HBB1 | 26:6:619:CHL:HMB1 | 1.79 | 0.65 |
| 22:2:220:ILE:HG22 | 25:9:612:CLA:HBB1 | 1.79 | 0.65 |
| 1:A:596:LEU:HD21 | 25:A:1128:CLA:HBC1 | 1.77 | 0.65 |
| 25:4:606:CLA:HBB1 | 25:4:606:CLA:HMB1 | 1.78 | 0.65 |
| 2:B:41:GLU:HG2 | 2:B:166:LEU:HB2 | 1.79 | 0.64 |
| 26:3:603:CHL:H43 | 26:3:608:CHL:HMD1 | 1.78 | 0.64 |
| 25:A:1117:CLA:HBB1 | 25:A:1117:CLA:HMB1 | 1.79 | 0.64 |
| 22:2:58:LEU:HD21 | 22:2:242:LEU:HD23 | 1.80 | 0.64 |
| 25:A:1012:CLA:H8 | 25:A:1012:CLA:H41 | 1.80 | 0.64 |
| 25:A:1102:CLA:HMA2 | 25:A:1109:CLA:HMD2 | 1.78 | 0.64 |
| 25:A:1110:CLA:HHC | 25:A:1110:CLA:HBB1 | 1.78 | 0.64 |
| 21:8:139:TRP:CE3 | 53:8:810:LAP:H193 | 2.33 | 0.64 |
| 26:4:609:CHL:O1A | 19:6:130:HIS:ND1 | 2.31 | 0.64 |
| 2:B:443:VAL:HG21 | 25:B:1230:CLA:HAC2 | 1.78 | 0.64 |
| 29:3:504:BCR:H10C | 26:3:611:CHL:HBA1 | 1.79 | 0.64 |
| 23:9:373:LYS:HG3 | 25:9:607:CLA:HED2 | 1.78 | 0.64 |
| 23:9:393:LEU:O | 23:9:396:ARG:NH1 | 2.31 | 0.64 |
| 4:D:198:THR:HG23 | 4:D:246:PRO:HB2 | 1.80 | 0.64 |
| 18:5:234:CYS:SG | 33:5:802:PTY:N1 | 2.68 | 0.64 |
| 43:7:501:LUT:H361 | 43:7:501:LUT:H28 | 1.80 | 0.63 |
| 26:1:613:CHL:HMB1 | 26:1:613:CHL:HBB1 | 1.78 | 0.63 |
| 17:4:77:GLY:HA3 | 17:4:187:ALA:HB1 | 1.80 | 0.63 |
| 20:7:111:VAL:HG21 | 29:7:503:BCR:H362 | 1.80 | 0.63 |
| 25:B:1219:CLA:HBB2 | 29:B:4004:BCR:H343 | 1.80 | 0.63 |
| 26:6:609:CHL:HMB1 | 26:6:609:CHL:HBB1 | 1.81 | 0.63 |
| 25:9:604:CLA:HBB1 | 25:9:604:CLA:HMB1 | 1.80 | 0.63 |
| 25:9:612:CLA:H171 | 25:9:612:CLA:H91 | 1.79 | 0.63 |
| 1:A:370:HIS:ND1 | 25:A:1116:CLA:OBD | 2.31 | 0.63 |
| 2:B:285:PHE:CE1 | 25:B:1216:CLA:HAB | 2.30 | 0.63 |
| 25:B:1212:CLA:H112 | 29:B:4001:BCR:H21C | 1.80 | 0.63 |
| 26:6:619:CHL:HMC | 37:6:803:PCW:H322 | 1.80 | 0.63 |
| 43:8:502:LUT:H32 | 26:8:604:CHL:CBB | 2.29 | 0.63 |
| 35:2:804:LMT:H3' | 25:2:615:CLA:HED1 | 1.80 | 0.63 |
| 50:9:504:XAT:H401 | 25:9:606:CLA:HMC2 | 1.81 | 0.63 |
| 30:A:5003:LHG:H201 | 16:3:448:CYS:HB3 | 1.80 | 0.63 |
| 25:B:1217:CLA:HBB1 | 25:B:1217:CLA:HHC | 1.80 | 0.63 |
| 29:7:503:BCR:H372 | 26:7:613:CHL:H102 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:7:606:CLA:HMA2 | 26:7:613:CHL:HBC3 | 1.81 | 0.63 |
| 15:1:35:ASN:C | 15:1:37:LEU:H | 2.02 | 0.63 |
| 25:3:602:CLA:HBB1 | 25:3:602:CLA:HMB1 | 1.80 | 0.63 |
| 18:5:254:PRO:HA | 33:5:802:PTY:HC31 | 1.79 | 0.63 |
| 43:8:501:LUT:H32 | 26:8:601:CHL:HBB1 | 1.80 | 0.63 |
| 25:A:1115:CLA:H51 | 10:K:109:LEU:HD13 | 1.81 | 0.62 |
| 2:B:192:THR:HG21 | 2:B:279:LEU:HB2 | 1.81 | 0.62 |
| 1:A:297:HIS:HB2 | 25:A:1116:CLA:C1B | 2.29 | 0.62 |
| 25:L:1502:CLA:HMA1 | 25:L:1503:CLA:HBC1 | 1.81 | 0.62 |
| 22:2:125:LEU:HD13 | 43:2:507:LUT:H163 | 1.80 | 0.62 |
| 11:L:451:TYR:HA | 25:L:1504:CLA:HMB1 | 1.81 | 0.62 |
| 22:2:77:GLY:O | 22:2:81:MET:HG3 | 1.99 | 0.62 |
| 30:B:5001:LHG:H351 | 47:8:807:PLM:HA1 | 1.81 | 0.62 |
| 14:O:131:GLN:HG2 | 25:O:1802:CLA:HBD | 1.82 | 0.62 |
| 2:B:27:ALA:HA | 25:B:1226:CLA:H43 | 1.80 | 0.62 |
| 17:4:130:PHE:HB3 | 25:4:612:CLA:HAB | 1.82 | 0.62 |
| 22:2:42:TYR:OH | 22:2:54:ASP:OD2 | 2.18 | 0.62 |
| 25:1:612:CLA:HMB2 | 35:1:804:LMT:H11 | 1.80 | 0.62 |
| 18:5:97:GLN:HG2 | 25:5:606:CLA:HED3 | 1.81 | 0.62 |
| 2:B:214:LEU:O | 23:9:396:ARG:NH2 | 2.32 | 0.62 |
| 43:1:501:LUT:H30 | 25:1:601:CLA:H52 | 1.80 | 0.62 |
| 43:2:507:LUT:H182 | 25:2:601:CLA:HAC2 | 1.80 | 0.62 |
| 26:A:1114:CHL:HBA1 | 33:A:5006:PTY:H112 | 1.81 | 0.62 |
| 26:7:609:CHL:H91 | 25:7:603:CLA:HBC3 | 1.80 | 0.62 |
| 26:7:617:CHL:H191 | 36:8:802:DGD:HB71 | 1.82 | 0.62 |
| 21:8:187:MET:HG3 | 21:8:191:LYS:HE3 | 1.82 | 0.62 |
| 22:2:51:TYR:HB2 | 25:2:604:CLA:HMD1 | 1.82 | 0.62 |
| 1:A:436:ALA:O | 1:A:440:HIS:ND1 | 2.27 | 0.62 |
| 1:A:17:VAL:HG11 | 1:A:184:ALA:HB1 | 1.82 | 0.62 |
| 25:B:1227:CLA:HBB2 | 25:B:1236:CLA:HMC2 | 1.82 | 0.62 |
| 26:5:610:CHL:HBB1 | 26:5:610:CHL:HHC | 1.82 | 0.62 |
| 1:A:465:LEU:HG | 25:B:1206:CLA:HMC3 | 1.82 | 0.61 |
| 43:1:501:LUT:H162 | 25:1:608:CLA:HBC1 | 1.82 | 0.61 |
| 1:A:677:PHE:CG | 29:A:4005:BCR:H363 | 2.36 | 0.61 |
| 11:L:330:ALA:HB2 | 25:L:1502:CLA:HMD1 | 1.82 | 0.61 |
| 26:2:609:CHL:HBB1 | 26:2:609:CHL:HHC | 1.81 | 0.61 |
| 2:B:378:TYR:CD2 | 25:B:1224:CLA:HAB | 2.36 | 0.61 |
| 19:6:46:PRO:HG2 | 19:6:49:LEU:HB2 | 1.83 | 0.61 |
| 1:A:72:LYS:HZ1 | 25:A:1109:CLA:HED2 | 1.65 | 0.61 |
| 25:A:1132:CLA:HMA2 | 11:L:359:LEU:HB3 | 1.82 | 0.61 |
| 11:L:302:VAL:HA | 11:L:312:GLU:HG3 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:1:609:CHL:HMA2 | 21:8:136:ILE:HD13 | 1.83 | 0.61 |
| 25:7:604:CLA:H172 | 25:7:605:CLA:HBB1 | 1.83 | 0.61 |
| 1:A:666:SER:HB2 | 2:B:446:ALA:HB1 | 1.83 | 0.61 |
| 16:3:478:LEU:HB2 | 26:3:603:CHL:H11 | 1.82 | 0.61 |
| 17:4:150:ASP:OD1 | 17:4:154:ASN:N | 2.33 | 0.61 |
| 23:9:282:TRP:HZ2 | 25:9:612:CLA:HAA1 | 1.65 | 0.61 |
| 25:A:1112:CLA:HBA2 | 26:A:1114:CHL:HMB3 | 1.82 | 0.61 |
| 25:A:1115:CLA:HMD1 | 25:A:1134:CLA:HED2 | 1.81 | 0.61 |
| 44:7:504:AXT:H383 | 21:8:247:GLY:HA3 | 1.82 | 0.61 |
| 2:B:67:PHE:HZ | 12:M:8:VAL:HG13 | 1.65 | 0.61 |
| 25:1:612:CLA:HMA1 | 35:1:804:LMT:H5' | 1.83 | 0.61 |
| 7:G:1228:LEU:HD23 | 7:G:1317:SER:HB2 | 1.83 | 0.61 |
| 22:2:57:ARG:HH22 | 30:2:802:LHG:HC32 | 1.66 | 0.61 |
| 1:A:736:ILE:HG21 | 25:A:1126:CLA:HMC2 | 1.83 | 0.60 |
| 4:D:287:HIS:HB3 | 4:D:288:PRO:HD3 | 1.82 | 0.60 |
| 13:I:28:LEU:HD12 | 32:I:5001:SQD:H242 | 1.82 | 0.60 |
| 29:4:503:BCR:H282 | 25:4:616:CLA:HMB1 | 1.83 | 0.60 |
| 26:8:603:CHL:HBC1 | 47:8:806:PLM:H81 | 1.83 | 0.60 |
| 23:9:390:VAL:HG12 | 26:9:603:CHL:HMD3 | 1.83 | 0.60 |
| 25:B:1204:CLA:H12 | 13:I:14:VAL:HG21 | 1.82 | 0.60 |
| 11:L:358:LYS:HG2 | 25:L:1503:CLA:HMA1 | 1.81 | 0.60 |
| 15:1:35:ASN:O | 15:1:37:LEU:N | 2.32 | 0.60 |
| 25:A:1106:CLA:H71 | 25:A:1128:CLA:H171 | 1.83 | 0.60 |
| 43:8:502:LUT:H30 | 26:8:604:CHL:H72 | 1.83 | 0.60 |
| 25:B:1221:CLA:HMA2 | 25:B:1221:CLA:H2 | 1.84 | 0.60 |
| 5:E:54:TRP:NE1 | 5:E:79:LYS:O | 2.27 | 0.60 |
| 47:4:804:PLM:HD2 | 25:8:602:CLA:H42 | 1.83 | 0.60 |
| 6:F:479:VAL:HG21 | 6:F:482:ARG:HH22 | 1.66 | 0.60 |
| 22:2:81:MET:SD | 25:2:601:CLA:HAB | 2.42 | 0.60 |
| 26:3:608:CHL:HHC | 26:3:608:CHL:HBB1 | 1.81 | 0.60 |
| 26:5:617:CHL:HHC | 26:5:617:CHL:HBB1 | 1.82 | 0.60 |
| 19:6:192:MET:SD | 25:6:604:CLA:HBB1 | 2.42 | 0.60 |
| 25:A:1108:CLA:H12 | 25:A:1110:CLA:H43 | 1.83 | 0.60 |
| 25:6:615:CLA:HMC3 | 26:6:619:CHL:HBC3 | 1.82 | 0.60 |
| 25:8:605:CLA:H62 | 36:8:803:DGD:HA51 | 1.84 | 0.60 |
| 25:2:604:CLA:HBC1 | 30:2:801:LHG:H111 | 1.83 | 0.60 |
| 17:4:45:ARG:O | 17:4:51:ASN:ND2 | 2.33 | 0.60 |
| 1:A:501:ASN:HB2 | 25:A:1134:CLA:HED3 | 1.84 | 0.60 |
| 1:A:598:TRP:HH2 | 25:B:1022:CLA:HAB | 1.66 | 0.60 |
| 25:A:1113:CLA:H112 | 29:A:4002:BCR:H282 | 1.84 | 0.60 |
| 7:G:1248:PHE:HB3 | 43:1:503:LUT:H221 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:3:373:ILE:HG23 | 26:7:609:CHL:H11 | 1.83 | 0.60 |
| 26:4:609:CHL:HHC | 26:4:609:CHL:HBB1 | 1.84 | 0.60 |
| 23:9:276:ASP:HB3 | 23:9:279:ARG:HB2 | 1.84 | 0.60 |
| 1:A:689:GLY:HA3 | 2:B:570:ASP:HB2 | 1.83 | 0.59 |
| 26:1:609:CHL:HMD1 | 21:8:154:PHE:HE1 | 1.66 | 0.59 |
| 26:9:603:CHL:H142 | 30:9:801:LHG:H281 | 1.83 | 0.59 |
| 2:B:107:ARG:NH2 | 2:B:114:VAL:O | 2.35 | 0.59 |
| 25:A:1131:CLA:H51 | 29:B:4007:BCR:H372 | 1.84 | 0.59 |
| 2:B:87:PRO:HB2 | 2:B:117:SER:HB3 | 1.83 | 0.59 |
| 2:B:423:LEU:HD13 | 2:B:533:LEU:HA | 1.82 | 0.59 |
| 2:B:692:VAL:HG11 | 25:B:1237:CLA:HAB | 1.84 | 0.59 |
| 15:1:125:THR:O | 15:1:129:ILE:HG13 | 2.02 | 0.59 |
| 21:8:143:LYS:HE3 | 36:8:803:DGD:HD3 | 1.83 | 0.59 |
| 25:A:1118:CLA:HBA1 | 10:K:91:VAL:HG23 | 1.84 | 0.59 |
| 8:H:83:ARG:HG3 | 11:L:388:LEU:HD21 | 1.83 | 0.59 |
| 26:3:604:CHL:H2 | 26:3:604:CHL:O1A | 2.01 | 0.59 |
| 30:4:801:LHG:HC91 | 30:4:801:LHG:H271 | 1.85 | 0.59 |
| 25:7:603:CLA:H2 | 25:7:608:CLA:HMD1 | 1.83 | 0.59 |
| 43:9:501:LUT:H32 | 26:9:601:CHL:HAB | 1.85 | 0.59 |
| 14:O:69:ILE:HD11 | 14:O:79:LEU:HD13 | 1.85 | 0.59 |
| 26:7:615:CHL:HHC | 26:7:615:CHL:HBB1 | 1.84 | 0.59 |
| 1:A:305:PHE:HE1 | 25:A:1119:CLA:HAB | 1.66 | 0.59 |
| 8:H:106:ALA:HA | 8:H:113:VAL:HG21 | 1.82 | 0.59 |
| 18:5:62:ASN:HB3 | 18:5:65:MET:HB2 | 1.85 | 0.59 |
| 18:5:147:ASN:ND2 | 18:5:159:ASN:OD1 | 2.32 | 0.59 |
| 26:6:617:CHL:HHC | 26:6:617:CHL:HBB1 | 1.85 | 0.59 |
| 1:A:392:THR:HG23 | 1:A:607:ILE:HG21 | 1.85 | 0.59 |
| 2:B:168:TRP:CZ2 | 25:B:1208:CLA:HMA1 | 2.38 | 0.59 |
| 22:2:30:ARG:NH1 | 22:2:44:ASP:O | 2.35 | 0.59 |
| 22:2:79:TRP:CZ2 | 43:2:507:LUT:H7 | 2.38 | 0.59 |
| 15:1:92:GLU:OE2 | 15:1:197:SER:OG | 2.19 | 0.59 |
| 25:1:606:CLA:HMB1 | 25:1:606:CLA:HBB1 | 1.85 | 0.59 |
| 43:9:502:LUT:H32 | 25:9:604:CLA:CAB | 2.33 | 0.59 |
| 25:B:1236:CLA:HED2 | 25:B:1236:CLA:H2A | 1.84 | 0.58 |
| 8:H:43:ASP:H | 8:H:50:THR:HG21 | 1.68 | 0.58 |
| 26:1:611:CHL:HHC | 26:1:611:CHL:HBB1 | 1.86 | 0.58 |
| 29:3:503:BCR:H383 | 25:3:606:CLA:HAB | 1.85 | 0.58 |
| 26:2:610:CHL:HHC | 26:2:610:CHL:HBB1 | 1.86 | 0.58 |
| 2:B:273:ASP:HB3 | 25:B:1214:CLA:HMA1 | 1.85 | 0.58 |
| 19:6:133:GLU:OE1 | 19:6:136:ARG:NH1 | 2.35 | 0.58 |
| 26:9:613:CHL:HHC | 26:9:613:CHL:HBB1 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:114:SER:HB2 | 1:A:131:VAL:HG11 | 1.85 | 0.58 |
| 1:A:349:TRP:HB3 | 25:A:1103:CLA:HAC1 | 1.85 | 0.58 |
| 10:K:38:ASN:HD21 | 25:K:1401:CLA:HED2 | 1.68 | 0.58 |
| 25:K:1401:CLA:HBB1 | 29:K:4002:BCR:H10C | 1.85 | 0.58 |
| 15:1:178:ARG:HB3 | 26:1:604:CHL:HBC3 | 1.85 | 0.58 |
| 26:6:611:CHL:HHC | 26:6:611:CHL:HBB1 | 1.86 | 0.58 |
| 1:A:566:LYS:NZ | 2:B:674:GLU:OE2 | 2.37 | 0.58 |
| 25:B:1224:CLA:H161 | 36:B:5003:DGD:HAG2 | 1.86 | 0.58 |
| 16:3:292:CYS:SG | 26:3:604:CHL:HAA2 | 2.43 | 0.58 |
| 4:D:229:GLU:HA | 4:D:242:MET:O | 2.04 | 0.58 |
| 19:6:90:VAL:HG11 | 43:6:501:LUT:H12 | 1.84 | 0.58 |
| 2:B:6:PHE:O | 2:B:8:LYS:N | 2.36 | 0.58 |
| 2:B:620:TRP:HB3 | 25:B:1021:CLA:H101 | 1.86 | 0.58 |
| 7:G:1307:HIS:NE2 | 29:G:4001:BCR:H352 | 2.19 | 0.58 |
| 15:1:39:GLY:HA3 | 21:8:147:SER:HB3 | 1.85 | 0.58 |
| 16:3:383:TRP:CD1 | 25:3:612:CLA:HMA2 | 2.38 | 0.58 |
| 26:7:617:CHL:HHC | 26:7:617:CHL:HBB1 | 1.86 | 0.58 |
| 36:8:802:DGD:HBT1 | 25:8:607:CLA:C1C | 2.34 | 0.58 |
| 26:9:608:CHL:HHC | 26:9:608:CHL:HBB1 | 1.85 | 0.58 |
| 26:9:610:CHL:HHC | 26:9:610:CHL:HBB1 | 1.86 | 0.58 |
| 25:A:1106:CLA:H101 | 29:J:4001:BCR:H10C | 1.86 | 0.58 |
| 25:A:1140:CLA:HMC2 | 29:B:4006:BCR:H381 | 1.85 | 0.58 |
| 2:B:151:LEU:HD22 | 12:M:22:ALA:HA | 1.85 | 0.58 |
| 25:B:1237:CLA:H72 | 25:B:1238:CLA:H43 | 1.86 | 0.58 |
| 19:6:78:SER:HB2 | 25:6:612:CLA:HED2 | 1.85 | 0.58 |
| 26:8:610:CHL:HBB1 | 26:8:610:CHL:HHC | 1.86 | 0.58 |
| 2:B:412:ILE:HA | 2:B:415:HIS:CE1 | 2.38 | 0.58 |
| 1:A:121:ILE:HG23 | 1:A:122:VAL:HG22 | 1.84 | 0.57 |
| 22:2:193:HIS:CG | 25:2:603:CLA:HAA1 | 2.39 | 0.57 |
| 25:A:1118:CLA:HMB2 | 10:K:94:LEU:HD22 | 1.86 | 0.57 |
| 30:A:5002:LHG:H161 | 25:A:1101:CLA:HMB2 | 1.86 | 0.57 |
| 11:L:318:SER:HB3 | 11:L:321:ILE:HB | 1.85 | 0.57 |
| 18:5:132:VAL:HG11 | 29:5:503:BCR:H16C | 1.85 | 0.57 |
| 22:2:126:GLU:HG3 | 25:2:612:CLA:C1B | 2.34 | 0.57 |
| 25:A:1129:CLA:HBB2 | 25:A:1137:CLA:HMC2 | 1.86 | 0.57 |
| 2:B:60:LEU:HD12 | 42:M:4001:ECH:H37A | 1.84 | 0.57 |
| 25:B:1223:CLA:H122 | 29:B:4004:BCR:H373 | 1.86 | 0.57 |
| 15:1:134:MET:HG3 | 25:1:612:CLA:HMC3 | 1.85 | 0.57 |
| 1:A:95:GLY:O | 1:A:99:SER:OG | 2.22 | 0.57 |
| 25:A:1130:CLA:HBA1 | 2:B:687:PRO:HD3 | 1.86 | 0.57 |
| 25:A:1138:CLA:HMC1 | 25:A:1101:CLA:H41 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 43:1:503:LUT:H10 | 26:1:613:CHL:HBA1 | 1.85 | 0.57 |
| 2:B:549:PRO:HB3 | 6:F:481:PRO:HG2 | 1.87 | 0.57 |
| 17:4:230:SER:HB2 | 17:4:231:PRO:HD3 | 1.85 | 0.57 |
| 26:2:609:CHL:HBC3 | 30:2:801:LHG:HC5 | 1.85 | 0.57 |
| 30:2:802:LHG:H291 | 30:2:802:LHG:H192 | 1.87 | 0.57 |
| 1:A:305:PHE:CE1 | 25:A:1119:CLA:HAB | 2.39 | 0.57 |
| 15:1:119:VAL:HG11 | 26:1:613:CHL:HMD1 | 1.86 | 0.57 |
| 23:9:245:ARG:NH1 | 23:9:265:ASP:OD1 | 2.37 | 0.57 |
| 18:5:125:GLU:HA | 26:5:613:CHL:HMA3 | 1.86 | 0.57 |
| 19:6:170:ALA:HB2 | 25:6:601:CLA:HBD | 1.86 | 0.57 |
| 1:A:343:GLU:O | 1:A:347:THR:OG1 | 2.20 | 0.57 |
| 1:A:435:ASP:OD2 | 1:A:561:ARG:NH1 | 2.36 | 0.57 |
| 25:A:1105:CLA:HMA1 | 25:A:1106:CLA:HMB3 | 1.87 | 0.57 |
| 25:B:1224:CLA:HBC3 | 36:B:5003:DGD:HBG3 | 1.86 | 0.57 |
| 22:2:81:MET:HB2 | 25:2:601:CLA:HMC3 | 1.86 | 0.57 |
| 23:9:249:LEU:HD12 | 23:9:250:PRO:HD2 | 1.85 | 0.57 |
| 25:H:1701:CLA:CBB | 29:L:4003:BCR:H10C | 2.34 | 0.57 |
| 23:9:378:GLY:O | 23:9:382:MET:HG3 | 2.04 | 0.57 |
| 2:B:429:PHE:CE1 | 25:B:1235:CLA:HAB | 2.40 | 0.57 |
| 17:4:215:HIS:CG | 25:4:603:CLA:HAA2 | 2.39 | 0.57 |
| 29:5:503:BCR:H272 | 47:5:804:PLM:HE1 | 1.87 | 0.57 |
| 26:8:613:CHL:HHC | 26:8:613:CHL:HBB1 | 1.86 | 0.57 |
| 25:A:1106:CLA:HHC | 25:A:1106:CLA:HBB1 | 1.87 | 0.56 |
| 43:7:501:LUT:H30 | 25:7:601:CLA:H72 | 1.86 | 0.56 |
| 1:A:453:PHE:HE1 | 25:B:1022:CLA:HMA1 | 1.70 | 0.56 |
| 25:A:1140:CLA:HHC | 25:A:1140:CLA:HBB1 | 1.87 | 0.56 |
| 34:A:5007:3PH:H2A2 | 34:A:5007:3PH:H372 | 1.86 | 0.56 |
| 54:A:6020:HOH:O | 2:B:622:ARG:NH1 | 2.38 | 0.56 |
| 2:B:304:GLU:HG3 | 7:G:1261:ALA:HA | 1.87 | 0.56 |
| 15:1:51:ALA:HB2 | 15:1:171:THR:HA | 1.86 | 0.56 |
| 21:8:205:PHE:CD2 | 43:8:502:LUT:H12 | 2.40 | 0.56 |
| 25:A:1113:CLA:HBA2 | 16:3:485:ILE:HD13 | 1.87 | 0.56 |
| 16:3:416:GLN:NE2 | 18:5:55:ASP:O | 2.36 | 0.56 |
| 19:6:132:VAL:HG11 | 29:6:503:BCR:H16C | 1.86 | 0.56 |
| 26:9:610:CHL:HHB | 41:9:804:SPH:H152 | 1.86 | 0.56 |
| 2:B:352:HIS:ND1 | 25:B:1214:CLA:OBD | 2.37 | 0.56 |
| 25:B:1231:CLA:H2 | 25:B:1232:CLA:HMB2 | 1.88 | 0.56 |
| 22:2:165:GLY:O | 22:2:169:MET:HG3 | 2.05 | 0.56 |
| 2:B:524:ILE:HG21 | 25:B:1234:CLA:HAB | 1.87 | 0.56 |
| 25:1:612:CLA:H203 | 30:1:802:LHG:H321 | 1.88 | 0.56 |
| 16:3:446:ILE:HG22 | 26:3:603:CHL:HBB1 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:5:56:PRO:HD2 | 43:5:502:LUT:H23 | 1.87 | 0.56 |
| 44:7:504:AXT:H393 | 30:7:803:LHG:H131 | 1.86 | 0.56 |
| 1:A:375:PRO:HG3 | 1:A:381:ALA:HB2 | 1.88 | 0.56 |
| 2:B:371:ALA:HB1 | 25:B:1224:CLA:HMA1 | 1.88 | 0.56 |
| 48:2:803:DGA:HBW1 | 48:2:803:DGA:HAF2 | 1.87 | 0.56 |
| 1:A:453:PHE:CE1 | 25:B:1022:CLA:HMA1 | 2.41 | 0.56 |
| 1:A:746:ARG:O | 1:A:750:VAL:HG22 | 2.06 | 0.56 |
| 17:4:164:PRO:HD3 | 25:4:611:CLA:HMD2 | 1.87 | 0.56 |
| 2:B:657:ILE:HG12 | 25:B:1239:CLA:HMB3 | 1.87 | 0.56 |
| 25:B:1216:CLA:HMB2 | 25:B:1221:CLA:HMA3 | 1.86 | 0.56 |
| 25:B:1236:CLA:H43 | 29:B:4005:BCR:H10C | 1.87 | 0.56 |
| 18:5:236:VAL:O | 18:5:257:GLN:NE2 | 2.39 | 0.56 |
| 1:A:680:ALA:HB3 | 25:A:1013:CLA:HBB2 | 1.88 | 0.56 |
| 10:K:58:PRO:HG2 | 29:K:4001:BCR:H291 | 1.87 | 0.56 |
| 25:5:603:CLA:HBC3 | 30:5:801:LHG:H372 | 1.88 | 0.56 |
| 26:2:613:CHL:HHC | 26:2:613:CHL:HBB1 | 1.88 | 0.56 |
| 1:A:356:ASN:ND2 | 25:A:1103:CLA:OBD | 2.26 | 0.56 |
| 25:A:1012:CLA:HAB | 2:B:583:TRP:HH2 | 1.70 | 0.56 |
| 15:1:193:ALA:HB2 | 25:1:615:CLA:HED3 | 1.88 | 0.56 |
| 20:7:59:MET:SD | 25:7:601:CLA:HAB | 2.46 | 0.56 |
| 25:A:1113:CLA:H42 | 29:3:505:BCR:H10C | 1.86 | 0.55 |
| 11:L:405:LYS:HG2 | 11:L:411:SER:HA | 1.89 | 0.55 |
| 1:A:448:LEU:HB3 | 1:A:541:PHE:HB2 | 1.87 | 0.55 |
| 26:A:1114:CHL:HHC | 26:A:1114:CHL:HBB1 | 1.87 | 0.55 |
| 21:8:137:LYS:HD3 | 25:8:611:CLA:HMC3 | 1.88 | 0.55 |
| 1:A:325:ILE:O | 1:A:329:HIS:ND1 | 2.38 | 0.55 |
| 1:A:474:ASP:OD1 | 1:A:480:GLN:NE2 | 2.39 | 0.55 |
| 25:A:1127:CLA:H2 | 29:A:4002:BCR:HC7 | 1.88 | 0.55 |
| 17:4:130:PHE:CG | 25:4:612:CLA:HMC3 | 2.40 | 0.55 |
| 20:7:105:ILE:HG23 | 25:7:612:CLA:HBB2 | 1.88 | 0.55 |
| 43:8:501:LUT:H34 | 26:8:601:CHL:CBB | 2.36 | 0.55 |
| 25:B:1219:CLA:HMB3 | 25:B:1240:CLA:C1D | 2.36 | 0.55 |
| 2:B:390:HIS:HA | 2:B:393:ILE:HD12 | 1.88 | 0.55 |
| 15:1:197:SER:OG | 15:1:200:GLU:HG3 | 2.06 | 0.55 |
| 15:1:99:TRP:HB2 | 44:1:502:AXT:H3 | 1.87 | 0.55 |
| 23:9:354:PHE:HD1 | 50:9:504:XAT:H242 | 1.72 | 0.55 |
| 1:A:484:ALA:HA | 25:A:1135:CLA:HBA1 | 1.89 | 0.55 |
| 1:A:533:PHE:HA | 25:A:1136:CLA:HED1 | 1.89 | 0.55 |
| 25:A:1107:CLA:HMB1 | 25:A:1107:CLA:HBB1 | 1.87 | 0.55 |
| 12:M:12:LEU:HB3 | 25:2:615:CLA:HBB2 | 1.88 | 0.55 |
| 26:4:618:CHL:HBB1 | 26:4:618:CHL:HHC | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:L:363:ARG:HA | 11:L:368:VAL:HG21 | 1.88 | 0.55 |
| 29:4:503:BCR:H24C | 26:4:613:CHL:HAA1 | 1.89 | 0.55 |
| 18:5:138:GLN:OE1 | 18:5:141:ARG:NH1 | 2.38 | 0.55 |
| 22:2:81:MET:HB3 | 50:2:501:XAT:C35 | 2.37 | 0.55 |
| 18:5:45:ASP:OD1 | 18:5:46:GLY:N | 2.40 | 0.55 |
| 25:7:612:CLA:HBC2 | 26:7:613:CHL:HMB1 | 1.87 | 0.55 |
| 1:A:584:CYS:N | 2:B:669:ARG:O | 2.40 | 0.54 |
| 25:A:1128:CLA:HBB1 | 25:A:1128:CLA:HMB1 | 1.88 | 0.54 |
| 8:H:88:GLY:HA3 | 32:H:5001:SQD:H262 | 1.88 | 0.54 |
| 1:A:322:LEU:HD13 | 25:A:1123:CLA:HAC2 | 1.90 | 0.54 |
| 1:A:396:TRP:HB3 | 25:A:1126:CLA:HMC3 | 1.89 | 0.54 |
| 2:B:388:PHE:CZ | 25:B:1222:CLA:HAB | 2.42 | 0.54 |
| 16:3:380:LEU:HD13 | 26:7:609:CHL:HMA2 | 1.89 | 0.54 |
| 43:4:502:LUT:H30 | 25:4:604:CLA:H72 | 1.88 | 0.54 |
| 25:A:1119:CLA:HMB2 | 25:A:1123:CLA:HMA3 | 1.88 | 0.54 |
| 25:2:605:CLA:HBC1 | 26:2:610:CHL:HAB | 1.88 | 0.54 |
| 1:A:265:PHE:HA | 25:K:1401:CLA:HBC3 | 1.88 | 0.54 |
| 30:B:5001:LHG:H242 | 15:1:60:LEU:HD21 | 1.89 | 0.54 |
| 26:1:609:CHL:HHC | 26:1:609:CHL:HBB1 | 1.89 | 0.54 |
| 26:3:604:CHL:H162 | 25:3:605:CLA:HBB1 | 1.89 | 0.54 |
| 43:4:502:LUT:H372 | 26:7:617:CHL:H152 | 1.90 | 0.54 |
| 29:7:503:BCR:C21 | 26:7:613:CHL:H2 | 2.35 | 0.54 |
| 25:2:604:CLA:H3A | 25:2:604:CLA:CGA | 2.38 | 0.54 |
| 26:7:611:CHL:HHC | 26:7:611:CHL:HBB1 | 1.88 | 0.54 |
| 2:B:126:TYR:O | 2:B:131:ARG:NH1 | 2.38 | 0.54 |
| 2:B:659:ALA:C | 25:B:1023:CLA:HAB | 2.28 | 0.54 |
| 8:H:90:VAL:HG11 | 11:L:385:THR:HB | 1.89 | 0.54 |
| 26:1:611:CHL:HBA1 | 45:1:803:OLA:H162 | 1.90 | 0.54 |
| 16:3:291:LEU:HD13 | 26:3:604:CHL:H42 | 1.89 | 0.54 |
| 18:5:197:PHE:CE1 | 43:5:502:LUT:H10 | 2.43 | 0.54 |
| 25:B:1209:CLA:HMC1 | 29:B:4002:BCR:H10C | 1.88 | 0.54 |
| 25:B:1240:CLA:HED2 | 25:B:1240:CLA:H2A | 1.90 | 0.54 |
| 26:3:603:CHL:H41 | 26:3:603:CHL:H72 | 1.89 | 0.54 |
| 21:8:203:VAL:HG12 | 26:8:603:CHL:HBB1 | 1.89 | 0.54 |
| 1:A:75:SER:OG | 1:A:181:TYR:HB2 | 2.08 | 0.54 |
| 17:4:203:ALA:HB2 | 25:4:615:CLA:HED3 | 1.90 | 0.54 |
| 43:2:502:LUT:H12 | 25:2:604:CLA:CAB | 2.38 | 0.54 |
| 25:1:605:CLA:H141 | 25:1:605:CLA:H202 | 1.89 | 0.54 |
| 26:7:609:CHL:HBB1 | 26:7:609:CHL:HHC | 1.89 | 0.54 |
| 2:B:520:VAL:HG21 | 2:B:594:TYR:HB2 | 1.90 | 0.54 |
| 8:H:86:ILE:HG23 | 11:L:388:LEU:HD22 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:A:1119:CLA:H41 | 29:A:4004:BCR:H16C | 1.90 | 0.53 |
| 25:A:1138:CLA:H2 | 25:B:1229:CLA:H42 | 1.89 | 0.53 |
| 25:H:1701:CLA:HMB2 | 25:L:1501:CLA:HAA2 | 1.90 | 0.53 |
| 29:4:503:BCR:H271 | 25:4:606:CLA:NB | 2.22 | 0.53 |
| 21:8:144:LYS:HB3 | 21:8:147:SER:OG | 2.08 | 0.53 |
| 25:B:1021:CLA:HMB3 | 25:B:1022:CLA:CAD | 2.38 | 0.53 |
| 25:B:1240:CLA:HMA1 | 30:B:5001:LHG:HC91 | 1.91 | 0.53 |
| 25:9:605:CLA:HMA2 | 25:9:605:CLA:H2 | 1.90 | 0.53 |
| 25:A:1106:CLA:HBB2 | 25:A:1126:CLA:H202 | 1.89 | 0.53 |
| 15:1:169:LEU:HB3 | 25:1:601:CLA:HMA1 | 1.90 | 0.53 |
| 18:5:190:GLY:O | 18:5:194:MET:HG3 | 2.08 | 0.53 |
| 19:6:233:PRO:HA | 47:6:804:PLM:H71 | 1.90 | 0.53 |
| 43:8:501:LUT:H32 | 26:8:601:CHL:CBB | 2.39 | 0.53 |
| 20:7:116:LEU:HD13 | 25:7:612:CLA:HMA2 | 1.91 | 0.53 |
| 21:8:226:HIS:CG | 26:8:603:CHL:HAA2 | 2.43 | 0.53 |
| 22:2:105:VAL:HG13 | 43:2:507:LUT:H383 | 1.90 | 0.53 |
| 1:A:250:MET:HG3 | 1:A:257:PHE:HD2 | 1.74 | 0.53 |
| 12:M:3:ILE:O | 13:I:2:SER:OG | 2.19 | 0.53 |
| 43:5:505:LUT:H371 | 43:5:505:LUT:H28 | 1.90 | 0.53 |
| 2:B:340:ALA:HB2 | 29:B:4005:BCR:H372 | 1.91 | 0.53 |
| 25:B:1021:CLA:HMB3 | 25:B:1022:CLA:OBD | 2.08 | 0.53 |
| 4:D:231:ILE:HG12 | 4:D:241:ILE:HG12 | 1.89 | 0.53 |
| 16:3:314:CYS:HB3 | 16:3:441:GLY:HA3 | 1.91 | 0.53 |
| 1:A:598:TRP:HE1 | 25:B:1023:CLA:C1D | 2.21 | 0.53 |
| 25:A:1130:CLA:H72 | 25:L:1502:CLA:H12 | 1.89 | 0.53 |
| 2:B:341:SER:O | 2:B:345:ILE:HG12 | 2.08 | 0.53 |
| 25:G:1601:CLA:C1B | 29:G:4001:BCR:H353 | 2.39 | 0.53 |
| 16:3:381:LYS:HD3 | 26:3:611:CHL:CBB | 2.39 | 0.53 |
| 25:B:1212:CLA:C1B | 29:B:4001:BCR:H271 | 2.39 | 0.53 |
| 30:B:5001:LHG:H342 | 47:8:807:PLM:HF1 | 1.90 | 0.53 |
| 15:1:210:MET:CE | 25:1:608:CLA:HMA1 | 2.39 | 0.53 |
| 25:1:608:CLA:H11 | 26:1:609:CHL:H42 | 1.91 | 0.53 |
| 17:4:56:PRO:HB2 | 26:7:617:CHL:H42 | 1.91 | 0.53 |
| 26:4:613:CHL:HHC | 26:4:613:CHL:HBB1 | 1.90 | 0.53 |
| 18:5:130:HIS:ND1 | 26:6:609:CHL:O1A | 2.42 | 0.53 |
| 18:5:137:TRP:CE2 | 18:5:141:ARG:HD2 | 2.43 | 0.53 |
| 22:2:180:ALA:HB2 | 35:2:804:LMT:H32 | 1.90 | 0.53 |
| 2:B:286:ILE:HG23 | 2:B:290:HIS:HE1 | 1.74 | 0.53 |
| 19:6:164:TYR:HB3 | 25:6:601:CLA:HED3 | 1.90 | 0.53 |
| 37:6:803:PCW:H19 | 25:7:602:CLA:HMC3 | 1.90 | 0.53 |
| 3:C:27:GLU:OE2 | 3:C:43:PRO:HG3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:263:GLN:O | 4:D:267:LYS:HB2 | 2.09 | 0.53 |
| 6:F:453:GLU:OE2 | 21:8:58:ASN:ND2 | 2.41 | 0.53 |
| 25:B:1230:CLA:HMA1 | 33:B:5005:PTY:H161 | 1.90 | 0.52 |
| 15:1:57:PRO:HG3 | 47:8:807:PLM:H81 | 1.91 | 0.52 |
| 22:2:58:LEU:HD12 | 25:2:604:CLA:H12 | 1.91 | 0.52 |
| 1:A:430:VAL:HA | 1:A:433:HIS:CE1 | 2.44 | 0.52 |
| 26:A:1114:CHL:HMD2 | 16:3:353:PRO:HG3 | 1.91 | 0.52 |
| 2:B:70:ALA:HB2 | 2:B:136:LEU:HB2 | 1.91 | 0.52 |
| 2:B:460:PHE:HB3 | 25:B:1234:CLA:H11 | 1.91 | 0.52 |
| 8:H:100:TRP:O | 8:H:105:ALA:N | 2.31 | 0.52 |
| 43:1:503:LUT:H203 | 26:1:611:CHL:HMA1 | 1.92 | 0.52 |
| 19:6:180:LEU:HB3 | 25:6:601:CLA:HMA1 | 1.92 | 0.52 |
| 19:6:195:PHE:CD2 | 43:6:502:LUT:H12 | 2.44 | 0.52 |
| 19:6:265:PRO:HD2 | 25:6:615:CLA:HED2 | 1.90 | 0.52 |
| 20:7:101:LEU:HD21 | 25:7:610:CLA:H141 | 1.90 | 0.52 |
| 26:7:613:CHL:HHC | 26:7:613:CHL:HBB1 | 1.90 | 0.52 |
| 1:A:610:PHE:O | 1:A:614:MET:HG2 | 2.09 | 0.52 |
| 2:B:659:ALA:HB3 | 25:B:1023:CLA:HBB2 | 1.92 | 0.52 |
| 7:G:1288:THR:HG21 | 7:G:1295:THR:HA | 1.91 | 0.52 |
| 11:L:447:ILE:HG22 | 11:L:448:LEU:H | 1.75 | 0.52 |
| 42:M:4001:ECH:H8 | 25:2:615:CLA:CBB | 2.38 | 0.52 |
| 29:5:503:BCR:H282 | 47:5:804:PLM:HC1 | 1.91 | 0.52 |
| 32:G:5001:SQD:H81 | 32:G:5001:SQD:H242 | 1.90 | 0.52 |
| 15:1:126:LEU:HD11 | 26:1:613:CHL:HMD3 | 1.90 | 0.52 |
| 15:1:214:PHE:CE1 | 25:1:608:CLA:HED2 | 2.45 | 0.52 |
| 17:4:132:TRP:CD1 | 29:4:503:BCR:H14C | 2.45 | 0.52 |
| 18:5:84:VAL:HG11 | 43:5:501:LUT:H12 | 1.91 | 0.52 |
| 25:6:605:CLA:HMD3 | 25:6:615:CLA:H172 | 1.92 | 0.52 |
| 30:2:802:LHG:H222 | 30:2:802:LHG:H302 | 1.92 | 0.52 |
| 1:A:178:TRP:HB2 | 25:A:1109:CLA:HMC3 | 1.92 | 0.52 |
| 25:A:1109:CLA:CHA | 25:A:1109:CLA:HBA1 | 2.39 | 0.52 |
| 26:A:1114:CHL:HBC2 | 25:3:610:CLA:HAB | 1.91 | 0.52 |
| 25:A:1139:CLA:C4C | 27:A:2001:PQN:H262 | 2.40 | 0.52 |
| 25:B:1229:CLA:HBB1 | 29:B:4006:BCR:H323 | 1.90 | 0.52 |
| 29:L:4001:BCR:H14C | 13:I:27:PHE:HB2 | 1.90 | 0.52 |
| 17:4:194:PHE:CE1 | 43:4:502:LUT:H10 | 2.44 | 0.52 |
| 18:5:161:GLU:HG3 | 18:5:164:TYR:HD2 | 1.74 | 0.52 |
| 21:8:227:LEU:HD11 | 25:8:608:CLA:HMC3 | 1.90 | 0.52 |
| 25:A:1137:CLA:HBB1 | 25:A:1137:CLA:HHC | 1.91 | 0.52 |
| 4:D:277:VAL:HG22 | 4:D:283:VAL:HG22 | 1.90 | 0.52 |
| 25:G:1603:CLA:HHC | 25:G:1603:CLA:HBB1 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:1:37:LEU:HD23 | 15:1:40:SER:HB3 | 1.91 | 0.52 |
| 15:1:141:ARG:HA | 26:1:611:CHL:HBC2 | 1.92 | 0.52 |
| 15:1:157:ASP:OD1 | 25:1:601:CLA:HBA2 | 2.10 | 0.52 |
| 26:9:601:CHL:H92 | 25:9:602:CLA:HMA1 | 1.91 | 0.52 |
| 1:A:580:ARG:NH1 | 4:D:255:GLU:OE2 | 2.43 | 0.52 |
| 2:B:258:PHE:CD1 | 25:B:1214:CLA:HMB2 | 2.44 | 0.52 |
| 25:B:1202:CLA:H2 | 25:B:1202:CLA:HAA2 | 1.92 | 0.52 |
| 25:B:1211:CLA:HMB1 | 25:B:1211:CLA:HBB1 | 1.91 | 0.52 |
| 26:3:611:CHL:HHC | 26:3:611:CHL:HBB1 | 1.92 | 0.52 |
| 29:5:503:BCR:H343 | 26:5:617:CHL:HAB | 1.92 | 0.52 |
| 25:A:1117:CLA:H92 | 25:A:1127:CLA:H91 | 1.92 | 0.52 |
| 2:B:404:ASN:OD1 | 2:B:407:ASN:ND2 | 2.39 | 0.52 |
| 1:A:441:LEU:HG | 1:A:548:LEU:HB2 | 1.91 | 0.51 |
| 25:B:1201:CLA:HMB1 | 25:B:1201:CLA:HBB1 | 1.93 | 0.51 |
| 14:O:102:ASP:H | 14:O:105:TRP:HD1 | 1.56 | 0.51 |
| 25:4:616:CLA:H12 | 25:4:616:CLA:HBD | 1.92 | 0.51 |
| 25:A:1125:CLA:CED | 25:A:1133:CLA:HAB | 2.41 | 0.51 |
| 12:M:5:ASP:OD1 | 35:2:804:LMT:O3B | 2.23 | 0.51 |
| 14:O:69:ILE:HG23 | 14:O:80:PHE:HB2 | 1.92 | 0.51 |
| 25:1:605:CLA:HBC1 | 25:1:612:CLA:HAC1 | 1.92 | 0.51 |
| 18:5:174:PHE:HD2 | 25:5:601:CLA:H11 | 1.75 | 0.51 |
| 25:5:605:CLA:OBD | 25:5:612:CLA:HBA2 | 2.10 | 0.51 |
| 22:2:223:CYS:SG | 25:9:612:CLA:HMA1 | 2.50 | 0.51 |
| 25:A:1102:CLA:HAB | 25:A:1104:CLA:CAD | 2.41 | 0.51 |
| 25:B:1204:CLA:H102 | 29:I:4001:BCR:HC41 | 1.93 | 0.51 |
| 25:4:604:CLA:H71 | 25:4:605:CLA:HMA1 | 1.91 | 0.51 |
| 26:6:610:CHL:HHC | 26:6:610:CHL:HBB1 | 1.92 | 0.51 |
| 6:F:378:LEU:HD23 | 6:F:386:PRO:HB3 | 1.93 | 0.51 |
| 11:L:295:LYS:N | 14:O:133:TYR:OH | 2.35 | 0.51 |
| 43:5:505:LUT:H183 | 25:7:608:CLA:HAB | 1.92 | 0.51 |
| 2:B:646:VAL:HG21 | 25:B:1205:CLA:HAC1 | 1.92 | 0.51 |
| 18:5:222:PRO:HG3 | 25:5:608:CLA:HMB3 | 1.93 | 0.51 |
| 29:5:503:BCR:H16C | 26:5:611:CHL:HMB3 | 1.93 | 0.51 |
| 25:5:605:CLA:HMD2 | 25:5:612:CLA:C1D | 2.40 | 0.51 |
| 25:B:1236:CLA:HHC | 25:B:1236:CLA:HBB1 | 1.92 | 0.51 |
| 3:C:17:CYS:HB3 | 28:C:3003:SF4:S4 | 2.49 | 0.51 |
| 18:5:149:ASP:HB3 | 18:5:152:ASN:O | 2.11 | 0.51 |
| 18:5:152:ASN:OD1 | 18:5:154:ASN:ND2 | 2.39 | 0.51 |
| 25:6:608:CLA:H2 | 26:6:609:CHL:H122 | 1.93 | 0.51 |
| 25:A:1108:CLA:HBB1 | 25:A:1111:CLA:H112 | 1.93 | 0.51 |
| 25:A:1126:CLA:O1D | 25:A:1127:CLA:HHB | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:669:ARG:HB2 | 27:B:2002:PQN:H7 | 1.91 | 0.51 |
| 25:B:1204:CLA:H61 | 29:I:4001:BCR:HC31 | 1.92 | 0.51 |
| 26:5:618:CHL:HHC | 26:5:618:CHL:HBB1 | 1.92 | 0.51 |
| 25:B:1023:CLA:H201 | 25:B:1239:CLA:H52 | 1.92 | 0.51 |
| 25:1:607:CLA:HBB1 | 29:8:503:BCR:HC21 | 1.93 | 0.51 |
| 7:G:1294:PHE:CE2 | 7:G:1299:VAL:HG22 | 2.46 | 0.51 |
| 26:1:609:CHL:HMD1 | 21:8:154:PHE:CE1 | 2.46 | 0.51 |
| 20:7:50:ALA:HB2 | 25:7:612:CLA:HED2 | 1.91 | 0.51 |
| 1:A:320:SER:HB3 | 1:A:325:ILE:HD11 | 1.93 | 0.51 |
| 25:A:1012:CLA:HBC2 | 2:B:586:ASN:HB2 | 1.93 | 0.51 |
| 2:B:49:ALA:HB3 | 12:M:29:LEU:HD21 | 1.93 | 0.51 |
| 2:B:667:SER:HB3 | 2:B:672:TRP:HE1 | 1.76 | 0.51 |
| 25:B:1216:CLA:HED2 | 25:B:1220:CLA:HED2 | 1.92 | 0.51 |
| 18:5:202:ILE:HG22 | 25:5:603:CLA:HMD3 | 1.92 | 0.51 |
| 22:2:230:ARG:HB2 | 23:9:347:LYS:HE3 | 1.93 | 0.51 |
| 1:A:695:GLU:OE2 | 2:B:551:LYS:NZ | 2.33 | 0.50 |
| 25:A:1110:CLA:H12 | 16:3:291:LEU:HD21 | 1.91 | 0.50 |
| 2:B:374:THR:HG23 | 2:B:592:THR:HG21 | 1.93 | 0.50 |
| 25:B:1201:CLA:H12 | 25:B:1201:CLA:H121 | 1.92 | 0.50 |
| 17:4:223:HIS:HB2 | 25:4:608:CLA:HED3 | 1.93 | 0.50 |
| 25:5:603:CLA:HMA1 | 25:5:608:CLA:HBC3 | 1.93 | 0.50 |
| 22:2:166:ARG:HB3 | 25:2:604:CLA:CBC | 2.42 | 0.50 |
| 35:2:804:LMT:H22 | 48:2:803:DGA:HA72 | 1.93 | 0.50 |
| 25:B:1207:CLA:H101 | 11:L:378:ALA:HB2 | 1.92 | 0.50 |
| 26:5:611:CHL:HBB1 | 26:5:611:CHL:HHC | 1.93 | 0.50 |
| 2:B:6:PHE:HB2 | 13:I:30:ILE:HA | 1.92 | 0.50 |
| 2:B:499:LEU:HA | 2:B:502:ILE:HG22 | 1.93 | 0.50 |
| 25:B:1205:CLA:O1A | 25:B:1224:CLA:HBD | 2.11 | 0.50 |
| 20:7:59:MET:HB2 | 25:7:601:CLA:HMC3 | 1.92 | 0.50 |
| 1:A:711:PRO:HA | 6:F:426:LEU:HD11 | 1.94 | 0.50 |
| 25:A:1012:CLA:H42 | 29:A:4005:BCR:H362 | 1.94 | 0.50 |
| 25:A:1130:CLA:HMB1 | 25:B:1237:CLA:HAA2 | 1.94 | 0.50 |
| 2:B:375:HIS:HB2 | 25:B:1224:CLA:C1B | 2.41 | 0.50 |
| 8:H:66:ASN:HB3 | 8:H:69:GLN:HG2 | 1.92 | 0.50 |
| 11:L:371:ILE:O | 11:L:375:ILE:HG12 | 2.11 | 0.50 |
| 14:O:98:PRO:HD2 | 25:O:1803:CLA:HMD3 | 1.93 | 0.50 |
| 25:4:612:CLA:HMB2 | 26:4:618:CHL:C1C | 2.41 | 0.50 |
| 43:6:501:LUT:H383 | 26:6:611:CHL:H12 | 1.94 | 0.50 |
| 25:8:618:CLA:HMD3 | 53:8:810:LAP:H181 | 1.94 | 0.50 |
| 1:A:679:TRP:O | 1:A:682:SER:OG | 2.21 | 0.50 |
| 1:A:733:LEU:HD22 | 25:A:1139:CLA:HMA1 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:A:1011:CL0:H15 | 24:A:1011:CL0:H11 | 1.93 | 0.50 |
| 25:A:1113:CLA:H92 | 29:A:4001:BCR:H393 | 1.94 | 0.50 |
| 3:C:24:ASP:OD1 | 4:D:287:HIS:HA | 2.12 | 0.50 |
| 15:1:172:LYS:HG3 | 25:1:607:CLA:HED2 | 1.93 | 0.50 |
| 17:4:59:LEU:HD13 | 25:4:604:CLA:H42 | 1.93 | 0.50 |
| 25:A:1122:CLA:H92 | 29:A:4003:BCR:H15C | 1.92 | 0.50 |
| 27:A:2001:PQN:H191 | 25:A:1101:CLA:H42 | 1.93 | 0.50 |
| 2:B:84:HIS:ND1 | 8:H:125:GLY:O | 2.39 | 0.50 |
| 25:B:1201:CLA:HMA2 | 12:M:29:LEU:HD22 | 1.93 | 0.50 |
| 25:1:612:CLA:HBC1 | 26:1:613:CHL:HBB1 | 1.93 | 0.50 |
| 33:A:5006:PTY:C30 | 33:A:5006:PTY:H111 | 2.42 | 0.50 |
| 25:B:1221:CLA:HBB1 | 25:B:1221:CLA:HMB1 | 1.93 | 0.50 |
| 29:B:4002:BCR:H322 | 25:9:612:CLA:H141 | 1.93 | 0.50 |
| 4:D:228:LYS:HA | 4:D:244:GLN:HG3 | 1.94 | 0.50 |
| 6:F:397:ARG:NH2 | 25:F:1301:CLA:OBD | 2.45 | 0.50 |
| 8:H:86:ILE:HD11 | 11:L:384:LEU:HD21 | 1.92 | 0.50 |
| 25:4:605:CLA:HED2 | 25:4:605:CLA:H2A | 1.93 | 0.50 |
| 26:9:603:CHL:HHC | 26:9:603:CHL:HBB1 | 1.92 | 0.50 |
| 25:A:1013:CLA:H121 | 29:A:4005:BCR:H23C | 1.93 | 0.50 |
| 25:A:1111:CLA:H191 | 25:3:605:CLA:H51 | 1.94 | 0.50 |
| 14:O:61:LEU:HB2 | 14:O:119:LEU:HD23 | 1.94 | 0.50 |
| 14:O:69:ILE:HG21 | 14:O:111:TRP:HE1 | 1.75 | 0.50 |
| 19:6:223:THR:O | 19:6:228:LYS:NZ | 2.34 | 0.50 |
| 1:A:367:VAL:O | 1:A:371:MET:HG3 | 2.12 | 0.50 |
| 25:B:1208:CLA:HED2 | 25:B:1208:CLA:H2A | 1.94 | 0.50 |
| 30:F:5002:LHG:H281 | 45:8:809:OLA:H51 | 1.92 | 0.50 |
| 33:3:802:PTY:H352 | 48:3:803:DGA:HB21 | 1.94 | 0.50 |
| 43:6:501:LUT:H28 | 25:6:601:CLA:H43 | 1.92 | 0.50 |
| 22:2:172:PHE:CZ | 43:2:502:LUT:H30 | 2.46 | 0.50 |
| 30:F:5001:LHG:HC62 | 25:8:609:CLA:HMA1 | 1.94 | 0.49 |
| 16:3:457:MET:SD | 26:3:603:CHL:HMD1 | 2.52 | 0.49 |
| 25:2:607:CLA:C3C | 30:2:801:LHG:HC62 | 2.42 | 0.49 |
| 1:A:190:TRP:CZ2 | 25:A:1108:CLA:HMA1 | 2.47 | 0.49 |
| 25:B:1224:CLA:O1D | 25:B:1225:CLA:HMA1 | 2.12 | 0.49 |
| 17:4:179:TRP:HB3 | 25:4:601:CLA:HMA1 | 1.94 | 0.49 |
| 23:9:331:GLU:HA | 26:9:613:CHL:HMA3 | 1.93 | 0.49 |
| 25:A:1128:CLA:H101 | 25:A:1139:CLA:HAA2 | 1.93 | 0.49 |
| 2:B:429:PHE:HZ | 25:B:1235:CLA:HMC3 | 1.77 | 0.49 |
| 2:B:698:PRO:O | 3:C:81:TYR:OH | 2.21 | 0.49 |
| 25:B:1201:CLA:H18 | 25:B:1204:CLA:H203 | 1.94 | 0.49 |
| 25:F:1302:CLA:H61 | 51:7:807:4RF:H35 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:1:502:AXT:H34 | 26:1:604:CHL:CBB | 2.42 | 0.49 |
| 25:9:604:CLA:HBC2 | 25:9:609:CLA:HBB2 | 1.94 | 0.49 |
| 1:A:435:ASP:OD1 | 1:A:556:TYR:OH | 2.25 | 0.49 |
| 11:L:382:LEU:O | 11:L:385:THR:HG22 | 2.13 | 0.49 |
| 23:9:362:PRO:O | 43:9:501:LUT:O23 | 2.28 | 0.49 |
| 1:A:547:VAL:HG11 | 25:A:1137:CLA:HMB3 | 1.94 | 0.49 |
| 3:C:29:VAL:HG12 | 4:D:301:ARG:HB2 | 1.95 | 0.49 |
| 43:4:501:LUT:H361 | 43:4:501:LUT:H28 | 1.94 | 0.49 |
| 21:8:196:ARG:HD2 | 25:8:607:CLA:O1D | 2.13 | 0.49 |
| 1:A:43:PRO:HG3 | 6:F:440:ILE:HD13 | 1.93 | 0.49 |
| 1:A:247:PRO:HG2 | 16:3:487:LYS:HG3 | 1.93 | 0.49 |
| 1:A:459:ASN:HB3 | 1:A:641:THR:HG22 | 1.95 | 0.49 |
| 1:A:589:TRP:CD1 | 25:A:1128:CLA:HMD1 | 2.48 | 0.49 |
| 25:A:1129:CLA:HAB | 25:A:1137:CLA:CBB | 2.42 | 0.49 |
| 25:B:1226:CLA:HMB1 | 25:B:1226:CLA:HBB1 | 1.94 | 0.49 |
| 30:B:5001:LHG:H251 | 15:1:58:LEU:HD13 | 1.94 | 0.49 |
| 18:5:133:GLU:OE1 | 18:5:136:ARG:NH2 | 2.35 | 0.49 |
| 21:8:154:PHE:CE2 | 21:8:161:PHE:HE2 | 2.30 | 0.49 |
| 1:A:59:PHE:CD2 | 25:A:1103:CLA:HMC2 | 2.47 | 0.49 |
| 30:A:5003:LHG:H171 | 29:3:505:BCR:H19C | 1.95 | 0.49 |
| 2:B:646:VAL:HA | 25:B:1206:CLA:CBC | 2.43 | 0.49 |
| 25:B:1219:CLA:HAA2 | 35:B:5006:LMT:H1' | 1.94 | 0.49 |
| 10:K:111:LEU:HB3 | 10:K:117:LEU:HB2 | 1.95 | 0.49 |
| 25:1:603:CLA:HMA1 | 25:1:608:CLA:HBC3 | 1.94 | 0.49 |
| 21:8:230:PRO:HG3 | 25:8:608:CLA:HMB3 | 1.95 | 0.49 |
| 23:9:298:VAL:HG11 | 43:9:501:LUT:H12 | 1.95 | 0.49 |
| 43:9:502:LUT:C11 | 25:9:605:CLA:HBC3 | 2.42 | 0.49 |
| 1:A:580:ARG:HA | 3:C:77:MET:HA | 1.94 | 0.49 |
| 25:A:1117:CLA:H2 | 25:A:1127:CLA:H92 | 1.94 | 0.49 |
| 2:B:277:HIS:HB2 | 25:B:1214:CLA:C1B | 2.43 | 0.49 |
| 25:B:1224:CLA:CGA | 25:B:1224:CLA:H3A | 2.39 | 0.49 |
| 11:L:353:VAL:CG1 | 11:L:376:ASN:HD22 | 2.20 | 0.49 |
| 32:I:5001:SQD:H461 | 22:2:243:PRO:HG2 | 1.95 | 0.49 |
| 30:6:801:LHG:H341 | 41:6:806:SPH:H181 | 1.95 | 0.49 |
| 1:A:107:ASP:HB3 | 1:A:111:ILE:HD12 | 1.95 | 0.49 |
| 25:A:1119:CLA:HED2 | 25:A:1122:CLA:HED2 | 1.93 | 0.49 |
| 25:A:1130:CLA:HBB1 | 25:A:1136:CLA:H192 | 1.94 | 0.49 |
| 25:B:1231:CLA:HHC | 25:B:1231:CLA:HBB1 | 1.95 | 0.49 |
| 7:G:1238:CYS:HB2 | 7:G:1310:ALA:HB2 | 1.95 | 0.49 |
| 15:1:202:LEU:HD13 | 25:1:608:CLA:HBC2 | 1.95 | 0.49 |
| 23:9:255:PRO:HB2 | 23:9:257:HIS:CE1 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:A:1011:CL0:H13 | 25:A:1012:CLA:OBD | 2.13 | 0.49 |
| 25:B:1215:CLA:HHC | 25:B:1215:CLA:HBB1 | 1.94 | 0.49 |
| 25:B:1230:CLA:H12 | 33:B:5005:PTY:H111 | 1.95 | 0.49 |
| 19:6:250:GLN:HB2 | 29:6:504:BCR:H343 | 1.95 | 0.49 |
| 25:B:1222:CLA:H51 | 25:B:1234:CLA:H62 | 1.94 | 0.48 |
| 4:D:310:ARG:HB2 | 4:D:313:GLN:HG3 | 1.95 | 0.48 |
| 21:8:76:ASN:ND2 | 25:8:612:CLA:OBD | 2.46 | 0.48 |
| 22:2:163:LYS:HD3 | 25:2:607:CLA:O1D | 2.13 | 0.48 |
| 1:A:377:TYR:CE2 | 25:A:1127:CLA:HED2 | 2.49 | 0.48 |
| 25:1:612:CLA:HBA2 | 35:1:804:LMT:H3' | 1.95 | 0.48 |
| 44:7:504:AXT:H171 | 44:7:504:AXT:H8 | 1.95 | 0.48 |
| 22:2:166:ARG:HB3 | 25:2:604:CLA:HBC3 | 1.95 | 0.48 |
| 2:B:5:LEU:HA | 2:B:14:ALA:HB1 | 1.95 | 0.48 |
| 2:B:653:PHE:O | 2:B:657:ILE:HG13 | 2.13 | 0.48 |
| 3:C:26:LEU:HA | 3:C:41:SER:O | 2.13 | 0.48 |
| 8:H:65:TYR:OH | 11:L:343:GLU:OE1 | 2.17 | 0.48 |
| 15:1:217:ASN:ND2 | 25:1:603:CLA:OBD | 2.47 | 0.48 |
| 25:1:605:CLA:H203 | 25:1:612:CLA:H13 | 1.96 | 0.48 |
| 1:A:278:PHE:HD1 | 25:A:1116:CLA:HMB2 | 1.78 | 0.48 |
| 16:3:311:VAL:HG22 | 16:3:438:ILE:HD11 | 1.95 | 0.48 |
| 25:9:602:CLA:HBB1 | 25:9:602:CLA:HMB1 | 1.95 | 0.48 |
| 25:9:609:CLA:HMB1 | 25:9:609:CLA:HBB1 | 1.95 | 0.48 |
| 2:B:9:PHE:HB2 | 2:B:35:HIS:CG | 2.48 | 0.48 |
| 2:B:11:GLN:N | 2:B:36:ASP:OD2 | 2.39 | 0.48 |
| 25:B:1021:CLA:HHC | 25:B:1021:CLA:HBB1 | 1.94 | 0.48 |
| 5:E:45:VAL:O | 5:E:58:THR:HA | 2.14 | 0.48 |
| 8:H:34:LYS:N | 8:H:46:ASP:OD2 | 2.46 | 0.48 |
| 25:L:1503:CLA:HBA1 | 25:L:1503:CLA:H3A | 1.64 | 0.48 |
| 25:1:605:CLA:H3A | 25:1:605:CLA:HBA1 | 1.63 | 0.48 |
| 18:5:64:LYS:NZ | 36:7:806:DGD:HD3 | 2.28 | 0.48 |
| 20:7:60:THR:HG22 | 25:7:606:CLA:HAB | 1.96 | 0.48 |
| 23:9:311:LYS:HD3 | 23:9:313:PHE:CZ | 2.49 | 0.48 |
| 25:A:1105:CLA:H2 | 40:J:4002:RRX:H31 | 1.94 | 0.48 |
| 25:A:1128:CLA:H71 | 30:A:5002:LHG:H202 | 1.95 | 0.48 |
| 15:1:205:HIS:CG | 25:1:603:CLA:HAA2 | 2.49 | 0.48 |
| 25:7:610:CLA:H61 | 25:7:610:CLA:H102 | 1.48 | 0.48 |
| 26:8:601:CHL:H42 | 25:8:602:CLA:HBA1 | 1.96 | 0.48 |
| 1:A:584:CYS:HB2 | 2:B:668:TRP:HB3 | 1.96 | 0.48 |
| 25:A:1012:CLA:H172 | 25:A:1126:CLA:H152 | 1.96 | 0.48 |
| 2:B:286:ILE:HG23 | 2:B:290:HIS:CE1 | 2.48 | 0.48 |
| 2:B:317:GLY:HA3 | 2:B:411:ARG:HD2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:15:THR:HG22 | 3:C:28:MET:HG3 | 1.94 | 0.48 |
| 38:F:5003:LPX:H7A | 25:F:1301:CLA:ND | 2.28 | 0.48 |
| 32:I:5001:SQD:H82 | 25:2:621:CLA:HMA1 | 1.94 | 0.48 |
| 16:3:372:ALA:O | 16:3:376:ASN:HB2 | 2.14 | 0.48 |
| 20:7:177:ARG:HD2 | 25:7:607:CLA:O1D | 2.12 | 0.48 |
| 23:9:339:GLU:HG3 | 25:9:612:CLA:C4B | 2.44 | 0.48 |
| 1:A:363:LEU:O | 1:A:367:VAL:HG23 | 2.14 | 0.48 |
| 25:B:1219:CLA:H91 | 25:B:1219:CLA:H112 | 1.69 | 0.48 |
| 3:C:9:ASP:HB2 | 5:E:70:ARG:HD2 | 1.96 | 0.48 |
| 43:3:501:LUT:H383 | 26:3:611:CHL:H43 | 1.96 | 0.48 |
| 18:5:175:SER:O | 18:5:177:GLY:N | 2.45 | 0.48 |
| 29:6:503:BCR:H271 | 25:6:606:CLA:NB | 2.28 | 0.48 |
| 25:7:605:CLA:HMD2 | 25:7:612:CLA:C1D | 2.43 | 0.48 |
| 25:2:604:CLA:CHD | 26:2:609:CHL:HBB2 | 2.43 | 0.48 |
| 1:A:363:LEU:HD11 | 25:A:1117:CLA:H71 | 1.95 | 0.48 |
| 24:A:1011:CL0:H13 | 25:A:1012:CLA:CAD | 2.43 | 0.48 |
| 25:A:1108:CLA:H91 | 25:A:1108:CLA:H111 | 1.69 | 0.48 |
| 26:A:1114:CHL:H112 | 26:A:1114:CHL:CBB | 2.44 | 0.48 |
| 25:4:601:CLA:H41 | 25:4:601:CLA:H61 | 1.47 | 0.48 |
| 22:2:126:GLU:OE1 | 22:2:129:ARG:NH2 | 2.37 | 0.48 |
| 1:A:165:GLY:HA2 | 33:A:5006:PTY:H352 | 1.96 | 0.48 |
| 9:J:45:LEU:HD22 | 29:J:4001:BCR:H402 | 1.95 | 0.48 |
| 48:3:803:DGA:HA51 | 48:3:803:DGA:HA22 | 1.71 | 0.48 |
| 19:6:48:HIS:NE2 | 19:6:61:ASP:OD2 | 2.47 | 0.48 |
| 22:2:156:GLU:OE2 | 22:2:160:LYS:NZ | 2.30 | 0.48 |
| 1:A:479:LEU:HB2 | 1:A:530:THR:HG23 | 1.96 | 0.47 |
| 25:A:1126:CLA:H3A | 25:A:1126:CLA:HBA2 | 1.49 | 0.47 |
| 2:B:57:ILE:HD11 | 42:M:4001:ECH:H39A | 1.97 | 0.47 |
| 2:B:79:VAL:HG13 | 2:B:126:TYR:HE1 | 1.79 | 0.47 |
| 37:B:5004:PCW:H121 | 37:B:5004:PCW:H152 | 1.55 | 0.47 |
| 33:G:5002:PTY:H132 | 15:1:128:ALA:HB1 | 1.96 | 0.47 |
| 25:K:1402:CLA:H51 | 25:K:1402:CLA:H11 | 1.70 | 0.47 |
| 25:1:607:CLA:H72 | 25:1:607:CLA:H112 | 1.58 | 0.47 |
| 26:1:609:CHL:HBA2 | 25:8:618:CLA:O1D | 2.12 | 0.47 |
| 16:3:387:LYS:NZ | 33:3:802:PTY:O12 | 2.41 | 0.47 |
| 43:5:501:LUT:H30 | 25:5:601:CLA:H52 | 1.96 | 0.47 |
| 25:B:1209:CLA:C3D | 25:B:1210:CLA:HMC3 | 2.45 | 0.47 |
| 25:B:1215:CLA:HBA2 | 25:B:1215:CLA:H3A | 1.58 | 0.47 |
| 15:1:34:GLY:HA3 | 15:1:53:TYR:CD2 | 2.50 | 0.47 |
| 25:4:607:CLA:HMB1 | 19:6:151:ILE:HG23 | 1.95 | 0.47 |
| 26:5:610:CHL:HBB2 | 25:5:612:CLA:HBC1 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2:227:ALA:HB2 | 30:9:802:LHG:H262 | 1.95 | 0.47 |
| 43:9:501:LUT:H373 | 26:9:601:CHL:H42 | 1.95 | 0.47 |
| 1:A:72:LYS:NZ | 25:A:1109:CLA:OBD | 2.39 | 0.47 |
| 25:A:1116:CLA:CGA | 25:A:1116:CLA:H3A | 2.44 | 0.47 |
| 25:A:1120:CLA:HMD2 | 29:K:4001:BCR:H23C | 1.97 | 0.47 |
| 25:B:1218:CLA:H43 | 35:1:804:LMT:H12 | 1.96 | 0.47 |
| 17:4:134:GLU:HG3 | 25:4:612:CLA:NB | 2.29 | 0.47 |
| 21:8:183:SER:OG | 21:8:185:GLU:OE1 | 2.27 | 0.47 |
| 1:A:426:LEU:HD13 | 25:A:1122:CLA:C1C | 2.45 | 0.47 |
| 25:B:1232:CLA:HMC1 | 30:1:802:LHG:H201 | 1.97 | 0.47 |
| 25:3:606:CLA:H192 | 25:5:604:CLA:H202 | 1.96 | 0.47 |
| 1:A:574:PRO:HB3 | 1:A:720:ILE:HB | 1.97 | 0.47 |
| 25:A:1138:CLA:H41 | 29:B:4006:BCR:H21C | 1.96 | 0.47 |
| 25:B:1205:CLA:H121 | 25:B:1224:CLA:H193 | 1.94 | 0.47 |
| 25:B:1216:CLA:H93 | 25:B:1216:CLA:H111 | 1.75 | 0.47 |
| 25:B:1207:CLA:HBB1 | 25:B:1207:CLA:HHC | 1.96 | 0.47 |
| 15:1:46:LEU:HA | 15:1:49:LEU:HD12 | 1.97 | 0.47 |
| 25:4:610:CLA:H202 | 25:4:610:CLA:H161 | 1.71 | 0.47 |
| 18:5:141:ARG:HE | 48:5:803:DGA:HB42 | 1.79 | 0.47 |
| 1:A:438:ILE:HG13 | 1:A:556:TYR:HE2 | 1.79 | 0.47 |
| 25:L:1502:CLA:H93 | 25:L:1502:CLA:H111 | 1.78 | 0.47 |
| 14:O:61:LEU:CD2 | 14:O:122:GLY:HA3 | 2.45 | 0.47 |
| 1:A:670:LEU:HD13 | 25:A:1107:CLA:HMC1 | 1.97 | 0.47 |
| 25:A:1122:CLA:HBB1 | 25:A:1129:CLA:HBC2 | 1.96 | 0.47 |
| 25:A:1130:CLA:H61 | 25:A:1130:CLA:H41 | 1.40 | 0.47 |
| 25:A:1101:CLA:H102 | 25:A:1101:CLA:H13 | 1.65 | 0.47 |
| 25:B:1228:CLA:C1C | 39:F:4001:NEX:H35 | 2.45 | 0.47 |
| 6:F:335:LYS:HB2 | 6:F:370:PHE:CD1 | 2.50 | 0.47 |
| 7:G:1300:MET:HA | 29:G:4001:BCR:H14C | 1.97 | 0.47 |
| 14:O:69:ILE:HA | 29:O:4001:BCR:H313 | 1.97 | 0.47 |
| 16:3:260:VAL:O | 30:3:801:LHG:HC11 | 2.14 | 0.47 |
| 25:3:616:CLA:H51 | 25:5:615:CLA:HAA2 | 1.96 | 0.47 |
| 25:6:601:CLA:H91 | 25:6:601:CLA:H112 | 1.80 | 0.47 |
| 29:7:503:BCR:H10C | 25:8:609:CLA:H52 | 1.97 | 0.47 |
| 26:8:603:CHL:H62 | 26:8:603:CHL:H41 | 1.72 | 0.47 |
| 30:2:801:LHG:HC61 | 30:2:801:LHG:H102 | 1.95 | 0.47 |
| 26:9:610:CHL:CBB | 26:9:613:CHL:HBB2 | 2.44 | 0.47 |
| 1:A:29:TRP:NE1 | 25:A:1109:CLA:O1A | 2.48 | 0.47 |
| 1:A:338:HIS:HB3 | 1:A:341:LEU:HD12 | 1.96 | 0.47 |
| 25:A:1112:CLA:HBA1 | 29:A:4001:BCR:H342 | 1.97 | 0.47 |
| 2:B:181:ALA:HB2 | 2:B:289:GLY:HA3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:595:TRP:CD1 | 25:B:1234:CLA:HBC2 | 2.50 | 0.47 |
| 25:B:1227:CLA:HBC1 | 29:B:4004:BCR:H21C | 1.96 | 0.47 |
| 25:B:1207:CLA:HMA2 | 25:B:1207:CLA:H2 | 1.97 | 0.47 |
| 17:4:224:PHE:CE1 | 25:4:608:CLA:HED2 | 2.49 | 0.47 |
| 19:6:68:ASN:HB3 | 19:6:71:ARG:HB2 | 1.97 | 0.47 |
| 29:7:503:BCR:H292 | 32:7:805:SQD:H251 | 1.97 | 0.47 |
| 21:8:137:LYS:CD | 25:8:611:CLA:HMC3 | 2.45 | 0.47 |
| 48:8:804:DGA:HB42 | 48:8:804:DGA:HA41 | 1.97 | 0.47 |
| 1:A:119:TRP:O | 1:A:124:GLN:NE2 | 2.35 | 0.47 |
| 25:A:1119:CLA:HBC3 | 25:A:1125:CLA:H193 | 1.97 | 0.47 |
| 25:A:1138:CLA:HED2 | 2:B:421:SER:HB3 | 1.97 | 0.47 |
| 2:B:295:ILE:HG12 | 25:B:1209:CLA:HMA2 | 1.97 | 0.47 |
| 6:F:454:GLY:O | 6:F:457:TRP:HB3 | 2.15 | 0.47 |
| 8:H:68:LEU:HD11 | 29:H:4001:BCR:H312 | 1.96 | 0.47 |
| 26:1:610:CHL:HAB | 26:1:613:CHL:HBB2 | 1.97 | 0.47 |
| 18:5:90:GLN:NE2 | 18:5:99:TRP:HB3 | 2.30 | 0.47 |
| 21:8:131:PHE:HA | 21:8:134:VAL:HG22 | 1.97 | 0.47 |
| 43:8:502:LUT:H35 | 43:8:502:LUT:H401 | 1.80 | 0.47 |
| 25:9:605:CLA:OBD | 25:9:612:CLA:H2 | 2.15 | 0.47 |
| 1:A:223:PRO:HD3 | 1:A:250:MET:HE1 | 1.97 | 0.47 |
| 25:A:1111:CLA:H41 | 25:A:1111:CLA:H61 | 1.46 | 0.47 |
| 25:A:1117:CLA:H203 | 25:A:1125:CLA:HBA2 | 1.97 | 0.47 |
| 25:B:1238:CLA:HBB2 | 27:B:2002:PQN:H141 | 1.97 | 0.47 |
| 17:4:231:PRO:O | 17:4:233:LEU:N | 2.43 | 0.47 |
| 29:5:503:BCR:C16 | 26:5:611:CHL:HMB3 | 2.45 | 0.47 |
| 25:7:604:CLA:H162 | 25:7:604:CLA:H193 | 1.71 | 0.47 |
| 43:2:507:LUT:H201 | 43:2:507:LUT:H15 | 1.66 | 0.47 |
| 1:A:744:LEU:HD23 | 1:A:744:LEU:HA | 1.78 | 0.46 |
| 25:A:1117:CLA:HBA2 | 25:A:1117:CLA:H3A | 1.56 | 0.46 |
| 25:A:1119:CLA:HBA1 | 25:A:1123:CLA:C3B | 2.45 | 0.46 |
| 4:D:249:LEU:HD23 | 4:D:260:LEU:HD22 | 1.97 | 0.46 |
| 9:J:40:VAL:HA | 25:J:1901:CLA:HBB2 | 1.97 | 0.46 |
| 11:L:351:LEU:HD22 | 25:L:1503:CLA:HBC3 | 1.97 | 0.46 |
| 25:1:612:CLA:H91 | 25:1:612:CLA:H111 | 1.64 | 0.46 |
| 25:7:610:CLA:H121 | 25:7:610:CLA:H8 | 1.72 | 0.46 |
| 1:A:403:VAL:HG11 | 1:A:596:LEU:HG | 1.97 | 0.46 |
| 25:A:1111:CLA:HMB1 | 25:A:1111:CLA:HBB1 | 1.98 | 0.46 |
| 29:B:4005:BCR:H15C | 29:B:4005:BCR:H351 | 1.74 | 0.46 |
| 7:G:1229:ALA:HB1 | 7:G:1234:VAL:HG21 | 1.97 | 0.46 |
| 19:6:89:GLY:HA2 | 43:6:502:LUT:H181 | 1.97 | 0.46 |
| 26:7:613:CHL:HHD | 26:7:613:CHL:HBC2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:2:223:CYS:SG | 30:9:802:LHG:H272 | 2.55 | 0.46 |
| 1:A:338:HIS:CE1 | 30:A:5001:LHG:HC11 | 2.49 | 0.46 |
| 25:A:1126:CLA:O1D | 25:A:1127:CLA:HMA1 | 2.15 | 0.46 |
| 33:A:5006:PTY:H182 | 33:A:5006:PTY:H362 | 1.97 | 0.46 |
| 15:1:145:GLU:O | 15:1:149:ARG:HG3 | 2.16 | 0.46 |
| 25:1:602:CLA:HMD2 | 25:1:607:CLA:C1D | 2.45 | 0.46 |
| 25:3:606:CLA:H51 | 25:3:613:CLA:HBD | 1.96 | 0.46 |
| 25:4:612:CLA:H41 | 25:4:612:CLA:H61 | 1.49 | 0.46 |
| 19:6:114:LEU:HD12 | 26:6:613:CHL:HMD3 | 1.97 | 0.46 |
| 25:A:1124:CLA:H51 | 25:A:1135:CLA:H11 | 1.96 | 0.46 |
| 25:B:1202:CLA:HBA1 | 25:B:1202:CLA:H3A | 1.46 | 0.46 |
| 25:B:1220:CLA:HBA2 | 25:B:1220:CLA:H3A | 1.60 | 0.46 |
| 25:B:1222:CLA:O1A | 25:B:1234:CLA:HMA1 | 2.15 | 0.46 |
| 25:K:1402:CLA:HED2 | 25:K:1402:CLA:H2A | 1.97 | 0.46 |
| 16:3:257:VAL:HG12 | 16:3:264:TYR:O | 2.15 | 0.46 |
| 18:5:142:LYS:O | 18:5:145:SER:OG | 2.21 | 0.46 |
| 21:8:199:ARG:O | 21:8:203:VAL:HG23 | 2.15 | 0.46 |
| 25:8:602:CLA:H11 | 25:8:602:CLA:H51 | 1.69 | 0.46 |
| 25:A:1112:CLA:HBB1 | 25:A:1112:CLA:HMB1 | 1.98 | 0.46 |
| 25:H:1703:CLA:H61 | 25:H:1703:CLA:H41 | 1.46 | 0.46 |
| 9:J:32:VAL:O | 9:J:36:LEU:HD23 | 2.15 | 0.46 |
| 15:1:191:HIS:ND1 | 15:1:196:ALA:O | 2.49 | 0.46 |
| 18:5:41:PRO:HD2 | 18:5:44:LEU:HD12 | 1.97 | 0.46 |
| 25:7:603:CLA:H13 | 25:7:603:CLA:H171 | 1.50 | 0.46 |
| 1:A:29:TRP:HE1 | 25:A:1109:CLA:CHB | 2.28 | 0.46 |
| 1:A:128:ASN:HB3 | 1:A:136:GLN:HB3 | 1.98 | 0.46 |
| 1:A:460:ASP:OD1 | 1:A:641:THR:HB | 2.15 | 0.46 |
| 25:A:1125:CLA:H111 | 25:A:1125:CLA:H152 | 1.44 | 0.46 |
| 2:B:719:VAL:HG21 | 25:B:1224:CLA:HMC2 | 1.98 | 0.46 |
| 25:B:1201:CLA:H142 | 25:B:1201:CLA:H112 | 1.77 | 0.46 |
| 5:E:88:ASN:HB3 | 5:E:90:TYR:CE1 | 2.51 | 0.46 |
| 14:O:105:TRP:O | 14:O:109:ILE:HG13 | 2.15 | 0.46 |
| 25:3:602:CLA:HED2 | 25:3:602:CLA:H2A | 1.97 | 0.46 |
| 25:3:610:CLA:H41 | 25:3:610:CLA:H62 | 1.57 | 0.46 |
| 33:3:802:PTY:H322 | 33:3:802:PTY:H141 | 1.98 | 0.46 |
| 17:4:135:LEU:HD23 | 17:4:135:LEU:HA | 1.71 | 0.46 |
| 17:4:223:HIS:C | 17:4:225:ILE:H | 2.14 | 0.46 |
| 25:4:606:CLA:HBA2 | 25:4:616:CLA:HMB3 | 1.97 | 0.46 |
| 25:5:602:CLA:H62 | 25:5:602:CLA:H41 | 1.50 | 0.46 |
| 22:2:113:THR:O | 22:2:117:ILE:HG12 | 2.16 | 0.46 |
| 1:A:718:LEU:HD21 | 27:A:2001:PQN:H151 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:B:1214:CLA:H102 | 25:B:1214:CLA:H61 | 1.50 | 0.46 |
| 25:B:1228:CLA:HMC2 | 39:F:4001:NEX:H14 | 1.98 | 0.46 |
| 25:K:1401:CLA:HBB1 | 29:K:4002:BCR:C11 | 2.45 | 0.46 |
| 15:1:98:ASN:OD1 | 15:1:101:ASP:HB2 | 2.16 | 0.46 |
| 47:4:804:PLM:H22 | 21:8:182:SER:HB3 | 1.97 | 0.46 |
| 18:5:35:PHE:HB3 | 18:5:38:VAL:CG1 | 2.46 | 0.46 |
| 25:5:606:CLA:HBC3 | 47:5:804:PLM:HG3 | 1.97 | 0.46 |
| 44:7:504:AXT:H163 | 25:7:612:CLA:C1B | 2.46 | 0.46 |
| 22:2:240:ARG:NH2 | 22:2:243:PRO:O | 2.48 | 0.46 |
| 1:A:77:HIS:ND1 | 25:A:1111:CLA:OBD | 2.46 | 0.46 |
| 1:A:474:ASP:O | 1:A:478:GLN:NE2 | 2.48 | 0.46 |
| 1:A:687:PHE:CD1 | 2:B:665:LEU:HB3 | 2.51 | 0.46 |
| 25:A:1127:CLA:HHC | 25:A:1127:CLA:HBB1 | 1.98 | 0.46 |
| 2:B:280:ALA:HA | 25:B:1213:CLA:HMC3 | 1.96 | 0.46 |
| 26:1:609:CHL:OBD | 21:8:137:LYS:NZ | 2.46 | 0.46 |
| 25:4:601:CLA:H92 | 25:4:601:CLA:H62 | 1.76 | 0.46 |
| 18:5:124:TRP:HA | 25:6:608:CLA:O1A | 2.15 | 0.46 |
| 19:6:256:ALA:HA | 26:6:610:CHL:CGA | 2.44 | 0.46 |
| 44:7:504:AXT:HC22 | 25:7:612:CLA:H2 | 1.97 | 0.46 |
| 25:7:605:CLA:HBC1 | 25:7:610:CLA:HBB2 | 1.98 | 0.46 |
| 25:A:1121:CLA:H143 | 25:A:1121:CLA:H112 | 1.73 | 0.46 |
| 2:B:178:HIS:CG | 25:B:1210:CLA:HMC2 | 2.51 | 0.46 |
| 26:3:603:CHL:HBB1 | 26:3:603:CHL:HHC | 1.98 | 0.46 |
| 19:6:84:ARG:NH1 | 26:6:611:CHL:OBD | 2.47 | 0.46 |
| 22:2:55:PRO:HD2 | 43:2:502:LUT:H3 | 1.98 | 0.46 |
| 2:B:5:LEU:O | 2:B:5:LEU:HD23 | 2.16 | 0.46 |
| 25:B:1201:CLA:H203 | 25:B:1201:CLA:H162 | 1.68 | 0.46 |
| 25:B:1201:CLA:HMC3 | 25:B:1203:CLA:HED2 | 1.97 | 0.46 |
| 25:B:1234:CLA:H62 | 25:B:1234:CLA:H2 | 1.66 | 0.46 |
| 6:F:462:PHE:HZ | 36:8:803:DGD:HB21 | 1.80 | 0.46 |
| 25:3:601:CLA:HBA2 | 25:3:601:CLA:H3A | 1.55 | 0.46 |
| 20:7:152:GLY:O | 20:7:162:ARG:NH1 | 2.48 | 0.46 |
| 21:8:220:LEU:HD22 | 48:8:804:DGA:HBN2 | 1.98 | 0.46 |
| 50:9:507:XAT:H203 | 25:9:606:CLA:H92 | 1.97 | 0.46 |
| 25:A:1111:CLA:HMA2 | 25:A:1111:CLA:C2 | 2.47 | 0.45 |
| 25:A:1112:CLA:H62 | 29:A:4001:BCR:H343 | 1.98 | 0.45 |
| 25:A:1120:CLA:H2 | 25:K:1403:CLA:CHB | 2.45 | 0.45 |
| 2:B:518:PHE:HA | 25:B:1235:CLA:HED1 | 1.98 | 0.45 |
| 25:B:1209:CLA:H51 | 25:B:1209:CLA:NC | 2.31 | 0.45 |
| 25:B:1228:CLA:HBA2 | 25:B:1228:CLA:H3A | 1.59 | 0.45 |
| 4:D:197:ASP:O | 8:H:40:ARG:NE | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:3:606:CLA:H141 | 25:3:606:CLA:H161 | 1.69 | 0.45 |
| 25:4:604:CLA:HAC2 | 30:4:801:LHG:H252 | 1.98 | 0.45 |
| 20:7:124:SER:HB2 | 21:8:37:GLY:HA2 | 1.98 | 0.45 |
| 23:9:282:TRP:CZ2 | 25:9:612:CLA:HAA1 | 2.48 | 0.45 |
| 1:A:687:PHE:HB2 | 25:A:1013:CLA:HBC1 | 1.98 | 0.45 |
| 25:A:1126:CLA:C1C | 29:A:4005:BCR:HC22 | 2.46 | 0.45 |
| 25:A:1134:CLA:HMB1 | 29:A:4004:BCR:H282 | 1.98 | 0.45 |
| 25:B:1205:CLA:H143 | 25:B:1205:CLA:H161 | 1.70 | 0.45 |
| 25:F:1302:CLA:H61 | 25:F:1302:CLA:H2 | 1.63 | 0.45 |
| 16:3:322:ALA:HB1 | 29:3:504:BCR:H21C | 1.97 | 0.45 |
| 25:3:616:CLA:H61 | 25:3:616:CLA:H41 | 1.64 | 0.45 |
| 26:5:613:CHL:H62 | 26:5:613:CHL:H41 | 1.59 | 0.45 |
| 43:6:502:LUT:H32 | 25:6:604:CLA:CBB | 2.46 | 0.45 |
| 20:7:217:VAL:HG13 | 20:7:223:VAL:HG21 | 1.99 | 0.45 |
| 21:8:227:LEU:HD22 | 48:8:804:DGA:HA62 | 1.97 | 0.45 |
| 25:8:618:CLA:HBD | 47:8:807:PLM:HD2 | 1.97 | 0.45 |
| 24:A:1011:CL0:H41 | 24:A:1011:CL0:H49 | 1.66 | 0.45 |
| 25:A:1116:CLA:H61 | 25:A:1116:CLA:H41 | 1.75 | 0.45 |
| 32:A:5005:SQD:H301 | 32:A:5005:SQD:H272 | 1.51 | 0.45 |
| 5:E:41:ARG:HG2 | 5:E:63:SER:HA | 1.99 | 0.45 |
| 25:G:1602:CLA:H101 | 25:G:1602:CLA:H61 | 1.75 | 0.45 |
| 43:5:505:LUT:H11 | 43:5:505:LUT:H191 | 1.70 | 0.45 |
| 25:2:602:CLA:HBB1 | 25:2:607:CLA:H152 | 1.98 | 0.45 |
| 1:A:13:VAL:N | 1:A:315:ASN:OD1 | 2.48 | 0.45 |
| 25:A:1138:CLA:H203 | 25:A:1140:CLA:H52 | 1.97 | 0.45 |
| 2:B:296:PHE:CD2 | 25:B:1217:CLA:HBD | 2.52 | 0.45 |
| 25:B:1201:CLA:CHA | 25:B:1201:CLA:HBA1 | 2.47 | 0.45 |
| 25:B:1231:CLA:H122 | 25:B:1231:CLA:H162 | 1.81 | 0.45 |
| 6:F:346:LEU:HA | 6:F:359:LEU:HD13 | 1.98 | 0.45 |
| 43:4:502:LUT:H32 | 25:4:604:CLA:CAB | 2.47 | 0.45 |
| 25:6:604:CLA:H102 | 25:6:605:CLA:HMB3 | 1.99 | 0.45 |
| 1:A:196:SER:O | 1:A:200:HIS:ND1 | 2.31 | 0.45 |
| 32:A:5005:SQD:H312 | 32:A:5005:SQD:H341 | 1.72 | 0.45 |
| 2:B:271:LEU:HD23 | 2:B:274:MET:HE3 | 1.99 | 0.45 |
| 25:B:1209:CLA:HMC2 | 25:B:1209:CLA:H92 | 1.97 | 0.45 |
| 25:B:1225:CLA:H52 | 29:B:4002:BCR:H23C | 1.99 | 0.45 |
| 8:H:80:LEU:HG | 8:H:86:ILE:HD13 | 1.99 | 0.45 |
| 11:L:357:ILE:CA | 11:L:372:VAL:HG21 | 2.44 | 0.45 |
| 25:L:1502:CLA:HMB3 | 25:L:1503:CLA:HBC2 | 1.98 | 0.45 |
| 16:3:433:LEU:HB3 | 25:3:601:CLA:HMA1 | 1.98 | 0.45 |
| 19:6:173:VAL:HA | 25:6:601:CLA:O1A | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:6:178:GLU:HG2 | 19:6:179:GLU:N | 2.31 | 0.45 |
| 25:7:605:CLA:OBD | 25:7:612:CLA:HBA2 | 2.17 | 0.45 |
| 21:8:84:VAL:HG11 | 43:8:501:LUT:H12 | 1.98 | 0.45 |
| 6:F:390:ALA:HB2 | 6:F:404:VAL:HG21 | 1.98 | 0.45 |
| 25:F:1302:CLA:HBB1 | 25:F:1302:CLA:HMB1 | 1.99 | 0.45 |
| 25:L:1504:CLA:HMA2 | 25:L:1504:CLA:H2 | 1.98 | 0.45 |
| 23:9:270:PRO:HD2 | 43:9:502:LUT:H23 | 1.98 | 0.45 |
| 23:9:385:PHE:CZ | 43:9:502:LUT:H10 | 2.51 | 0.45 |
| 25:A:1103:CLA:H91 | 25:A:1103:CLA:H111 | 1.67 | 0.45 |
| 25:A:1106:CLA:H101 | 29:J:4001:BCR:C10 | 2.47 | 0.45 |
| 25:A:1112:CLA:H51 | 26:A:1114:CHL:H42 | 1.99 | 0.45 |
| 25:A:1133:CLA:HED2 | 25:A:1133:CLA:H2A | 1.98 | 0.45 |
| 2:B:441:ASN:O | 2:B:445:GLN:HG2 | 2.17 | 0.45 |
| 2:B:464:ILE:HD12 | 25:B:1234:CLA:O1A | 2.16 | 0.45 |
| 2:B:726:LEU:O | 2:B:730:THR:HG22 | 2.17 | 0.45 |
| 25:B:1220:CLA:H41 | 25:B:1220:CLA:H61 | 1.63 | 0.45 |
| 12:M:5:ASP:OD2 | 12:M:5:ASP:N | 2.49 | 0.45 |
| 12:M:24:ARG:HD2 | 30:2:802:LHG:C7 | 2.46 | 0.45 |
| 43:1:501:LUT:H35 | 43:1:501:LUT:H401 | 1.81 | 0.45 |
| 29:4:503:BCR:H24C | 26:4:613:CHL:CAA | 2.46 | 0.45 |
| 18:5:144:ASP:OD1 | 18:5:147:ASN:ND2 | 2.49 | 0.45 |
| 19:6:260:LEU:HD22 | 19:6:263:LEU:HD23 | 1.97 | 0.45 |
| 1:A:250:MET:HG3 | 1:A:257:PHE:CD2 | 2.50 | 0.45 |
| 25:A:1108:CLA:HED2 | 16:3:298:GLY:O | 2.17 | 0.45 |
| 25:B:1213:CLA:H52 | 25:B:1213:CLA:C1C | 2.46 | 0.45 |
| 3:C:30:PRO:HG3 | 4:D:299:ALA:HA | 1.97 | 0.45 |
| 25:3:601:CLA:H203 | 25:5:609:CLA:HMC3 | 1.98 | 0.45 |
| 29:5:504:BCR:H383 | 26:5:610:CHL:H52 | 1.98 | 0.45 |
| 26:5:610:CHL:HBB2 | 25:5:612:CLA:CBC | 2.46 | 0.45 |
| 29:6:504:BCR:H351 | 29:6:504:BCR:H15C | 1.60 | 0.45 |
| 25:2:621:CLA:H192 | 25:2:621:CLA:H162 | 1.71 | 0.45 |
| 1:A:300:ALA:HA | 25:A:1115:CLA:HMC3 | 1.98 | 0.45 |
| 2:B:48:PHE:CE2 | 2:B:52:PHE:HE2 | 2.35 | 0.45 |
| 2:B:632:LEU:HD22 | 2:B:725:PHE:HA | 1.98 | 0.45 |
| 25:B:1222:CLA:HAA2 | 25:B:1223:CLA:OBD | 2.16 | 0.45 |
| 25:1:612:CLA:H91 | 25:1:612:CLA:H143 | 1.97 | 0.45 |
| 25:3:605:CLA:H62 | 25:3:605:CLA:H93 | 1.71 | 0.45 |
| 17:4:39:PRO:O | 17:4:41:HIS:N | 2.46 | 0.45 |
| 33:5:802:PTY:H371 | 33:5:802:PTY:H402 | 1.72 | 0.45 |
| 21:8:123:LEU:HD21 | 26:8:613:CHL:CHD | 2.47 | 0.45 |
| 29:8:503:BCR:H402 | 25:8:606:CLA:H61 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:251:ALA:HA | 1:A:254:TYR:O | 2.17 | 0.45 |
| 1:A:326:LEU:O | 1:A:338:HIS:HB2 | 2.16 | 0.45 |
| 25:A:1124:CLA:H3A | 25:A:1124:CLA:HBA2 | 1.55 | 0.45 |
| 25:B:1212:CLA:H51 | 25:B:1212:CLA:H11 | 1.72 | 0.45 |
| 25:B:1231:CLA:H62 | 25:B:1231:CLA:H93 | 1.66 | 0.45 |
| 3:C:74:THR:HG21 | 4:D:217:GLU:OE1 | 2.17 | 0.45 |
| 29:H:4001:BCR:H351 | 29:H:4001:BCR:H15C | 1.79 | 0.45 |
| 26:1:604:CHL:HBB1 | 26:1:604:CHL:HHC | 1.99 | 0.45 |
| 25:3:601:CLA:H151 | 25:3:601:CLA:H18 | 1.74 | 0.45 |
| 17:4:152:PHE:CE2 | 25:4:617:CLA:HMA3 | 2.52 | 0.45 |
| 21:8:208:PHE:HE1 | 43:8:501:LUT:H41 | 1.81 | 0.45 |
| 26:8:603:CHL:HBB1 | 26:8:603:CHL:HHC | 1.99 | 0.45 |
| 25:8:620:CLA:HAA1 | 48:8:804:DGA:HBH1 | 1.98 | 0.45 |
| 1:A:409:ALA:HB1 | 29:A:4003:BCR:H271 | 1.99 | 0.44 |
| 1:A:473:SER:HB3 | 1:A:640:ASN:HD22 | 1.81 | 0.44 |
| 25:A:1101:CLA:H162 | 25:A:1101:CLA:H141 | 1.70 | 0.44 |
| 25:B:1236:CLA:HBA2 | 25:B:1240:CLA:H193 | 1.98 | 0.44 |
| 3:C:61:ASP:HA | 3:C:62:PHE:HA | 1.82 | 0.44 |
| 15:1:56:ASP:HA | 44:1:502:AXT:O24 | 2.16 | 0.44 |
| 25:1:606:CLA:H92 | 25:1:606:CLA:H61 | 1.80 | 0.44 |
| 16:3:309:SER:HA | 25:3:612:CLA:HED2 | 1.99 | 0.44 |
| 43:5:501:LUT:H35 | 43:5:501:LUT:H401 | 1.86 | 0.44 |
| 25:8:605:CLA:HMD2 | 25:8:612:CLA:C1D | 2.47 | 0.44 |
| 22:2:55:PRO:O | 22:2:241:PRO:HG2 | 2.17 | 0.44 |
| 26:9:603:CHL:CGA | 26:9:603:CHL:C1A | 2.95 | 0.44 |
| 1:A:541:PHE:HZ | 25:B:1022:CLA:HBB2 | 1.81 | 0.44 |
| 1:A:558:ARG:O | 1:A:567:ALA:N | 2.50 | 0.44 |
| 1:A:578:PRO:HG2 | 3:C:69:LEU:HD11 | 1.99 | 0.44 |
| 25:A:1013:CLA:H3A | 25:A:1013:CLA:CGA | 2.47 | 0.44 |
| 2:B:96:HIS:CE1 | 25:B:1206:CLA:HMB3 | 2.52 | 0.44 |
| 25:B:1229:CLA:H203 | 25:B:1235:CLA:H161 | 1.99 | 0.44 |
| 10:K:47:LEU:HB3 | 25:K:1403:CLA:HMC1 | 1.98 | 0.44 |
| 25:5:602:CLA:C1D | 25:5:607:CLA:H71 | 2.47 | 0.44 |
| 25:5:606:CLA:HMA2 | 26:5:613:CHL:HAC2 | 1.98 | 0.44 |
| 19:6:259:PHE:HB2 | 29:6:504:BCR:H282 | 1.97 | 0.44 |
| 25:7:610:CLA:CAB | 26:7:613:CHL:HBB2 | 2.48 | 0.44 |
| 25:A:1102:CLA:HMC1 | 30:A:5002:LHG:H171 | 1.99 | 0.44 |
| 25:A:1133:CLA:C2D | 25:A:1134:CLA:HAB | 2.47 | 0.44 |
| 2:B:290:HIS:CD2 | 29:B:4001:BCR:H352 | 2.53 | 0.44 |
| 8:H:75:ARG:HG3 | 25:H:1703:CLA:HED2 | 1.98 | 0.44 |
| 17:4:130:PHE:CD2 | 25:4:612:CLA:HMC3 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:4:601:CLA:H92 | 25:4:602:CLA:HMA1 | 1.99 | 0.44 |
| 25:B:1021:CLA:H121 | 25:B:1021:CLA:H161 | 1.55 | 0.44 |
| 25:B:1229:CLA:HMC3 | 33:B:5005:PTY:H211 | 1.99 | 0.44 |
| 25:1:612:CLA:HBA2 | 25:1:612:CLA:H3A | 1.52 | 0.44 |
| 20:7:55:GLY:O | 20:7:59:MET:HG3 | 2.18 | 0.44 |
| 25:8:618:CLA:HBA1 | 25:8:618:CLA:H3A | 1.71 | 0.44 |
| 22:2:160:LYS:HG3 | 25:2:607:CLA:HED2 | 1.99 | 0.44 |
| 1:A:43:PRO:HB3 | 1:A:48:TRP:CE3 | 2.53 | 0.44 |
| 25:A:1105:CLA:H8 | 32:A:5005:SQD:H132 | 1.99 | 0.44 |
| 25:A:1122:CLA:H42 | 29:A:4004:BCR:H363 | 2.00 | 0.44 |
| 25:A:1130:CLA:H41 | 25:A:1130:CLA:H92 | 1.99 | 0.44 |
| 6:F:334:ARG:O | 6:F:338:GLU:HG3 | 2.18 | 0.44 |
| 26:4:618:CHL:H93 | 26:4:618:CHL:HBC3 | 1.99 | 0.44 |
| 18:5:133:GLU:HG3 | 25:5:612:CLA:C4B | 2.48 | 0.44 |
| 43:7:501:LUT:H32 | 25:7:601:CLA:CAB | 2.48 | 0.44 |
| 21:8:154:PHE:HE2 | 21:8:161:PHE:HE2 | 1.63 | 0.44 |
| 25:2:604:CLA:H102 | 25:2:605:CLA:H91 | 2.00 | 0.44 |
| 43:9:502:LUT:H11 | 25:9:605:CLA:HBC3 | 2.00 | 0.44 |
| 1:A:60:ASP:OD2 | 1:A:350:HIS:NE2 | 2.48 | 0.44 |
| 1:A:419:PRO:HG3 | 4:D:233:GLU:HB2 | 2.00 | 0.44 |
| 1:A:646:LEU:HD22 | 2:B:652:LEU:HD21 | 2.00 | 0.44 |
| 1:A:690:ARG:H | 2:B:569:CYS:HB2 | 1.81 | 0.44 |
| 2:B:211:ASP:HA | 33:9:803:PTY:H312 | 2.00 | 0.44 |
| 25:B:1205:CLA:CGA | 25:B:1205:CLA:C1A | 2.96 | 0.44 |
| 30:F:5002:LHG:H312 | 26:8:610:CHL:H52 | 1.98 | 0.44 |
| 16:3:357:TYR:CZ | 16:3:359:LYS:HB2 | 2.53 | 0.44 |
| 25:6:615:CLA:H92 | 25:6:615:CLA:H61 | 1.80 | 0.44 |
| 48:8:804:DGA:HA52 | 48:8:804:DGA:HB91 | 1.99 | 0.44 |
| 50:2:501:XAT:H391 | 50:2:501:XAT:H31 | 1.70 | 0.44 |
| 25:A:1108:CLA:H13 | 29:A:4002:BCR:H372 | 1.99 | 0.44 |
| 32:A:5005:SQD:H461 | 32:A:5005:SQD:H241 | 1.79 | 0.44 |
| 2:B:345:ILE:HD12 | 25:B:1215:CLA:H101 | 1.98 | 0.44 |
| 25:B:1220:CLA:CMD | 25:B:1221:CLA:HAB | 2.48 | 0.44 |
| 33:J:5001:PTY:H332 | 33:J:5001:PTY:H361 | 1.66 | 0.44 |
| 43:1:501:LUT:H15 | 43:1:501:LUT:H201 | 1.84 | 0.44 |
| 16:3:397:PHE:CE2 | 26:3:611:CHL:HBB2 | 2.52 | 0.44 |
| 17:4:90:GLN:NE2 | 17:4:105:VAL:O | 2.38 | 0.44 |
| 25:6:615:CLA:HMD2 | 30:6:801:LHG:H223 | 1.99 | 0.44 |
| 21:8:170:PRO:HB3 | 25:8:611:CLA:HBC2 | 2.00 | 0.44 |
| 22:2:241:PRO:O | 22:2:243:PRO:HD3 | 2.18 | 0.44 |
| 1:A:89:SER:HB2 | 1:A:166:ALA:HB3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:217:GLN:HB3 | 1:A:295:VAL:HG22 | 1.99 | 0.44 |
| 1:A:300:ALA:HB1 | 25:A:1115:CLA:HBC2 | 2.00 | 0.44 |
| 1:A:677:PHE:HB2 | 25:A:1012:CLA:O1A | 2.18 | 0.44 |
| 1:A:681:PHE:HZ | 25:A:1139:CLA:HBC2 | 1.82 | 0.44 |
| 25:A:1115:CLA:CHD | 25:A:1116:CLA:HBB2 | 2.48 | 0.44 |
| 25:A:1123:CLA:HBA1 | 25:A:1127:CLA:H203 | 2.00 | 0.44 |
| 2:B:5:LEU:HD22 | 13:I:35:ILE:HG12 | 2.00 | 0.44 |
| 2:B:436:GLY:HA3 | 25:B:1230:CLA:HAB | 1.99 | 0.44 |
| 25:B:1231:CLA:H12 | 29:B:4005:BCR:HC42 | 2.00 | 0.44 |
| 6:F:457:TRP:CD1 | 6:F:458:PRO:HD3 | 2.53 | 0.44 |
| 25:G:1603:CLA:H3A | 25:G:1603:CLA:HBA2 | 1.54 | 0.44 |
| 8:H:82:ARG:HB3 | 8:H:85:TYR:CD2 | 2.53 | 0.44 |
| 25:K:1404:CLA:H3A | 25:K:1404:CLA:HBA1 | 1.76 | 0.44 |
| 12:M:20:ILE:O | 12:M:23:VAL:HG12 | 2.17 | 0.44 |
| 18:5:141:ARG:HH21 | 48:5:803:DGA:HB51 | 1.83 | 0.44 |
| 1:A:299:LEU:HD21 | 25:A:1115:CLA:HAB | 1.99 | 0.44 |
| 1:A:605:ILE:HD12 | 24:A:1011:CL0:H53 | 2.00 | 0.44 |
| 43:3:502:LUT:H391 | 26:3:603:CHL:H202 | 1.98 | 0.44 |
| 25:3:607:CLA:H143 | 25:3:607:CLA:H161 | 1.75 | 0.44 |
| 21:8:111:TYR:HB3 | 26:8:613:CHL:HBC1 | 1.99 | 0.44 |
| 2:B:90:HIS:ND1 | 2:B:91:ALA:O | 2.51 | 0.43 |
| 2:B:429:PHE:CD1 | 25:B:1235:CLA:HAB | 2.53 | 0.43 |
| 2:B:508:SER:HA | 2:B:511:LEU:HD21 | 2.00 | 0.43 |
| 2:B:536:VAL:HG22 | 29:B:4004:BCR:H291 | 2.00 | 0.43 |
| 11:L:379:ALA:O | 11:L:383:ILE:HG12 | 2.18 | 0.43 |
| 14:O:92:ALA:O | 14:O:94:PHE:N | 2.51 | 0.43 |
| 25:O:1802:CLA:H41 | 25:O:1802:CLA:H62 | 1.37 | 0.43 |
| 25:1:605:CLA:HMC3 | 25:1:612:CLA:H201 | 2.00 | 0.43 |
| 17:4:141:TYR:HA | 17:4:161:LEU:HD11 | 2.00 | 0.43 |
| 43:4:501:LUT:H35 | 43:4:501:LUT:H401 | 1.74 | 0.43 |
| 18:5:161:GLU:HG3 | 18:5:164:TYR:CD2 | 2.52 | 0.43 |
| 25:6:602:CLA:H51 | 25:6:602:CLA:H11 | 1.78 | 0.43 |
| 20:7:135:LYS:HG2 | 20:7:145:VAL:HG23 | 1.98 | 0.43 |
| 22:2:157:THR:HG22 | 25:2:601:CLA:HMA1 | 2.00 | 0.43 |
| 23:9:385:PHE:CE1 | 43:9:502:LUT:H10 | 2.52 | 0.43 |
| 30:9:801:LHG:H102 | 30:9:801:LHG:H132 | 1.86 | 0.43 |
| 25:A:1105:CLA:HHC | 25:A:1105:CLA:HBB1 | 1.99 | 0.43 |
| 25:A:1108:CLA:H61 | 25:A:1108:CLA:H41 | 1.59 | 0.43 |
| 25:A:1115:CLA:H91 | 25:A:1115:CLA:H111 | 1.71 | 0.43 |
| 25:A:1120:CLA:C4D | 29:K:4001:BCR:H271 | 2.49 | 0.43 |
| 25:A:1120:CLA:C3D | 29:K:4001:BCR:H271 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:637:ASN:HB2 | 2:B:638:PRO:HD2 | 1.99 | 0.43 |
| 30:F:5001:LHG:C6 | 25:8:609:CLA:HMA1 | 2.48 | 0.43 |
| 8:H:56:MET:HG2 | 8:H:57:TYR:CE2 | 2.53 | 0.43 |
| 15:1:61:ALA:HB2 | 26:1:604:CHL:HBA1 | 1.99 | 0.43 |
| 43:3:501:LUT:H15 | 43:3:501:LUT:H201 | 1.88 | 0.43 |
| 26:9:601:CHL:H3A | 26:9:601:CHL:HBA2 | 1.37 | 0.43 |
| 25:A:1127:CLA:H61 | 25:A:1127:CLA:H41 | 1.72 | 0.43 |
| 2:B:646:VAL:HA | 25:B:1206:CLA:HBC2 | 2.00 | 0.43 |
| 25:B:1209:CLA:H141 | 25:B:1209:CLA:H161 | 1.76 | 0.43 |
| 7:G:1294:PHE:CE2 | 25:G:1602:CLA:HMB2 | 2.53 | 0.43 |
| 25:G:1602:CLA:H112 | 25:9:609:CLA:HAC1 | 2.01 | 0.43 |
| 8:H:34:LYS:HG3 | 8:H:50:THR:HG22 | 2.00 | 0.43 |
| 8:H:70:SER:O | 8:H:74:GLU:HG2 | 2.18 | 0.43 |
| 18:5:209:LYS:HB2 | 18:5:214:ASN:HD21 | 1.84 | 0.43 |
| 19:6:149:ASP:HB3 | 19:6:152:PHE:O | 2.18 | 0.43 |
| 21:8:79:TRP:CE2 | 25:8:612:CLA:HBC3 | 2.53 | 0.43 |
| 48:2:803:DGA:HA81 | 48:2:803:DGA:HA52 | 1.51 | 0.43 |
| 1:A:245:LEU:HD21 | 26:A:1114:CHL:H192 | 2.01 | 0.43 |
| 1:A:689:GLY:O | 1:A:693:TRP:HD1 | 2.01 | 0.43 |
| 25:A:1133:CLA:H121 | 25:A:1133:CLA:H161 | 1.69 | 0.43 |
| 25:A:1133:CLA:H93 | 25:A:1133:CLA:H112 | 1.82 | 0.43 |
| 34:A:5007:3PH:H282 | 48:3:803:DGA:HB62 | 2.00 | 0.43 |
| 10:K:112:LYS:HB3 | 10:K:117:LEU:HD23 | 2.00 | 0.43 |
| 30:1:801:LHG:H102 | 30:1:801:LHG:H271 | 2.00 | 0.43 |
| 18:5:79:TRP:HD1 | 25:5:612:CLA:HMD3 | 1.84 | 0.43 |
| 44:7:504:AXT:H11 | 44:7:504:AXT:H191 | 1.73 | 0.43 |
| 44:7:504:AXT:O3 | 25:7:612:CLA:H52 | 2.18 | 0.43 |
| 25:2:603:CLA:H62 | 25:2:603:CLA:H41 | 1.81 | 0.43 |
| 30:2:801:LHG:H341 | 23:9:337:PHE:CD2 | 2.54 | 0.43 |
| 1:A:264:PHE:HB2 | 1:A:272:TYR:HE2 | 1.84 | 0.43 |
| 25:A:1103:CLA:HMC3 | 25:A:1128:CLA:HMA1 | 2.00 | 0.43 |
| 25:B:1021:CLA:HBA2 | 25:B:1021:CLA:H3A | 1.52 | 0.43 |
| 25:B:1022:CLA:H203 | 25:B:1207:CLA:HMC2 | 2.00 | 0.43 |
| 29:H:4001:BCR:H24C | 11:L:440:TRP:NE1 | 2.22 | 0.43 |
| 32:H:5001:SQD:H252 | 25:2:612:CLA:H11 | 1.99 | 0.43 |
| 25:3:605:CLA:H2 | 25:3:605:CLA:H61 | 1.71 | 0.43 |
| 25:3:616:CLA:HBC3 | 18:5:227:TRP:CH2 | 2.53 | 0.43 |
| 19:6:265:PRO:HB2 | 26:6:619:CHL:HAB | 1.99 | 0.43 |
| 37:6:803:PCW:H20 | 37:6:803:PCW:H171 | 1.66 | 0.43 |
| 20:7:214:THR:HG22 | 25:7:603:CLA:HED1 | 2.00 | 0.43 |
| 22:2:148:ASP:OD2 | 22:2:153:ARG:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:2:603:CLA:HBA1 | 25:2:603:CLA:CBD | 2.46 | 0.43 |
| 43:9:501:LUT:H32 | 26:9:601:CHL:CAB | 2.49 | 0.43 |
| 24:A:1011:CL0:H53 | 24:A:1011:CL0:H61 | 1.73 | 0.43 |
| 2:B:465:GLN:NE2 | 25:B:1234:CLA:OBD | 2.36 | 0.43 |
| 2:B:517:ASP:HA | 2:B:520:VAL:HG12 | 1.99 | 0.43 |
| 7:G:1324:ASN:OD1 | 25:G:1603:CLA:HAC2 | 2.18 | 0.43 |
| 9:J:29:THR:HB | 9:J:31:PRO:HD2 | 1.99 | 0.43 |
| 29:4:503:BCR:H351 | 29:4:503:BCR:H15C | 1.64 | 0.43 |
| 29:4:503:BCR:H19C | 26:4:613:CHL:O1A | 2.18 | 0.43 |
| 50:7:502:XAT:H31 | 50:7:502:XAT:H391 | 1.74 | 0.43 |
| 25:8:609:CLA:H92 | 25:8:609:CLA:H62 | 1.82 | 0.43 |
| 1:A:72:LYS:NZ | 1:A:181:TYR:OH | 2.48 | 0.43 |
| 1:A:360:PHE:CE2 | 25:A:1104:CLA:HMB1 | 2.53 | 0.43 |
| 1:A:587:SER:OG | 1:A:590:ASP:OD2 | 2.34 | 0.43 |
| 25:A:1119:CLA:H141 | 25:A:1119:CLA:H161 | 1.71 | 0.43 |
| 25:B:1224:CLA:H91 | 25:B:1224:CLA:H111 | 1.70 | 0.43 |
| 27:B:2002:PQN:H251 | 27:B:2002:PQN:H211 | 1.90 | 0.43 |
| 8:H:90:VAL:HG12 | 32:I:5001:SQD:H322 | 2.01 | 0.43 |
| 10:K:32:TYR:HB3 | 37:K:5001:PCW:H32 | 1.99 | 0.43 |
| 15:1:141:ARG:O | 15:1:149:ARG:HG2 | 2.18 | 0.43 |
| 15:1:212:VAL:HG12 | 25:1:603:CLA:HED1 | 2.01 | 0.43 |
| 25:4:615:CLA:HAA2 | 25:4:615:CLA:H2 | 2.00 | 0.43 |
| 18:5:52:ARG:HB2 | 25:5:604:CLA:HMD1 | 2.00 | 0.43 |
| 25:5:602:CLA:HMD2 | 25:5:607:CLA:C1D | 2.49 | 0.43 |
| 25:5:612:CLA:H203 | 25:5:612:CLA:H162 | 1.72 | 0.43 |
| 36:7:806:DGD:HO2E | 36:7:806:DGD:HO4D | 1.65 | 0.43 |
| 25:7:602:CLA:HMD3 | 25:7:607:CLA:H52 | 2.01 | 0.43 |
| 23:9:327:LEU:HD21 | 26:9:613:CHL:CHD | 2.49 | 0.43 |
| 25:9:605:CLA:H112 | 25:9:605:CLA:H91 | 1.70 | 0.43 |
| 25:A:1106:CLA:C3D | 25:A:1126:CLA:HBA1 | 2.49 | 0.43 |
| 25:A:1111:CLA:H141 | 25:A:1111:CLA:H161 | 1.79 | 0.43 |
| 25:A:1119:CLA:H62 | 25:A:1123:CLA:HMB1 | 2.00 | 0.43 |
| 25:A:1125:CLA:HED2 | 25:A:1133:CLA:HAB | 1.99 | 0.43 |
| 25:A:1131:CLA:CAD | 29:L:4002:BCR:H10C | 2.49 | 0.43 |
| 6:F:442:ILE:HB | 9:J:33:LEU:HD12 | 2.00 | 0.43 |
| 25:G:1603:CLA:ND | 33:G:5003:PTY:H142 | 2.33 | 0.43 |
| 25:1:601:CLA:H92 | 25:1:601:CLA:H61 | 1.69 | 0.43 |
| 16:3:250:ASP:O | 16:3:252:ALA:N | 2.48 | 0.43 |
| 25:5:609:CLA:HBA2 | 30:5:801:LHG:HC62 | 2.01 | 0.43 |
| 26:5:618:CHL:HED1 | 30:6:801:LHG:H332 | 2.01 | 0.43 |
| 20:7:73:LYS:HD3 | 20:7:202:ASP:OD1 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:7:135:LYS:HG2 | 20:7:145:VAL:CG2 | 2.48 | 0.43 |
| 23:9:383:THR:HG22 | 26:9:603:CHL:HBB1 | 2.01 | 0.43 |
| 25:A:1129:CLA:HAB | 25:A:1137:CLA:HBB2 | 2.00 | 0.43 |
| 2:B:577:PHE:O | 2:B:581:VAL:HG23 | 2.19 | 0.43 |
| 2:B:649:TRP:HH2 | 25:B:1022:CLA:H111 | 1.83 | 0.43 |
| 2:B:701:LEU:HD11 | 25:B:1239:CLA:HMD3 | 2.00 | 0.43 |
| 25:B:1239:CLA:H192 | 25:B:1239:CLA:H161 | 1.80 | 0.43 |
| 25:1:608:CLA:H42 | 26:1:609:CHL:H12 | 2.01 | 0.43 |
| 21:8:136:ILE:HG12 | 53:8:810:LAP:H191 | 2.00 | 0.43 |
| 1:A:412:PHE:CD1 | 1:A:416:ASP:HB2 | 2.54 | 0.43 |
| 1:A:453:PHE:CZ | 1:A:457:ILE:HD11 | 2.54 | 0.43 |
| 25:A:1119:CLA:H3A | 25:A:1119:CLA:HBA2 | 1.64 | 0.43 |
| 25:A:1139:CLA:HBA2 | 25:A:1139:CLA:H3A | 1.35 | 0.43 |
| 27:A:2001:PQN:H222 | 27:A:2001:PQN:H261 | 1.80 | 0.43 |
| 29:A:4003:BCR:H313 | 14:O:117:LEU:HA | 2.01 | 0.43 |
| 32:A:5005:SQD:O47 | 32:A:5005:SQD:O2 | 2.28 | 0.43 |
| 25:B:1220:CLA:H101 | 29:B:4004:BCR:C11 | 2.48 | 0.43 |
| 11:L:314:PRO:O | 11:L:318:SER:HB2 | 2.18 | 0.43 |
| 26:1:604:CHL:HMD2 | 26:1:609:CHL:CBB | 2.49 | 0.43 |
| 25:4:615:CLA:H91 | 25:4:615:CLA:H112 | 1.75 | 0.43 |
| 25:6:615:CLA:HAB | 37:6:803:PCW:C37 | 2.49 | 0.43 |
| 44:7:504:AXT:H15 | 25:8:615:CLA:HBC1 | 2.01 | 0.43 |
| 30:9:802:LHG:H212 | 30:9:802:LHG:H182 | 1.72 | 0.43 |
| 25:9:604:CLA:H102 | 25:9:605:CLA:HMB3 | 2.01 | 0.43 |
| 1:A:439:SER:HB3 | 2:B:678:THR:HG22 | 2.01 | 0.42 |
| 25:A:1103:CLA:H51 | 25:A:1111:CLA:H12 | 2.01 | 0.42 |
| 25:A:1105:CLA:ND | 32:A:5005:SQD:H142 | 2.33 | 0.42 |
| 25:A:1126:CLA:H193 | 25:A:1126:CLA:H162 | 1.72 | 0.42 |
| 25:B:1225:CLA:HBA2 | 25:B:1225:CLA:H3A | 1.36 | 0.42 |
| 25:B:1227:CLA:HAB | 25:B:1236:CLA:CBB | 2.49 | 0.42 |
| 25:B:1230:CLA:H41 | 25:B:1230:CLA:H61 | 1.84 | 0.42 |
| 6:F:372:LYS:NZ | 9:J:54:ASP:O | 2.39 | 0.42 |
| 43:5:501:LUT:C11 | 25:5:602:CLA:HMC2 | 2.49 | 0.42 |
| 48:5:803:DGA:HA22 | 48:5:803:DGA:HG12 | 1.84 | 0.42 |
| 19:6:205:THR:HG21 | 25:6:603:CLA:HED3 | 2.00 | 0.42 |
| 19:6:231:VAL:HB | 26:6:619:CHL:C1C | 2.49 | 0.42 |
| 50:9:504:XAT:H31 | 50:9:504:XAT:H391 | 1.72 | 0.42 |
| 1:A:55:ASP:OD2 | 30:A:5002:LHG:O2 | 2.36 | 0.42 |
| 25:A:1012:CLA:HMA2 | 2:B:617:LEU:HD13 | 2.00 | 0.42 |
| 30:A:5003:LHG:H261 | 25:3:610:CLA:HMC1 | 2.00 | 0.42 |
| 16:3:257:VAL:HG21 | 16:3:273:LEU:HD21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:3:421:LEU:HA | 18:5:38:VAL:HG12 | 2.00 | 0.42 |
| 17:4:195:LEU:HD23 | 25:4:603:CLA:HMC1 | 2.01 | 0.42 |
| 25:5:612:CLA:H62 | 25:5:612:CLA:H2 | 1.77 | 0.42 |
| 50:7:502:XAT:H15 | 50:7:502:XAT:H201 | 1.78 | 0.42 |
| 21:8:129:PHE:CE1 | 25:8:618:CLA:HMA1 | 2.53 | 0.42 |
| 25:8:612:CLA:H3A | 25:8:612:CLA:HBA2 | 1.45 | 0.42 |
| 1:A:245:LEU:HD11 | 26:A:1114:CHL:HAC1 | 2.01 | 0.42 |
| 1:A:305:PHE:HZ | 25:A:1117:CLA:H112 | 1.84 | 0.42 |
| 25:A:1012:CLA:C4 | 29:A:4005:BCR:H362 | 2.49 | 0.42 |
| 2:B:296:PHE:HA | 7:G:1285:ILE:HD13 | 2.01 | 0.42 |
| 2:B:333:PHE:CE1 | 29:B:4005:BCR:H291 | 2.54 | 0.42 |
| 2:B:485:ALA:H | 30:1:802:LHG:H122 | 1.85 | 0.42 |
| 25:B:1217:CLA:H51 | 25:B:1217:CLA:C4B | 2.49 | 0.42 |
| 25:B:1226:CLA:H201 | 29:B:4007:BCR:H10C | 2.02 | 0.42 |
| 5:E:49:ARG:CD | 5:E:51:GLU:HB2 | 2.49 | 0.42 |
| 10:K:32:TYR:OH | 25:K:1401:CLA:HMD1 | 2.19 | 0.42 |
| 14:O:73:ALA:O | 14:O:75:GLY:N | 2.53 | 0.42 |
| 15:1:210:MET:HE1 | 25:1:608:CLA:HMA1 | 2.01 | 0.42 |
| 15:1:211:ALA:O | 15:1:216:THR:HG21 | 2.19 | 0.42 |
| 25:1:603:CLA:H102 | 26:1:609:CHL:H61 | 2.02 | 0.42 |
| 47:8:807:PLM:H41 | 53:8:810:LAP:H202 | 2.00 | 0.42 |
| 1:A:402:ILE:HG23 | 29:A:4004:BCR:H343 | 2.01 | 0.42 |
| 25:A:1137:CLA:H112 | 29:A:4003:BCR:HC41 | 2.01 | 0.42 |
| 27:A:2001:PQN:H141 | 25:A:1140:CLA:HBB2 | 2.00 | 0.42 |
| 25:B:1225:CLA:ND | 29:B:4002:BCR:H281 | 2.33 | 0.42 |
| 15:1:60:LEU:HD12 | 26:1:604:CHL:H11 | 2.02 | 0.42 |
| 43:3:502:LUT:H15 | 43:3:502:LUT:H201 | 1.85 | 0.42 |
| 25:4:611:CLA:HHC | 25:4:611:CLA:HBB1 | 2.00 | 0.42 |
| 18:5:35:PHE:O | 18:5:38:VAL:HG22 | 2.19 | 0.42 |
| 18:5:131:PHE:HA | 26:6:609:CHL:HBA1 | 2.01 | 0.42 |
| 25:5:612:CLA:H101 | 26:5:618:CHL:CBB | 2.49 | 0.42 |
| 43:6:501:LUT:H35 | 43:6:501:LUT:H401 | 1.84 | 0.42 |
| 25:6:606:CLA:O1A | 26:6:613:CHL:HMD2 | 2.19 | 0.42 |
| 25:7:604:CLA:H71 | 25:7:605:CLA:HMA1 | 2.00 | 0.42 |
| 25:2:603:CLA:H142 | 25:2:603:CLA:H111 | 1.86 | 0.42 |
| 1:A:45:THR:HG22 | 1:A:714:GLN:HB2 | 2.00 | 0.42 |
| 1:A:221:SER:O | 1:A:225:ASN:HB2 | 2.19 | 0.42 |
| 1:A:737:ALA:HA | 29:A:4005:BCR:HC42 | 2.01 | 0.42 |
| 25:A:1132:CLA:H202 | 25:A:1132:CLA:H161 | 1.70 | 0.42 |
| 2:B:227:PHE:HB3 | 32:G:5001:SQD:H261 | 2.01 | 0.42 |
| 2:B:477:PHE:H | 2:B:480:SER:HB2 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:B:1202:CLA:HED2 | 25:B:1226:CLA:HBB2 | 2.01 | 0.42 |
| 27:B:2002:PQN:H142 | 29:B:4007:BCR:H271 | 2.02 | 0.42 |
| 10:K:33:LEU:HD23 | 37:K:5001:PCW:H321 | 2.01 | 0.42 |
| 15:1:35:ASN:C | 15:1:37:LEU:N | 2.71 | 0.42 |
| 16:3:390:GLY:O | 16:3:394:LYS:NZ | 2.32 | 0.42 |
| 25:3:613:CLA:H91 | 25:3:613:CLA:H111 | 1.72 | 0.42 |
| 17:4:163:TYR:HB3 | 25:4:601:CLA:O1D | 2.18 | 0.42 |
| 20:7:183:MET:SD | 25:7:604:CLA:HAB | 2.60 | 0.42 |
| 44:7:504:AXT:H201 | 25:8:615:CLA:HBC1 | 2.01 | 0.42 |
| 25:8:618:CLA:H143 | 25:8:618:CLA:H112 | 1.80 | 0.42 |
| 25:8:620:CLA:HED2 | 25:8:620:CLA:H2A | 2.01 | 0.42 |
| 22:2:76:ASN:ND2 | 25:2:612:CLA:OBD | 2.52 | 0.42 |
| 25:A:1115:CLA:H62 | 25:A:1115:CLA:H41 | 1.67 | 0.42 |
| 6:F:417:TRP:HD1 | 6:F:454:GLY:C | 2.22 | 0.42 |
| 29:K:4002:BCR:H15C | 29:K:4002:BCR:H351 | 1.83 | 0.42 |
| 15:1:72:GLU:HG2 | 25:1:612:CLA:HED3 | 2.02 | 0.42 |
| 15:1:169:LEU:HB3 | 25:1:601:CLA:CMA | 2.50 | 0.42 |
| 15:1:210:MET:HE2 | 25:1:608:CLA:HMA1 | 2.00 | 0.42 |
| 25:1:605:CLA:HMD3 | 35:1:804:LMT:H82 | 2.01 | 0.42 |
| 25:1:612:CLA:H111 | 25:1:612:CLA:H143 | 1.66 | 0.42 |
| 16:3:414:GLY:HA3 | 25:3:601:CLA:HED2 | 2.00 | 0.42 |
| 17:4:90:GLN:NE2 | 17:4:103:ALA:O | 2.53 | 0.42 |
| 18:5:209:LYS:HB2 | 18:5:214:ASN:ND2 | 2.34 | 0.42 |
| 25:5:607:CLA:H41 | 25:5:607:CLA:H61 | 1.70 | 0.42 |
| 25:5:614:CLA:CAD | 19:6:221:LEU:HD11 | 2.50 | 0.42 |
| 22:2:124:ILE:HG13 | 22:2:125:LEU:N | 2.34 | 0.42 |
| 2:B:339:LEU:HD22 | 2:B:383:ILE:HG23 | 2.01 | 0.42 |
| 2:B:430:LEU:HD11 | 25:B:1235:CLA:HMB3 | 2.01 | 0.42 |
| 2:B:556:TYR:HD2 | 25:B:1226:CLA:HED2 | 1.84 | 0.42 |
| 25:B:1228:CLA:HMB1 | 25:B:1228:CLA:HBB1 | 2.01 | 0.42 |
| 25:B:1229:CLA:CAB | 25:B:1230:CLA:HMB2 | 2.50 | 0.42 |
| 25:1:601:CLA:H62 | 25:1:601:CLA:H41 | 1.85 | 0.42 |
| 25:1:612:CLA:H192 | 30:1:802:LHG:H361 | 2.01 | 0.42 |
| 25:3:613:CLA:H11 | 25:3:613:CLA:H51 | 1.70 | 0.42 |
| 20:7:122:PRO:HB2 | 20:7:145:VAL:HG13 | 2.02 | 0.42 |
| 21:8:89:ILE:HB | 21:8:90:PRO:HD3 | 2.01 | 0.42 |
| 22:2:99:TRP:NE1 | 48:2:803:DGA:HB22 | 2.35 | 0.42 |
| 23:9:279:ARG:HH22 | 30:9:802:LHG:HC42 | 1.85 | 0.42 |
| 50:9:507:XAT:H30 | 25:9:606:CLA:CAD | 2.50 | 0.42 |
| 25:9:607:CLA:HBC1 | 30:9:801:LHG:H132 | 2.02 | 0.42 |
| 1:A:264:PHE:CZ | 29:K:4001:BCR:H343 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:535:VAL:HG21 | 1:A:609:HIS:HB2 | 2.02 | 0.42 |
| 1:A:685:PHE:HA | 27:A:2001:PQN:H9 | 2.01 | 0.42 |
| 25:A:1013:CLA:H151 | 25:A:1013:CLA:H112 | 1.44 | 0.42 |
| 25:A:1013:CLA:HBB1 | 25:A:1013:CLA:HMB1 | 2.02 | 0.42 |
| 25:A:1104:CLA:H161 | 25:A:1104:CLA:H193 | 1.76 | 0.42 |
| 25:A:1113:CLA:H122 | 25:A:1113:CLA:H8 | 1.68 | 0.42 |
| 2:B:91:ALA:HA | 2:B:114:VAL:HG12 | 2.02 | 0.42 |
| 25:B:1021:CLA:H142 | 25:B:1021:CLA:H111 | 1.81 | 0.42 |
| 25:B:1234:CLA:H93 | 25:B:1234:CLA:H61 | 1.71 | 0.42 |
| 33:B:5005:PTY:H342 | 9:J:48:ILE:HD11 | 2.01 | 0.42 |
| 39:F:4001:NEX:H373 | 39:F:4001:NEX:H23 | 1.84 | 0.42 |
| 16:3:423:LEU:HB2 | 25:3:601:CLA:HBA1 | 2.02 | 0.42 |
| 25:3:605:CLA:HED3 | 25:3:605:CLA:H72 | 2.02 | 0.42 |
| 19:6:203:GLN:HE22 | 29:6:504:BCR:H282 | 1.85 | 0.42 |
| 25:6:604:CLA:H192 | 25:6:604:CLA:H161 | 1.68 | 0.42 |
| 25:2:601:CLA:H91 | 25:2:601:CLA:H111 | 1.84 | 0.42 |
| 23:9:414:ASN:ND2 | 26:9:608:CHL:HED3 | 2.34 | 0.42 |
| 41:9:804:SPH:H161 | 41:9:804:SPH:H132 | 1.82 | 0.42 |
| 1:A:577:GLY:HA2 | 2:B:563:PRO:HD3 | 2.02 | 0.42 |
| 25:A:1118:CLA:H3A | 25:A:1118:CLA:HBA2 | 1.35 | 0.42 |
| 25:A:1124:CLA:HAA2 | 25:A:1125:CLA:OBD | 2.19 | 0.42 |
| 25:A:1131:CLA:H11 | 25:A:1131:CLA:H52 | 1.78 | 0.42 |
| 25:B:1204:CLA:HBC3 | 12:M:15:ALA:HB2 | 2.01 | 0.42 |
| 25:B:1224:CLA:H161 | 25:B:1224:CLA:H141 | 1.72 | 0.42 |
| 25:B:1240:CLA:HMC3 | 25:1:605:CLA:H2 | 2.01 | 0.42 |
| 32:G:5001:SQD:H271 | 32:G:5001:SQD:H302 | 1.79 | 0.42 |
| 14:O:61:LEU:HB3 | 14:O:119:LEU:HA | 2.02 | 0.42 |
| 25:4:602:CLA:HMD2 | 25:4:607:CLA:C1D | 2.50 | 0.42 |
| 26:4:609:CHL:H12 | 26:4:609:CHL:H51 | 1.73 | 0.42 |
| 25:6:608:CLA:HBC1 | 25:6:603:CLA:H192 | 2.01 | 0.42 |
| 25:6:602:CLA:H41 | 25:6:602:CLA:H62 | 1.59 | 0.42 |
| 25:6:615:CLA:H142 | 25:6:615:CLA:H111 | 1.82 | 0.42 |
| 43:7:501:LUT:H35 | 43:7:501:LUT:H401 | 1.83 | 0.42 |
| 50:7:502:XAT:H35 | 50:7:502:XAT:H401 | 1.91 | 0.42 |
| 26:7:617:CHL:H11 | 36:8:802:DGD:HA72 | 2.02 | 0.42 |
| 21:8:89:ILE:O | 21:8:93:LEU:HG | 2.20 | 0.42 |
| 22:2:57:ARG:HH12 | 30:2:802:LHG:HC2 | 1.85 | 0.42 |
| 22:2:110:ASP:HB3 | 22:2:113:THR:HG23 | 2.01 | 0.42 |
| 48:2:803:DGA:HAH2 | 48:2:803:DGA:HAT2 | 1.86 | 0.42 |
| 26:9:603:CHL:H71 | 26:9:603:CHL:CHC | 2.50 | 0.42 |
| 30:A:5002:LHG:H122 | 30:A:5002:LHG:H151 | 1.69 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:4:LYS:HZ1 | 2:B:21:ARG:HE | 1.67 | 0.42 |
| 25:B:1206:CLA:H122 | 25:B:1206:CLA:H161 | 1.44 | 0.42 |
| 25:B:1216:CLA:HBC2 | 25:B:1221:CLA:H18 | 2.02 | 0.42 |
| 29:B:4002:BCR:H321 | 29:B:4002:BCR:HC8 | 2.02 | 0.42 |
| 36:B:5003:DGD:HAE2 | 36:B:5003:DGD:HA81 | 1.75 | 0.42 |
| 25:1:601:CLA:HMD2 | 26:1:611:CHL:O1A | 2.20 | 0.42 |
| 30:1:801:LHG:H111 | 29:8:503:BCR:H313 | 2.02 | 0.42 |
| 25:4:604:CLA:HED2 | 25:4:604:CLA:H2A | 2.02 | 0.42 |
| 18:5:135:ARG:HD2 | 26:6:609:CHL:HED3 | 2.01 | 0.42 |
| 43:5:505:LUT:H15 | 43:5:505:LUT:H201 | 1.76 | 0.42 |
| 19:6:99:VAL:HG12 | 19:6:100:LYS:HG3 | 2.02 | 0.42 |
| 19:6:246:THR:HA | 19:6:255:PRO:O | 2.19 | 0.42 |
| 26:9:610:CHL:H2 | 33:9:803:PTY:C30 | 2.50 | 0.42 |
| 1:A:413:MET:HG3 | 1:A:558:ARG:HG3 | 2.02 | 0.41 |
| 25:A:1125:CLA:HBA1 | 25:A:1125:CLA:H3A | 1.51 | 0.41 |
| 11:L:393:VAL:HG23 | 13:I:28:LEU:HD23 | 2.02 | 0.41 |
| 29:3:504:BCR:H372 | 25:3:613:CLA:H151 | 2.01 | 0.41 |
| 29:5:504:BCR:H332 | 19:6:237:VAL:HG11 | 2.02 | 0.41 |
| 25:6:608:CLA:H2 | 26:6:609:CHL:H151 | 2.01 | 0.41 |
| 20:7:160:LEU:HD23 | 20:7:160:LEU:HA | 1.87 | 0.41 |
| 21:8:79:TRP:HD1 | 25:8:612:CLA:HMD3 | 1.84 | 0.41 |
| 21:8:92:GLU:OE2 | 21:8:95:ARG:NH2 | 2.37 | 0.41 |
| 21:8:194:GLU:HB2 | 26:8:601:CHL:C1B | 2.50 | 0.41 |
| 25:8:606:CLA:HED2 | 52:8:805:P5S:HB | 2.02 | 0.41 |
| 26:2:609:CHL:H62 | 26:2:609:CHL:H41 | 1.76 | 0.41 |
| 30:2:802:LHG:H321 | 30:2:802:LHG:H352 | 1.61 | 0.41 |
| 43:9:501:LUT:C30 | 26:9:601:CHL:H8 | 2.50 | 0.41 |
| 1:A:96:ALA:HB2 | 1:A:159:LEU:HB2 | 2.02 | 0.41 |
| 1:A:116:GLN:NE2 | 25:A:1107:CLA:OBD | 2.52 | 0.41 |
| 25:A:1113:CLA:H93 | 29:3:505:BCR:HC8 | 2.02 | 0.41 |
| 14:O:131:GLN:HG3 | 25:O:1802:CLA:HAA1 | 2.02 | 0.41 |
| 25:3:605:CLA:HMD2 | 25:3:612:CLA:C1D | 2.50 | 0.41 |
| 19:6:232:VAL:O | 19:6:234:GLY:N | 2.54 | 0.41 |
| 43:9:501:LUT:H35 | 43:9:501:LUT:H401 | 1.84 | 0.41 |
| 1:A:289:LEU:HD21 | 1:A:374:MET:HB3 | 2.00 | 0.41 |
| 1:A:366:ILE:HG12 | 25:A:1124:CLA:HED3 | 2.01 | 0.41 |
| 25:B:1230:CLA:HBA2 | 25:B:1230:CLA:H3A | 1.73 | 0.41 |
| 4:D:218:GLU:OE1 | 4:D:276:ARG:HD3 | 2.20 | 0.41 |
| 32:G:5001:SQD:H111 | 32:G:5001:SQD:H262 | 2.01 | 0.41 |
| 11:L:365:VAL:HG12 | 11:L:367:ASN:H | 1.85 | 0.41 |
| 40:3:506:RRX:H42 | 40:3:506:RRX:H47 | 1.76 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:4:610:CLA:H142 | 25:4:610:CLA:H111 | 1.69 | 0.41 |
| 25:5:601:CLA:H71 | 25:5:602:CLA:HMA1 | 2.03 | 0.41 |
| 25:6:603:CLA:H141 | 25:6:603:CLA:H161 | 1.85 | 0.41 |
| 20:7:171:TYR:HB3 | 25:7:601:CLA:HMA1 | 2.03 | 0.41 |
| 25:7:610:CLA:CBB | 26:7:613:CHL:HBB2 | 2.50 | 0.41 |
| 21:8:161:PHE:CZ | 25:8:611:CLA:HAB | 2.55 | 0.41 |
| 23:9:255:PRO:O | 23:9:257:HIS:N | 2.50 | 0.41 |
| 23:9:373:LYS:O | 23:9:377:ASN:ND2 | 2.37 | 0.41 |
| 1:A:687:PHE:HB2 | 25:A:1013:CLA:CBC | 2.50 | 0.41 |
| 25:A:1115:CLA:H3A | 25:A:1115:CLA:HBA2 | 1.80 | 0.41 |
| 25:A:1138:CLA:H93 | 25:A:1138:CLA:H61 | 1.90 | 0.41 |
| 2:B:158:LEU:HD23 | 2:B:158:LEU:HA | 1.94 | 0.41 |
| 25:G:1601:CLA:C2B | 29:G:4001:BCR:H353 | 2.50 | 0.41 |
| 13:I:18:PHE:CD1 | 25:2:621:CLA:H151 | 2.56 | 0.41 |
| 25:1:603:CLA:HMB1 | 25:1:603:CLA:HBB1 | 2.01 | 0.41 |
| 43:4:502:LUT:H35 | 43:4:502:LUT:H401 | 1.78 | 0.41 |
| 47:4:804:PLM:HG1 | 25:8:602:CLA:HED1 | 2.03 | 0.41 |
| 18:5:252:LEU:HD23 | 18:5:252:LEU:HA | 1.86 | 0.41 |
| 43:6:501:LUT:H15 | 43:6:501:LUT:H201 | 1.90 | 0.41 |
| 29:6:503:BCR:H351 | 29:6:503:BCR:H15C | 1.84 | 0.41 |
| 29:7:503:BCR:H15C | 29:7:503:BCR:H351 | 1.92 | 0.41 |
| 26:7:611:CHL:HMA2 | 26:7:613:CHL:H101 | 2.02 | 0.41 |
| 1:A:122:VAL:HB | 25:B:1230:CLA:HMD1 | 2.02 | 0.41 |
| 1:A:589:TRP:NE1 | 25:A:1128:CLA:HMD1 | 2.35 | 0.41 |
| 25:A:1132:CLA:HMA2 | 11:L:359:LEU:HD22 | 2.02 | 0.41 |
| 25:A:1138:CLA:C1B | 25:B:1229:CLA:H41 | 2.51 | 0.41 |
| 25:B:1023:CLA:H92 | 25:B:1023:CLA:H62 | 1.83 | 0.41 |
| 25:B:1217:CLA:H62 | 25:B:1217:CLA:H41 | 1.74 | 0.41 |
| 25:B:1220:CLA:H101 | 29:B:4004:BCR:C10 | 2.51 | 0.41 |
| 9:J:43:GLY:O | 9:J:47:GLU:HG2 | 2.19 | 0.41 |
| 11:L:443:LEU:O | 11:L:447:ILE:HG12 | 2.21 | 0.41 |
| 25:3:612:CLA:HBA2 | 25:3:612:CLA:H3A | 1.36 | 0.41 |
| 43:4:502:LUT:H15 | 43:4:502:LUT:H201 | 1.87 | 0.41 |
| 25:7:604:CLA:H152 | 25:7:604:CLA:H112 | 1.62 | 0.41 |
| 22:2:161:GLU:HB2 | 25:2:601:CLA:CHB | 2.51 | 0.41 |
| 1:A:510:TRP:CH2 | 25:A:1125:CLA:HBC2 | 2.54 | 0.41 |
| 25:A:1113:CLA:H3A | 25:A:1113:CLA:H12 | 2.03 | 0.41 |
| 25:B:1205:CLA:HAB | 25:B:1206:CLA:HAA2 | 2.03 | 0.41 |
| 25:B:1218:CLA:HMA1 | 25:B:1219:CLA:O1A | 2.20 | 0.41 |
| 25:B:1218:CLA:CMD | 29:B:4001:BCR:HC7 | 2.40 | 0.41 |
| 25:B:1207:CLA:H111 | 8:H:96:GLY:HA3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:L:383:ILE:HB | 29:L:4001:BCR:H401 | 2.03 | 0.41 |
| 42:M:4001:ECH:H35 | 42:M:4001:ECH:H15 | 1.81 | 0.41 |
| 14:O:131:GLN:CG | 25:O:1802:CLA:HBD | 2.49 | 0.41 |
| 26:4:609:CHL:H161 | 26:4:609:CHL:H122 | 1.98 | 0.41 |
| 43:5:502:LUT:H32 | 25:5:604:CLA:CAB | 2.50 | 0.41 |
| 19:6:195:PHE:CD1 | 43:6:502:LUT:H10 | 2.56 | 0.41 |
| 43:6:502:LUT:H15 | 43:6:502:LUT:H201 | 1.84 | 0.41 |
| 29:7:503:BCR:H332 | 25:8:609:CLA:H102 | 2.02 | 0.41 |
| 25:7:603:CLA:C1C | 25:7:603:CLA:H51 | 2.50 | 0.41 |
| 25:2:608:CLA:HBA1 | 25:2:608:CLA:H3A | 1.91 | 0.41 |
| 1:A:368:ALA:HB2 | 1:A:394:HIS:HB2 | 2.02 | 0.41 |
| 1:A:480:GLN:HA | 1:A:481:PRO:HD3 | 1.89 | 0.41 |
| 1:A:747:ILE:HD12 | 1:A:747:ILE:HA | 1.94 | 0.41 |
| 25:B:1213:CLA:H61 | 25:B:1213:CLA:H41 | 1.79 | 0.41 |
| 25:B:1215:CLA:H62 | 25:B:1215:CLA:H41 | 1.43 | 0.41 |
| 30:B:5002:LHG:H271 | 30:B:5002:LHG:H241 | 1.84 | 0.41 |
| 5:E:62:VAL:HB | 5:E:74:VAL:HG12 | 2.02 | 0.41 |
| 9:J:45:LEU:HD13 | 29:J:4001:BCR:H24C | 2.02 | 0.41 |
| 14:O:95:PRO:HB2 | 14:O:96:GLN:H | 1.77 | 0.41 |
| 15:1:130:GLU:OE1 | 26:1:610:CHL:HMC | 2.21 | 0.41 |
| 43:3:501:LUT:H11 | 43:3:501:LUT:H191 | 1.95 | 0.41 |
| 25:3:602:CLA:HMD2 | 25:3:607:CLA:C1D | 2.51 | 0.41 |
| 18:5:59:LEU:HD13 | 25:5:604:CLA:H42 | 2.02 | 0.41 |
| 18:5:101:THR:HB | 18:5:104:MET:CE | 2.51 | 0.41 |
| 25:6:615:CLA:H61 | 25:6:615:CLA:H41 | 1.76 | 0.41 |
| 21:8:170:PRO:O | 21:8:174:PHE:HB2 | 2.21 | 0.41 |
| 43:2:507:LUT:H31 | 43:2:507:LUT:H391 | 1.75 | 0.41 |
| 23:9:385:PHE:CD2 | 43:9:502:LUT:H12 | 2.56 | 0.41 |
| 1:A:227:LEU:HD12 | 1:A:237:ILE:HG23 | 2.02 | 0.41 |
| 1:A:532:ASP:HA | 1:A:535:VAL:HG12 | 2.03 | 0.41 |
| 25:A:1133:CLA:H193 | 25:A:1133:CLA:H162 | 1.87 | 0.41 |
| 2:B:286:ILE:O | 2:B:290:HIS:ND1 | 2.39 | 0.41 |
| 2:B:445:GLN:HG3 | 2:B:616:TYR:CD1 | 2.55 | 0.41 |
| 25:B:1207:CLA:H93 | 25:B:1207:CLA:H112 | 1.89 | 0.41 |
| 7:G:1295:THR:O | 7:G:1299:VAL:HG23 | 2.20 | 0.41 |
| 25:5:604:CLA:H71 | 25:5:605:CLA:HMA1 | 2.03 | 0.41 |
| 21:8:140:GLU:OE2 | 53:8:810:LAP:H192 | 2.21 | 0.41 |
| 21:8:195:ILE:HD12 | 21:8:195:ILE:HA | 1.87 | 0.41 |
| 22:2:175:PHE:CE1 | 22:2:186:PRO:HB3 | 2.54 | 0.41 |
| 43:9:501:LUT:H15 | 43:9:501:LUT:H201 | 1.84 | 0.41 |
| 1:A:15:ILE:HD13 | 25:A:1108:CLA:HAA2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:142:SER:HB2 | 25:A:1127:CLA:HMA2 | 2.03 | 0.41 |
| 1:A:486:TRP:HA | 14:O:101:THR:OG1 | 2.21 | 0.41 |
| 1:A:488:GLN:HG3 | 1:A:510:TRP:HA | 2.02 | 0.41 |
| 1:A:680:ALA:CB | 25:A:1013:CLA:HBB2 | 2.51 | 0.41 |
| 1:A:740:TRP:CG | 29:A:4005:BCR:HC41 | 2.56 | 0.41 |
| 25:A:1103:CLA:H112 | 25:A:1103:CLA:H152 | 1.62 | 0.41 |
| 25:A:1103:CLA:H2 | 25:A:1103:CLA:H62 | 1.80 | 0.41 |
| 25:A:1130:CLA:H8 | 25:L:1502:CLA:H91 | 2.02 | 0.41 |
| 25:A:1136:CLA:H51 | 25:A:1136:CLA:H11 | 1.77 | 0.41 |
| 2:B:54:GLN:HG2 | 25:B:1202:CLA:HMA1 | 2.03 | 0.41 |
| 2:B:168:TRP:CE2 | 25:B:1208:CLA:HMA1 | 2.56 | 0.41 |
| 2:B:352:HIS:HB3 | 25:B:1214:CLA:HED2 | 2.03 | 0.41 |
| 2:B:418:ALA:O | 2:B:422:HIS:ND1 | 2.49 | 0.41 |
| 2:B:462:GLN:HG2 | 2:B:473:TYR:CE1 | 2.55 | 0.41 |
| 25:B:1021:CLA:H162 | 25:B:1021:CLA:H202 | 1.75 | 0.41 |
| 25:B:1023:CLA:H3A | 25:B:1023:CLA:CGA | 2.50 | 0.41 |
| 25:B:1216:CLA:HMB1 | 25:B:1216:CLA:HBB1 | 2.03 | 0.41 |
| 25:B:1220:CLA:H72 | 29:B:4004:BCR:C10 | 2.46 | 0.41 |
| 25:B:1226:CLA:H61 | 25:B:1226:CLA:H92 | 1.82 | 0.41 |
| 25:B:1229:CLA:HBB2 | 29:B:4006:BCR:HC41 | 2.02 | 0.41 |
| 25:F:1302:CLA:O1D | 20:7:116:LEU:HD11 | 2.21 | 0.41 |
| 8:H:43:ASP:N | 8:H:50:THR:HG21 | 2.35 | 0.41 |
| 8:H:78:ASN:HD22 | 25:H:1703:CLA:HED3 | 1.86 | 0.41 |
| 42:M:4001:ECH:H20 | 42:M:4001:ECH:H36 | 1.77 | 0.41 |
| 14:O:61:LEU:CB | 14:O:119:LEU:HD23 | 2.51 | 0.41 |
| 25:1:605:CLA:H52 | 25:1:605:CLA:H11 | 1.98 | 0.41 |
| 29:3:503:BCR:C16 | 26:3:611:CHL:HMB3 | 2.50 | 0.41 |
| 29:3:505:BCR:H351 | 29:3:505:BCR:H15C | 1.81 | 0.41 |
| 25:3:612:CLA:HMB2 | 25:3:618:CLA:C1C | 2.51 | 0.41 |
| 17:4:131:ASN:HD22 | 26:4:618:CHL:HMA3 | 1.86 | 0.41 |
| 25:4:604:CLA:H142 | 25:4:604:CLA:H111 | 1.96 | 0.41 |
| 21:8:131:PHE:HB3 | 25:8:612:CLA:HAB | 2.02 | 0.41 |
| 43:8:501:LUT:H35 | 43:8:501:LUT:H401 | 1.87 | 0.41 |
| 25:8:609:CLA:H91 | 30:8:801:LHG:H311 | 2.03 | 0.41 |
| 22:2:99:TRP:CD1 | 48:2:803:DGA:HB22 | 2.55 | 0.41 |
| 23:9:342:ARG:HA | 23:9:358:PHE:CZ | 2.56 | 0.41 |
| 43:9:501:LUT:H11 | 43:9:501:LUT:H191 | 1.93 | 0.41 |
| 1:A:153:ILE:O | 1:A:155:SER:N | 2.49 | 0.41 |
| 1:A:304:LEU:HG | 25:A:1119:CLA:HMC1 | 2.02 | 0.41 |
| 2:B:396:VAL:HG11 | 2:B:556:TYR:HB2 | 2.03 | 0.41 |
| 25:B:1227:CLA:HMB2 | 25:B:1228:CLA:C2D | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:B:1236:CLA:C4 | 29:B:4005:BCR:H10C | 2.51 | 0.41 |
| 7:G:1294:PHE:HE2 | 7:G:1299:VAL:HG22 | 1.85 | 0.41 |
| 25:K:1402:CLA:H41 | 25:K:1402:CLA:H61 | 1.88 | 0.41 |
| 25:1:605:CLA:HMD2 | 25:1:612:CLA:C1D | 2.51 | 0.41 |
| 45:1:803:OLA:H81 | 45:1:803:OLA:H112 | 1.77 | 0.41 |
| 29:3:504:BCR:H362 | 25:3:601:CLA:H142 | 2.03 | 0.41 |
| 19:6:97:GLU:CD | 19:6:208:ASN:HB3 | 2.40 | 0.41 |
| 19:6:192:MET:SD | 25:6:604:CLA:HMC3 | 2.61 | 0.41 |
| 20:7:174:ASN:ND2 | 25:7:607:CLA:OBD | 2.50 | 0.41 |
| 23:9:358:PHE:HA | 23:9:359:PRO:HA | 1.91 | 0.41 |
| 26:9:601:CHL:HMB1 | 26:9:601:CHL:CBB | 2.50 | 0.41 |
| 25:A:1140:CLA:H92 | 6:F:451:LEU:HD12 | 2.02 | 0.40 |
| 2:B:87:PRO:HB3 | 2:B:122:TYR:CG | 2.55 | 0.40 |
| 2:B:176:LEU:HD23 | 2:B:176:LEU:HA | 1.91 | 0.40 |
| 25:B:1231:CLA:H121 | 25:B:1231:CLA:H8 | 1.91 | 0.40 |
| 33:J:5001:PTY:H312 | 51:7:807:4RF:H6 | 2.03 | 0.40 |
| 17:4:138:MET:SD | 25:4:612:CLA:HMA2 | 2.61 | 0.40 |
| 19:6:114:LEU:HD11 | 26:6:613:CHL:HHD | 2.04 | 0.40 |
| 19:6:124:PHE:O | 19:6:128:VAL:HG22 | 2.21 | 0.40 |
| 20:7:88:TYR:HB3 | 26:7:613:CHL:HBC1 | 2.03 | 0.40 |
| 23:9:374:GLU:HB2 | 26:9:601:CHL:C1B | 2.51 | 0.40 |
| 1:A:348:SER:OG | 1:A:416:ASP:OD2 | 2.30 | 0.40 |
| 25:A:1108:CLA:H202 | 25:A:1108:CLA:H161 | 1.79 | 0.40 |
| 2:B:311:PRO:HA | 2:B:312:PRO:HD3 | 1.97 | 0.40 |
| 25:B:1230:CLA:HED2 | 25:B:1230:CLA:H2A | 2.03 | 0.40 |
| 27:B:2002:PQN:H292 | 36:B:5003:DGD:HA81 | 2.04 | 0.40 |
| 6:F:392:PRO:HG3 | 39:F:4001:NEX:H42 | 2.02 | 0.40 |
| 25:H:1703:CLA:H3A | 25:2:612:CLA:HMA1 | 2.03 | 0.40 |
| 11:L:352:LEU:HD23 | 11:L:376:ASN:OD1 | 2.21 | 0.40 |
| 17:4:119:LYS:HD3 | 25:4:610:CLA:HBC3 | 2.03 | 0.40 |
| 43:5:501:LUT:H15 | 43:5:501:LUT:H201 | 1.88 | 0.40 |
| 25:7:601:CLA:HMD2 | 26:7:611:CHL:O1A | 2.21 | 0.40 |
| 22:2:184:LYS:HB2 | 22:2:189:CYS:SG | 2.60 | 0.40 |
| 50:9:507:XAT:H30 | 25:9:606:CLA:C3D | 2.51 | 0.40 |
| 25:A:1103:CLA:HBA1 | 25:A:1103:CLA:H3A | 1.46 | 0.40 |
| 25:A:1131:CLA:H141 | 25:A:1131:CLA:H161 | 1.84 | 0.40 |
| 30:A:5001:LHG:H171 | 30:A:5001:LHG:H201 | 1.86 | 0.40 |
| 2:B:79:VAL:HG13 | 2:B:126:TYR:CE1 | 2.55 | 0.40 |
| 2:B:495:LEU:HD23 | 2:B:495:LEU:HA | 1.77 | 0.40 |
| 25:H:1703:CLA:HBA2 | 25:H:1703:CLA:H12 | 1.95 | 0.40 |
| 15:1:178:ARG:HB3 | 26:1:604:CHL:CBC | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:1:609:CHL:H92 | 26:1:609:CHL:H62 | 1.79 | 0.40 |
| 16:3:314:CYS:CB | 16:3:441:GLY:HA3 | 2.51 | 0.40 |
| 43:5:502:LUT:H35 | 43:5:502:LUT:H401 | 1.85 | 0.40 |
| 30:7:803:LHG:H102 | 30:7:803:LHG:H132 | 1.84 | 0.40 |
| 22:2:69:TYR:HB3 | 25:2:604:CLA:HMA1 | 2.03 | 0.40 |
| 22:2:86:GLY:O | 22:2:90:THR:HG23 | 2.22 | 0.40 |
| 25:2:602:CLA:H11 | 25:2:602:CLA:H51 | 1.87 | 0.40 |
| 1:A:321:SER:HB3 | 1:A:324:GLU:HB2 | 2.02 | 0.40 |
| 1:A:410:ALA:HB1 | 1:A:588:ALA:HB1 | 2.04 | 0.40 |
| 1:A:413:MET:HE3 | 1:A:413:MET:HB2 | 1.93 | 0.40 |
| 25:A:1131:CLA:OBD | 29:L:4002:BCR:H10C | 2.21 | 0.40 |
| 29:A:4005:BCR:H351 | 29:A:4005:BCR:H15C | 1.95 | 0.40 |
| 35:A:5008:LMT:H31 | 35:A:5008:LMT:H62 | 1.77 | 0.40 |
| 2:B:66:LEU:HD11 | 29:B:4003:BCR:H281 | 2.03 | 0.40 |
| 2:B:416:LYS:HB2 | 2:B:540:LEU:HD13 | 2.04 | 0.40 |
| 2:B:490:GLY:O | 2:B:495:LEU:HB2 | 2.21 | 0.40 |
| 16:3:360:TYR:CE1 | 25:3:606:CLA:HAA2 | 2.56 | 0.40 |
| 17:4:151:PRO:HG2 | 29:4:503:BCR:H333 | 2.04 | 0.40 |
| 43:4:501:LUT:H11 | 43:4:501:LUT:H191 | 1.93 | 0.40 |
| 20:7:46:TRP:CE2 | 51:7:807:4RF:H39 | 2.56 | 0.40 |
| 20:7:62:VAL:HG11 | 43:7:501:LUT:H12 | 2.03 | 0.40 |
| 25:8:602:CLA:H61 | 25:8:602:CLA:H41 | 1.89 | 0.40 |
| 1:A:253:LEU:HD23 | 1:A:253:LEU:HA | 1.86 | 0.40 |
| 1:A:615:GLN:HB3 | 1:A:631:THR:HG23 | 2.03 | 0.40 |
| 1:A:650:LEU:O | 1:A:654:SER:HB2 | 2.20 | 0.40 |
| 25:A:1116:CLA:H3A | 25:A:1116:CLA:HBA2 | 1.85 | 0.40 |
| 25:A:1130:CLA:NC | 25:L:1502:CLA:H112 | 2.36 | 0.40 |
| 34:A:5007:3PH:H361 | 34:A:5007:3PH:H332 | 1.74 | 0.40 |
| 2:B:379:ILE:O | 2:B:383:ILE:HG13 | 2.21 | 0.40 |
| 2:B:594:TYR:HA | 2:B:620:TRP:HH2 | 1.86 | 0.40 |
| 4:D:258:LEU:HD12 | 4:D:258:LEU:HA | 1.85 | 0.40 |
| 41:J:5002:SPH:H5 | 41:J:5002:SPH:H82 | 1.73 | 0.40 |
| 26:1:611:CHL:HHD | 26:1:611:CHL:HBC3 | 2.04 | 0.40 |
| 25:4:611:CLA:H11 | 25:4:611:CLA:H51 | 1.73 | 0.40 |
| 25:5:605:CLA:HED2 | 25:5:605:CLA:H2A | 2.04 | 0.40 |
| 29:7:503:BCR:H23C | 26:7:613:CHL:H2 | 2.03 | 0.40 |
| 22:2:145:ALA:HB3 | 22:2:146:PRO:HD3 | 2.04 | 0.40 |
| 25:2:604:CLA:H11 | 25:2:604:CLA:H52 | 1.87 | 0.40 |
| 25:9:604:CLA:H3A | 25:9:604:CLA:CGA | 2.51 | 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 | 739/741 (100%) | 709 (96%) | 30 (4%) | 0 | 100 | 100 |
| 2 | B | 729/731 (100%) | 697 (96%) | 32 (4%) | 0 | 100 | 100 |
| 3 | C | 78/80 (98%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | D | 141/143 (99%) | 129 (92%) | 12 (8%) | 0 | 100 | 100 |
| 5 | E | 62/64 (97%) | 60 (97%) | 2 (3%) | 0 | 100 | 100 |
| 6 | F | 163/165 (99%) | 154 (94%) | 9 (6%) | 0 | 100 | 100 |
| 7 | G | 97/99 (98%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 8 | H | 92/94 (98%) | 80 (87%) | 11 (12%) | 1 (1%) | 14 | 34 |
| 9 | J | 39/41 (95%) | 39 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 84/86 (98%) | 79 (94%) | 5 (6%) | 0 | 100 | 100 |
| 11 | L | 155/157 (99%) | 144 (93%) | 10 (6%) | 1 (1%) | 25 | 50 |
| 12 | M | 29/31 (94%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 13 | I | 33/35 (94%) | 29 (88%) | 4 (12%) | 0 | 100 | 100 |
| 14 | O | 85/87 (98%) | 66 (78%) | 16 (19%) | 3 (4%) | 3 | 8 |
| 15 | 1 | 190/192 (99%) | 174 (92%) | 15 (8%) | 1 (0%) | 29 | 54 |
| 15 | a | 190/192 (99%) | 171 (90%) | 19 (10%) | 0 | 100 | 100 |
| 16 | 3 | 239/241 (99%) | 225 (94%) | 13 (5%) | 1 (0%) | 34 | 60 |
| 17 | 4 | 205/207 (99%) | 184 (90%) | 19 (9%) | 2 (1%) | 15 | 37 |
| 18 | 5 | 227/229 (99%) | 214 (94%) | 13 (6%) | 0 | 100 | 100 |
| 19 | 6 | 229/231 (99%) | 213 (93%) | 15 (7%) | 1 (0%) | 34 | 60 |
| 20 | 7 | 219/221 (99%) | 207 (94%) | 11 (5%) | 1 (0%) | 29 | 54 |
| 21 | 8 | 217/219 (99%) | 207 (95%) | 10 (5%) | 0 | 100 | 100 |
| 22 | 2 | 213/215 (99%) | 197 (92%) | 16 (8%) | 0 | 100 | 100 |
| 23 | 9 | 181/183 (99%) | 171 (94%) | 10 (6%) | 0 | 100 | 100 |
| All | All | 4636/4684 (99%) | 4348 (94%) | 277 (6%) | 11 (0%) | 50 | 73 |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 118 | PRO |
| 14 | O | 93 | ASN |
| 14 | O | 95 | PRO |
| 15 | 1 | 36 | TRP |
| 17 | 4 | 224 | PHE |
| 14 | O | 94 | PHE |
| 16 | 3 | 265 | LYS |
| 19 | 6 | 255 | PRO |
| 11 | L | 447 | ILE |
| 20 | 7 | 164 | SER |
| 17 | 4 | 218 | ASN |

### 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 | 600/600 (100%) | 600 (100%) | 0 | 100 | 100 |
| 2 | B | 588/588 (100%) | 588 (100%) | 0 | 100 | 100 |
| 3 | C | 69/69 (100%) | 69 (100%) | 0 | 100 | 100 |
| 4 | D | 121/121 (100%) | 121 (100%) | 0 | 100 | 100 |
| 5 | E | 55/55 (100%) | 55 (100%) | 0 | 100 | 100 |
| 6 | F | 126/126 (100%) | 126 (100%) | 0 | 100 | 100 |
| 7 | G | 71/71 (100%) | 71 (100%) | 0 | 100 | 100 |
| 8 | H | 71/71 (100%) | 71 (100%) | 0 | 100 | 100 |
| 9 | J | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 10 | K | 66/66 (100%) | 66 (100%) | 0 | 100 | 100 |
| 11 | L | 122/122 (100%) | 122 (100%) | 0 | 100 | 100 |
| 12 | M | 23/23 (100%) | 23 (100%) | 0 | 100 | 100 |
| 13 | I | 30/30 (100%) | 30 (100%) | 0 | 100 | 100 |
| 14 | O | 66/66 (100%) | 66 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 15 | 1 | 134/134 (100%) | 134 (100%) | 0 | 100 | 100 |
| 15 | a | 134/134 (100%) | 134 (100%) | 0 | 100 | 100 |
| 16 | 3 | 186/186 (100%) | 186 (100%) | 0 | 100 | 100 |
| 17 | 4 | 165/165 (100%) | 165 (100%) | 0 | 100 | 100 |
| 18 | 5 | 185/185 (100%) | 185 (100%) | 0 | 100 | 100 |
| 19 | 6 | 187/187 (100%) | 187 (100%) | 0 | 100 | 100 |
| 20 | 7 | 176/176 (100%) | 176 (100%) | 0 | 100 | 100 |
| 21 | 8 | 168/168 (100%) | 167 (99%) | 1 (1%) | 86 | 95 |
| 22 | 2 | 173/173 (100%) | 173 (100%) | 0 | 100 | 100 |
| 23 | 9 | 141/141 (100%) | 141 (100%) | 0 | 100 | 100 |
| All | All | 3692/3692 (100%) | 3691 (100%) | 1 (0%) | 100 | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | 8 | 31 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | O | 131 | GLN |
| 15 | a | 35 | ASN |
| 17 | 4 | 131 | 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)

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

403 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 | $\#\|Z\| > 2$ |
| 25 | CLA | a | 601 | - | 60,68,73 | 1.40 | 9 (15%) | 70,107,113 | 2.06 | 18 (25%) |
| 30 | LHG | 9 | 802 | - | 48,48,48 | 0.38 | 0 | 51,54,54 | 1.13 | 3 (5%) |
| 26 | CHL | 9 | 613 | - | 42,50,74 | 1.16 | 4 (9%) | 44,85,114 | 1.47 | 8 (18%) |
| 25 | CLA | B | 1232 | - | 45,53,73 | 1.62 | 8 (17%) | 52,89,113 | 2.10 | 13 (25%) |
| 52 | P5S | 8 | 805 | - | 35,36,53 | 1.16 | 3 (8%) | 39,43,60 | 1.22 | 2 (5%) |
| 29 | BCR | L | 4001 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.29 | 16 (28%) |
| 25 | CLA | 2 | 615 | - | 56,64,73 | 1.46 | 8 (14%) | 65,102,113 | 2.12 | 16 (24%) |
| 49 | 13X | 6 | 805 | - | 9,9,9 | 0.88 | 0 | 12,12,12 | 0.38 | 0 |
| 25 | CLA | H | 1703 | - | 55,63,73 | 1.47 | 8 (14%) | 64,101,113 | 2.09 | 15 (23%) |
| 25 | CLA | B | 1217 | - | 56,64,73 | 1.46 | 10 (17%) | 65,102,113 | 2.14 | 17 (26%) |
| 47 | PLM | 5 | 804 | - | 17,17,17 | 0.57 | 0 | 17,17,17 | 1.13 | 0 |
| 25 | CLA | 2 | 607 | 30 | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.99 | 16 (21%) |
| 25 | CLA | 7 | 606 | - | 54,62,73 | 1.48 | 7 (12%) | 63,100,113 | 2.09 | 15 (23%) |
| 25 | CLA | H | 1702 | 8 | 46,54,73 | 1.60 | 9 (19%) | 53,90,113 | 2.20 | 13 (24%) |
| 51 | 4RF | 7 | 807 | - | 36,36,56 | 1.07 | 6 (16%) | 39,39,59 | 1.14 | 3 (7%) |
| 48 | DGA | 3 | 803 | - | 23,23,43 | 1.41 | 3 (13%) | 25,25,45 | 1.34 | 2 (8%) |
| 25 | CLA | B | 1210 | - | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 2.00 | 19 (25%) |
| 43 | LUT | 7 | 501 | - | 42,43,43 | 2.38 | 1 (2%) | 51,60,60 | 2.06 | 11 (21%) |
| 25 | CLA | 4 | 612 | 17 | 62,70,73 | 1.37 | 7 (11%) | 72,109,113 | 2.07 | 17 (23%) |
| 26 | CHL | 7 | 613 | - | 61,69,74 | 0.92 | 4 (6%) | 67,108,114 | 1.23 | 11 (16%) |
| 27 | PQN | A | 2001 | - | 34,34,34 | 0.37 | 0 | 42,45,45 | 1.14 | 2 (4%) |
| 29 | BCR | 5 | 504 | - | 41,41,41 | 1.84 | 4 (9%) | 56,56,56 | 4.54 | 19 (33%) |
| 25 | CLA | 8 | 612 | - | 50,58,73 | 1.53 | 7 (14%) | 58,95,113 | 2.15 | 14 (24%) |
| 25 | CLA | 8 | 605 | - | 55,63,73 | 1.48 | 9 (16%) | 64,101,113 | 2.10 | 16 (25%) |
| 25 | CLA | A | 1126 | - | 65,73,73 | 1.37 | 9 (13%) | 76,113,113 | 1.98 | 17 (22%) |
| 25 | CLA | 2 | 604 | - | 56,64,73 | 1.44 | 7 (12%) | 65,102,113 | 2.18 | 18 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 29 | BCR | O | 4001 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.63 | 14 (25%) |
| 25 | CLA | 2 | 603 | 22 | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.17 | 20 (28%) |
| 29 | BCR | 5 | 503 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.34 | 17 (30%) |
| 25 | CLA | B | 1239 | - | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.95 | 17 (22%) |
| 25 | CLA | 3 | 602 | - | 46,54,73 | 1.58 | 8 (17%) | 53,90,113 | 2.15 | 16 (30%) |
| 43 | LUT | a | 503 | - | 42,43,43 | 2.36 | 1 (2%) | 51,60,60 | 2.28 | 15 (29%) |
| 43 | LUT | 5 | 501 | - | 42,43,43 | 2.34 | 1 (2%) | 51,60,60 | 1.92 | 14 (27%) |
| 25 | CLA | L | 1504 | - | 50,58,73 | 1.56 | 8 (16%) | 58,95,113 | 2.19 | 15 (25%) |
| 25 | CLA | a | 607 | - | 58,66,73 | 1.44 | 9 (15%) | 67,104,113 | 2.08 | 16 (23%) |
| 25 | CLA | A | 1141 | - | 45,53,73 | 1.62 | 9 (20%) | 52,89,113 | 2.21 | 12 (23%) |
| 25 | CLA | 5 | 601 | 18 | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.08 | 20 (28%) |
| 30 | LHG | 7 | 802 | - | 35,35,48 | 0.44 | 0 | 38,41,54 | 1.07 | 2 (5%) |
| 25 | CLA | 7 | 610 | - | 60,68,73 | 1.41 | 9 (15%) | 70,107,113 | 2.04 | 16 (22%) |
| 33 | PTY | a | 802 | - | 37,37,49 | 1.00 | 4 (10%) | 40,42,54 | 1.10 | 2 (5%) |
| 25 | CLA | 1 | 603 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 1.98 | 16 (21%) |
| 38 | LPX | F | 5003 | - | 29,29,29 | 1.00 | 2 (6%) | 31,33,33 | 0.93 | 1 (3%) |
| 25 | CLA | 1 | 607 | 30 | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 1.92 | 15 (19%) |
| 29 | BCR | J | 4001 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.26 | 17 (30%) |
| 50 | XAT | 9 | 507 | - | 39,47,47 | 0.69 | 1 (2%) | 54,74,74 | 1.98 | 14 (25%) |
| 24 | CL0 | A | 1011 | - | 65,73,73 | 2.37 | 18 (27%) | 76,113,113 | 2.50 | 21 (27%) |
| 25 | CLA | 4 | 601 | - | 60,68,73 | 1.39 | 7 (11%) | 70,107,113 | 2.09 | 19 (27%) |
| 25 | CLA | A | 1109 | 25 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 2.04 | 18 (23%) |
| 25 | CLA | 6 | 607 | 30 | 55,63,73 | 1.48 | 8 (14%) | 64,101,113 | 2.05 | 16 (25%) |
| 25 | CLA | A | 1110 | - | 54,62,73 | 1.49 | 10 (18%) | 62,99,113 | 2.13 | 16 (25%) |
| 25 | CLA | 7 | 605 | - | 43,52,73 | 1.65 | 8 (18%) | 49,88,113 | 2.06 | 15 (30%) |
| 37 | PCW | B | 5004 | - | 38,38,53 | 1.29 | 4 (10%) | 44,46,61 | 1.07 | 2 (4%) |
| 30 | LHG | a | 801 | - | 34,34,48 | 0.45 | 0 | 37,40,54 | 1.10 | 3 (8%) |
| 43 | LUT | 5 | 502 | - | 42,43,43 | 2.33 | 1 (2%) | 51,60,60 | 1.90 | 11 (21%) |
| 25 | CLA | 1 | 602 | - | 45,53,73 | 1.63 | 9 (20%) | 52,89,113 | 2.10 | 13 (25%) |
| 25 | CLA | B | 1229 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 2.00 | 19 (25%) |
| 25 | CLA | 8 | 602 | - | 52,60,73 | 1.51 | 8 (15%) | 60,97,113 | 2.16 | 16 (26%) |
| 25 | CLA | B | 1237 | - | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 1.92 | 15 (19%) |
| 25 | CLA | 4 | 615 | 17 | 60,68,73 | 1.42 | 8 (13%) | 70,107,113 | 1.96 | 15 (21%) |
| 25 | CLA | a | 603 | - | 65,73,73 | 1.35 | 7 (10%) | 76,113,113 | 2.05 | 17 (22%) |
| 43 | LUT | 4 | 501 | - | 42,43,43 | 2.36 | 1 (2%) | 51,60,60 | 2.01 | 12 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 43 | LUT | a | 501 | - | 42,43,43 | 2.36 | 1 (2%) | 51,60,60 | 2.07 | 12 (23%) |
| 25 | CLA | 3 | 606 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 1.96 | 15 (19%) |
| 26 | CHL | 6 | 611 | - | 51,59,74 | 0.97 | 3 (5%) | 55,96,114 | 1.43 | 11 (20%) |
| 43 | LUT | 5 | 505 | - | 42,43,43 | 2.38 | 1 (2%) | 51,60,60 | 2.28 | 14 (27%) |
| 50 | XAT | 9 | 504 | - | 39,47,47 | 0.66 | 1 (2%) | 54,74,74 | 6.69 | 16 (29%) |
| 33 | PTY | a | 803 | - | 37,37,49 | 1.00 | 4 (10%) | 40,42,54 | 1.08 | 2 (5%) |
| 26 | CHL | 1 | 604 | - | 66,74,74 | 0.92 | 4 (6%) | 73,114,114 | 1.32 | 9 (12%) |
| 25 | CLA | 2 | 608 | - | 45,53,73 | 1.63 | 8 (17%) | 52,89,113 | 2.10 | 12 (23%) |
| 25 | CLA | B | 1211 | - | 55,63,73 | 1.46 | 8 (14%) | 64,101,113 | 2.14 | 20 (31%) |
| 25 | CLA | K | 1402 | - | 60,68,73 | 1.42 | 9 (15%) | 70,107,113 | 2.05 | 17 (24%) |
| 28 | SF4 | C | 3002 | 3 | 0,12,12 | - | - | - | | |
| 30 | LHG | 1 | 802 | - | 48,48,48 | 0.40 | 0 | 51,54,54 | 1.00 | 3 (5%) |
| 25 | CLA | A | 1117 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 2.11 | 17 (22%) |
| 25 | CLA | B | 1238 | - | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 1.97 | 16 (21%) |
| 25 | CLA | A | 1119 | - | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.91 | 16 (21%) |
| 25 | CLA | 2 | 601 | - | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.18 | 18 (25%) |
| 26 | CHL | 8 | 601 | 21 | 61,69,74 | 0.99 | 4 (6%) | 67,108,114 | 1.41 | 9 (13%) |
| 43 | LUT | 3 | 501 | - | 42,43,43 | 2.36 | 1 (2%) | 51,60,60 | 1.96 | 14 (27%) |
| 39 | NEX | F | 4001 | - | 38,46,46 | 3.37 | 9 (23%) | 50,70,70 | 4.73 | 16 (32%) |
| 30 | LHG | 6 | 802 | - | 36,36,48 | 0.43 | 0 | 39,42,54 | 1.24 | 3 (7%) |
| 25 | CLA | A | 1108 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.91 | 16 (21%) |
| 25 | CLA | F | 1301 | - | 50,58,73 | 1.55 | 7 (14%) | 58,95,113 | 2.20 | 15 (25%) |
| 29 | BCR | 8 | 503 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.24 | 12 (21%) |
| 26 | CHL | 4 | 609 | 17 | 66,74,74 | 0.84 | 3 (4%) | 73,114,114 | 1.25 | 10 (13%) |
| 29 | BCR | A | 4002 | - | 41,41,41 | 1.80 | 4 (9%) | 56,56,56 | 4.10 | 14 (25%) |
| 25 | CLA | F | 1302 | - | 55,63,73 | 1.46 | 7 (12%) | 64,101,113 | 2.13 | 17 (26%) |
| 25 | CLA | G | 1601 | - | 50,58,73 | 1.55 | 8 (16%) | 58,95,113 | 2.18 | 16 (27%) |
| 25 | CLA | L | 1502 | - | 60,68,73 | 1.39 | 8 (13%) | 70,107,113 | 2.09 | 18 (25%) |
| 25 | CLA | 7 | 602 | - | 44,52,73 | 1.63 | 7 (15%) | 51,88,113 | 2.11 | 13 (25%) |
| 25 | CLA | A | 1135 | - | 51,59,73 | 1.55 | 9 (17%) | 59,96,113 | 2.20 | 17 (28%) |
| 25 | CLA | B | 1240 | 30 | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 2.00 | 18 (23%) |
| 32 | SQD | G | 5001 | - | 45,46,54 | 0.84 | 0 | 54,57,65 | 0.95 | 2 (3%) |
| 33 | PTY | G | 5002 | - | 27,27,49 | 1.03 | 2 (7%) | 28,31,54 | 1.07 | 1 (3%) |
| 25 | CLA | B | 1207 | - | 60,68,73 | 1.41 | 7 (11%) | 70,107,113 | 1.97 | 15 (21%) |
| 30 | LHG | F | 5001 | - | 42,42,48 | 0.42 | 0 | 45,48,54 | 1.10 | 2 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 43 | LUT | 2 | 507 | - | 42,43,43 | 2.38 | 1 (2%) | 51,60,60 | 2.56 | 18 (35%) |
| 25 | CLA | A | 1013 | - | 65,73,73 | 1.33 | 7 (10%) | 76,113,113 | 1.91 | 17 (22%) |
| 29 | BCR | A | 4005 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.22 | 13 (23%) |
| 26 | CHL | 6 | 609 | 19 | 66,74,74 | 0.77 | 2 (3%) | 73,114,114 | 1.25 | 12 (16%) |
| 36 | DGD | 8 | 803 | - | 47,47,67 | 0.81 | 1 (2%) | 61,61,81 | 1.09 | 3 (4%) |
| 25 | CLA | 2 | 612 | - | 50,58,73 | 1.56 | 9 (18%) | 58,95,113 | 2.14 | 15 (25%) |
| 30 | LHG | 2 | 801 | 25 | 48,48,48 | 0.36 | 0 | 51,54,54 | 1.03 | 2 (3%) |
| 25 | CLA | 8 | 615 | 21 | 46,54,73 | 1.60 | 8 (17%) | 53,90,113 | 2.19 | 14 (26%) |
| 25 | CLA | B | 1230 | - | 58,66,73 | 1.41 | 6 (10%) | 67,104,113 | 2.13 | 18 (26%) |
| 43 | LUT | 8 | 501 | - | 42,43,43 | 2.35 | 1 (2%) | 51,60,60 | 1.90 | 13 (25%) |
| 25 | CLA | 3 | 610 | 16 | 57,65,73 | 1.43 | 8 (14%) | 66,103,113 | 2.10 | 18 (27%) |
| 44 | AXT | 1 | 502 | - | 44,44,45 | 2.95 | 15 (34%) | 55,62,64 | 1.98 | 13 (23%) |
| 25 | CLA | A | 1125 | - | 65,73,73 | 1.38 | 10 (15%) | 76,113,113 | 1.93 | 16 (21%) |
| 25 | CLA | B | 1212 | - | 57,65,73 | 1.43 | 7 (12%) | 66,103,113 | 2.15 | 19 (28%) |
| 25 | CLA | 4 | 606 | - | 50,58,73 | 1.53 | 8 (16%) | 58,95,113 | 2.25 | 17 (29%) |
| 29 | BCR | 3 | 505 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.28 | 15 (26%) |
| 25 | CLA | B | 1213 | - | 55,63,73 | 1.45 | 7 (12%) | 64,101,113 | 2.13 | 17 (26%) |
| 47 | PLM | 8 | 806 | - | 16,16,17 | 0.42 | 0 | 15,15,17 | 0.92 | 0 |
| 25 | CLA | 8 | 608 | - | 52,60,73 | 1.51 | 7 (13%) | 60,97,113 | 2.18 | 17 (28%) |
| 29 | BCR | B | 4005 | - | 41,41,41 | 1.84 | 4 (9%) | 56,56,56 | 4.28 | 12 (21%) |
| 25 | CLA | 1 | 615 | 15 | 46,54,73 | 1.59 | 7 (15%) | 53,90,113 | 2.17 | 14 (26%) |
| 43 | LUT | 1 | 501 | - | 42,43,43 | 2.36 | 1 (2%) | 51,60,60 | 1.96 | 15 (29%) |
| 30 | LHG | F | 5002 | - | 35,35,48 | 0.43 | 0 | 38,41,54 | 1.19 | 3 (7%) |
| 25 | CLA | 1 | 608 | - | 60,68,73 | 1.40 | 9 (15%) | 70,107,113 | 1.99 | 14 (20%) |
| 30 | LHG | 4 | 801 | - | 48,48,48 | 0.39 | 0 | 51,54,54 | 0.99 | 2 (3%) |
| 25 | CLA | B | 1220 | - | 60,68,73 | 1.41 | 9 (15%) | 70,107,113 | 2.00 | 15 (21%) |
| 48 | DGA | 5 | 803 | - | 22,22,43 | 1.43 | 3 (13%) | 24,24,45 | 1.33 | 2 (8%) |
| 25 | CLA | A | 1128 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 2.02 | 16 (21%) |
| 25 | CLA | 4 | 611 | - | 56,64,73 | 1.46 | 7 (12%) | 65,102,113 | 2.11 | 17 (26%) |
| 25 | CLA | A | 1012 | - | 65,73,73 | 1.37 | 8 (12%) | 76,113,113 | 1.98 | 15 (19%) |
| 45 | OLA | 8 | 808 | - | 19,19,19 | 0.56 | 0 | 19,19,19 | 1.03 | 0 |
| 25 | CLA | A | 1101 | - | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.96 | 18 (23%) |
| 26 | CHL | 2 | 609 | 22 | 66,74,74 | 0.88 | 4 (6%) | 73,114,114 | 1.23 | 10 (13%) |
| 26 | CHL | 9 | 610 | - | 51,59,74 | 0.96 | 3 (5%) | 55,96,114 | 1.42 | 12 (21%) |
| 25 | CLA | B | 1201 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 4.36 | 21 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 26 | CHL | 8 | 613 | - | 51,59,74 | 0.97 | 3 (5%) | 55,96,114 | 1.39 | 9 (16%) |
| 25 | CLA | a | 615 | 15 | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.11 | 12 (22%) |
| 25 | CLA | 5 | 608 | - | 45,53,73 | 1.63 | 8 (17%) | 52,89,113 | 2.04 | 12 (23%) |
| 25 | CLA | a | 608 | - | 55,63,73 | 1.48 | 9 (16%) | 64,101,113 | 2.08 | 15 (23%) |
| 26 | CHL | 9 | 608 | - | 48,56,74 | 0.98 | 3 (6%) | 51,92,114 | 1.41 | 10 (19%) |
| 26 | CHL | 6 | 619 | 19 | 66,74,74 | 0.80 | 2 (3%) | 73,114,114 | 1.35 | 11 (15%) |
| 29 | BCR | A | 4001 | - | 41,41,41 | 1.82 | 4 (9%) | 56,56,56 | 4.26 | 17 (30%) |
| 25 | CLA | 5 | 614 | 18 | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.08 | 13 (24%) |
| 29 | BCR | L | 4003 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.35 | 15 (26%) |
| 30 | LHG | 8 | 801 | 25 | 36,36,48 | 0.44 | 0 | 39,42,54 | 1.15 | 3 (7%) |
| 25 | CLA | B | 1215 | - | 60,68,73 | 1.40 | 7 (11%) | 70,107,113 | 1.97 | 13 (18%) |
| 37 | PCW | K | 5001 | - | 40,40,53 | 1.26 | 4 (10%) | 46,48,61 | 1.08 | 2 (4%) |
| 25 | CLA | B | 1231 | - | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 1.92 | 14 (18%) |
| 25 | CLA | 6 | 612 | - | 50,58,73 | 1.54 | 8 (16%) | 58,95,113 | 2.19 | 15 (25%) |
| 26 | CHL | A | 1114 | - | 66,74,74 | 0.87 | 3 (4%) | 73,114,114 | 1.32 | 9 (12%) |
| 25 | CLA | 3 | 613 | - | 61,69,73 | 1.38 | 8 (13%) | 71,108,113 | 2.03 | 17 (23%) |
| 25 | CLA | A | 1121 | - | 60,68,73 | 1.41 | 8 (13%) | 70,107,113 | 2.10 | 18 (25%) |
| 29 | BCR | K | 4002 | - | 41,41,41 | 1.84 | 4 (9%) | 56,56,56 | 4.29 | 16 (28%) |
| 25 | CLA | 5 | 607 | - | 60,68,73 | 1.41 | 8 (13%) | 70,107,113 | 2.05 | 17 (24%) |
| 33 | PTY | A | 5006 | - | 33,33,49 | 1.05 | 4 (12%) | 36,38,54 | 1.10 | 2 (5%) |
| 25 | CLA | 6 | 603 | - | 65,73,73 | 1.35 | 10 (15%) | 76,113,113 | 1.97 | 16 (21%) |
| 32 | SQD | I | 5001 | - | 53,54,54 | 0.80 | 0 | 62,65,65 | 0.89 | 2 (3%) |
| 26 | CHL | 5 | 617 | 18 | 47,55,74 | 0.98 | 3 (6%) | 50,91,114 | 1.46 | 11 (22%) |
| 25 | CLA | 7 | 604 | 20 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 2.01 | 17 (22%) |
| 32 | SQD | A | 5005 | - | 53,54,54 | 0.79 | 0 | 62,65,65 | 0.91 | 2 (3%) |
| 27 | PQN | B | 2002 | - | 34,34,34 | 0.37 | 0 | 42,45,45 | 1.05 | 3 (7%) |
| 37 | PCW | K | 5002 | - | 35,35,53 | 1.31 | 4 (11%) | 41,43,61 | 1.07 | 2 (4%) |
| 25 | CLA | 8 | 618 | 21 | 60,68,73 | 1.41 | 8 (13%) | 70,107,113 | 2.09 | 16 (22%) |
| 25 | CLA | A | 1139 | - | 55,63,73 | 1.49 | 9 (16%) | 64,101,113 | 2.08 | 15 (23%) |
| 43 | LUT | 6 | 502 | - | 42,43,43 | 2.32 | 1 (2%) | 51,60,60 | 1.98 | 14 (27%) |
| 25 | CLA | A | 1137 | - | 60,68,73 | 1.42 | 8 (13%) | 70,107,113 | 2.06 | 20 (28%) |
| 26 | CHL | 1 | 613 | - | 48,56,74 | 0.92 | 2 (4%) | 51,92,114 | 1.39 | 9 (17%) |
| 25 | CLA | 1 | 612 | 15 | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.95 | 16 (21%) |
| 30 | LHG | 9 | 801 | - | 32,32,48 | 0.47 | 0 | 35,38,54 | 1.18 | 3 (8%) |
| 25 | CLA | 5 | 604 | 18 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.98 | 16 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 25 | CLA | 5 | 603 | 18 | 56,64,73 | 1.46 | 10 (17%) | 65,102,113 | 2.11 | 17 (26%) |
| 47 | PLM | 4 | 804 | - | 17,17,17 | 0.57 | 0 | 17,17,17 | 1.06 | 0 |
| 26 | CHL | 9 | 603 | - | 66,74,74 | 0.88 | 3 (4%) | 73,114,114 | 1.16 | 8 (10%) |
| 25 | CLA | A | 1123 | - | 65,73,73 | 1.36 | 10 (15%) | 76,113,113 | 2.02 | 16 (21%) |
| 25 | CLA | 8 | 609 | 21 | 60,68,73 | 1.41 | 8 (13%) | 70,107,113 | 2.08 | 17 (24%) |
| 25 | CLA | G | 1603 | - | 45,53,73 | 1.63 | 8 (17%) | 52,89,113 | 2.11 | 14 (26%) |
| 26 | CHL | 3 | 604 | 16 | 66,74,74 | 0.92 | 4 (6%) | 73,114,114 | 1.38 | 9 (12%) |
| 29 | BCR | B | 4002 | - | 41,41,41 | 1.84 | 4 (9%) | 56,56,56 | 4.34 | 14 (25%) |
| 25 | CLA | B | 1221 | - | 65,73,73 | 1.34 | 10 (15%) | 76,113,113 | 2.03 | 18 (23%) |
| 26 | CHL | 4 | 613 | - | 52,60,74 | 0.95 | 3 (5%) | 56,97,114 | 1.34 | 10 (17%) |
| 25 | CLA | a | 611 | - | 50,58,73 | 1.54 | 9 (18%) | 58,95,113 | 2.19 | 16 (27%) |
| 25 | CLA | A | 1103 | - | 65,73,73 | 1.33 | 7 (10%) | 76,113,113 | 2.01 | 16 (21%) |
| 25 | CLA | 3 | 616 | - | 56,64,73 | 1.45 | 7 (12%) | 65,102,113 | 2.15 | 17 (26%) |
| 25 | CLA | 8 | 607 | 30 | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.12 | 11 (20%) |
| 30 | LHG | B | 5002 | - | 48,48,48 | 0.39 | 0 | 51,54,54 | 1.07 | 3 (5%) |
| 30 | LHG | B | 5001 | 25 | 48,48,48 | 0.40 | 0 | 51,54,54 | 0.98 | 3 (5%) |
| 25 | CLA | B | 1214 | - | 59,67,73 | 1.43 | 8 (13%) | 68,105,113 | 2.09 | 16 (23%) |
| 41 | SPH | 9 | 804 | - | 19,20,20 | 0.65 | 0 | 18,21,21 | 1.08 | 0 |
| 43 | LUT | 4 | 502 | - | 42,43,43 | 2.34 | 1 (2%) | 51,60,60 | 1.93 | 13 (25%) |
| 29 | BCR | 3 | 504 | - | 41,41,41 | 1.84 | 4 (9%) | 56,56,56 | 4.33 | 17 (30%) |
| 29 | BCR | H | 4001 | - | 41,41,41 | 1.86 | 4 (9%) | 56,56,56 | 7.67 | 20 (35%) |
| 29 | BCR | G | 4001 | - | 41,41,41 | 1.87 | 4 (9%) | 56,56,56 | 4.42 | 15 (26%) |
| 29 | BCR | 3 | 503 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.31 | 15 (26%) |
| 33 | PTY | G | 5003 | - | 27,27,49 | 1.02 | 2 (7%) | 28,31,54 | 1.07 | 1 (3%) |
| 29 | BCR | B | 4004 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.26 | 15 (26%) |
| 25 | CLA | A | 1133 | - | 65,73,73 | 1.37 | 9 (13%) | 76,113,113 | 1.90 | 14 (18%) |
| 25 | CLA | B | 1235 | - | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 2.03 | 17 (22%) |
| 26 | CHL | 8 | 610 | - | 56,64,74 | 0.90 | 3 (5%) | 61,102,114 | 1.40 | 13 (21%) |
| 26 | CHL | a | 610 | - | 48,56,74 | 0.97 | 3 (6%) | 51,92,114 | 1.37 | 10 (19%) |
| 33 | PTY | 7 | 804 | - | 32,32,49 | 1.05 | 4 (12%) | 35,37,54 | 1.19 | 2 (5%) |
| 26 | CHL | 5 | 613 | - | 56,64,74 | 0.85 | 2 (3%) | 61,102,114 | 1.37 | 11 (18%) |
| 46 | QTB | a | 504 | - | 19,19,19 | 2.54 | 5 (26%) | 20,26,26 | 2.83 | 8 (40%) |
| 25 | CLA | B | 1206 | 2 | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 2.03 | 16 (21%) |
| 30 | LHG | A | 5002 | - | 48,48,48 | 0.39 | 0 | 51,54,54 | 1.00 | 3 (5%) |
| 25 | CLA | a | 612 | 15 | 57,65,73 | 1.45 | 9 (15%) | 66,103,113 | 2.02 | 15 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 25 | CLA | a | 605 | - | 55,63,73 | 1.46 | 8 (14%) | 64,101,113 | 2.14 | 18 (28%) |
| 26 | CHL | 1 | 611 | - | 56,64,74 | 0.92 | 3 (5%) | 61,102,114 | 1.33 | 9 (14%) |
| 25 | CLA | 9 | 612 | - | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 1.95 | 16 (21%) |
| 25 | CLA | 6 | 615 | 54 | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 2.02 | 16 (21%) |
| 30 | LHG | 5 | 801 | - | 48,48,48 | 0.38 | 0 | 51,54,54 | 1.08 | 3 (5%) |
| 26 | CHL | 7 | 609 | 20 | 62,70,74 | 0.89 | 3 (4%) | 68,109,114 | 1.26 | 10 (14%) |
| 47 | PLM | 8 | 807 | - | 17,17,17 | 0.56 | 0 | 17,17,17 | 1.13 | 0 |
| 25 | CLA | 6 | 608 | - | 55,63,73 | 1.47 | 10 (18%) | 64,101,113 | 2.14 | 16 (25%) |
| 25 | CLA | a | 602 | - | 50,58,73 | 1.55 | 8 (16%) | 58,95,113 | 2.17 | 17 (29%) |
| 25 | CLA | B | 1236 | - | 53,61,73 | 1.50 | 9 (16%) | 61,98,113 | 2.11 | 17 (27%) |
| 25 | CLA | B | 1208 | - | 54,62,73 | 1.41 | 7 (12%) | 67,100,113 | 2.11 | 18 (26%) |
| 29 | BCR | 6 | 504 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.42 | 17 (30%) |
| 25 | CLA | B | 1023 | - | 65,73,73 | 1.35 | 7 (10%) | 76,113,113 | 1.96 | 16 (21%) |
| 26 | CHL | 5 | 611 | - | 51,59,74 | 1.05 | 4 (7%) | 55,96,114 | 1.40 | 9 (16%) |
| 33 | PTY | 3 | 802 | - | 37,37,49 | 0.99 | 4 (10%) | 40,42,54 | 1.10 | 2 (5%) |
| 25 | CLA | A | 1112 | - | 55,63,73 | 1.46 | 6 (10%) | 64,101,113 | 2.22 | 17 (26%) |
| 26 | CHL | 1 | 609 | 15 | 66,74,74 | 0.86 | 3 (4%) | 73,114,114 | 1.16 | 9 (12%) |
| 28 | SF4 | A | 3001 | 1,2 | 0,12,12 | - | - | - | | |
| 26 | CHL | a | 604 | - | 61,69,74 | 0.97 | 4 (6%) | 67,108,114 | 1.39 | 9 (13%) |
| 25 | CLA | B | 1202 | - | 65,73,73 | 1.35 | 9 (13%) | 76,113,113 | 1.94 | 16 (21%) |
| 25 | CLA | 2 | 605 | - | 60,68,73 | 1.42 | 9 (15%) | 70,107,113 | 2.04 | 19 (27%) |
| 25 | CLA | 3 | 601 | 16 | 65,73,73 | 1.35 | 7 (10%) | 76,113,113 | 1.96 | 17 (22%) |
| 29 | BCR | B | 4001 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.28 | 13 (23%) |
| 26 | CHL | 3 | 603 | 16 | 66,74,74 | 0.92 | 4 (6%) | 73,114,114 | 1.16 | 8 (10%) |
| 25 | CLA | B | 1205 | - | 65,73,73 | 1.35 | 10 (15%) | 76,113,113 | 2.03 | 16 (21%) |
| 25 | CLA | 4 | 605 | - | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.11 | 13 (24%) |
| 25 | CLA | A | 1116 | - | 60,68,73 | 1.42 | 9 (15%) | 70,107,113 | 2.00 | 15 (21%) |
| 29 | BCR | 4 | 503 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.37 | 12 (21%) |
| 25 | CLA | B | 1218 | - | 55,63,73 | 1.46 | 7 (12%) | 64,101,113 | 2.23 | 18 (28%) |
| 25 | CLA | B | 1234 | - | 63,69,73 | 1.22 | 5 (7%) | 71,99,113 | 2.17 | 17 (23%) |
| 25 | CLA | A | 1111 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 2.02 | 18 (23%) |
| 25 | CLA | G | 1602 | 7 | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.05 | 18 (25%) |
| 30 | LHG | A | 5001 | - | 48,48,48 | 0.39 | 0 | 51,54,54 | 1.10 | 3 (5%) |
| 25 | CLA | 4 | 602 | - | 52,60,73 | 1.51 | 8 (15%) | 60,97,113 | 2.14 | 17 (28%) |
| 26 | CHL | a | 609 | 15 | 53,61,74 | 0.87 | 2 (3%) | 57,98,114 | 1.34 | 12 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 29 | BCR | K | 4001 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.32 | 15 (26%) |
| 29 | BCR | B | 4007 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.34 | 15 (26%) |
| 43 | LUT | a | 502 | - | 42,43,43 | 2.35 | 1 (2%) | 51,60,60 | 1.97 | 14 (27%) |
| 25 | CLA | B | 1203 | 2 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.91 | 15 (19%) |
| 45 | OLA | 1 | 803 | - | 19,19,19 | 0.56 | 0 | 19,19,19 | 1.03 | 0 |
| 25 | CLA | B | 1216 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 1.94 | 18 (23%) |
| 25 | CLA | B | 1204 | - | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 2.01 | 18 (23%) |
| 30 | LHG | 6 | 801 | 25 | 48,48,48 | 0.40 | 0 | 51,54,54 | 1.05 | 3 (5%) |
| 37 | PCW | 6 | 803 | - | 35,35,53 | 1.29 | 4 (11%) | 41,43,61 | 1.13 | 2 (4%) |
| 25 | CLA | 1 | 601 | - | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.03 | 17 (24%) |
| 34 | 3PH | A | 5007 | - | 32,32,47 | 1.02 | 4 (12%) | 36,37,52 | 1.20 | 2 (5%) |
| 30 | LHG | 3 | 801 | 25 | 48,48,48 | 0.40 | 0 | 51,54,54 | 1.03 | 3 (5%) |
| 25 | CLA | K | 1401 | - | 46,54,73 | 1.60 | 7 (15%) | 53,90,113 | 2.06 | 12 (22%) |
| 26 | CHL | 7 | 615 | 20 | 51,59,74 | 0.96 | 3 (5%) | 55,96,114 | 1.38 | 11 (20%) |
| 25 | CLA | 2 | 602 | - | 52,60,73 | 1.52 | 8 (15%) | 60,97,113 | 2.14 | 17 (28%) |
| 25 | CLA | A | 1105 | - | 57,65,73 | 1.45 | 9 (15%) | 66,103,113 | 2.07 | 15 (22%) |
| 25 | CLA | A | 1122 | - | 60,68,73 | 1.42 | 9 (15%) | 70,107,113 | 1.98 | 16 (22%) |
| 33 | PTY | 5 | 802 | - | 37,37,49 | 0.99 | 4 (10%) | 40,42,54 | 1.16 | 2 (5%) |
| 25 | CLA | A | 1120 | - | 49,57,73 | 1.55 | 8 (16%) | 55,93,113 | 2.26 | 16 (29%) |
| 25 | CLA | 5 | 612 | 18 | 65,73,73 | 1.34 | 9 (13%) | 76,113,113 | 1.97 | 17 (22%) |
| 30 | LHG | 1 | 801 | 25 | 34,34,48 | 0.44 | 0 | 37,40,54 | 1.15 | 3 (8%) |
| 25 | CLA | 4 | 610 | - | 65,73,73 | 1.37 | 8 (12%) | 76,113,113 | 2.01 | 16 (21%) |
| 25 | CLA | 8 | 611 | - | 50,58,73 | 1.52 | 7 (14%) | 58,95,113 | 2.21 | 17 (29%) |
| 53 | LAP | 8 | 810 | - | 28,28,28 | 1.22 | 2 (7%) | 33,35,35 | 0.99 | 1 (3%) |
| 44 | AXT | 7 | 504 | - | 44,44,45 | 2.41 | 17 (38%) | 55,62,64 | 2.40 | 17 (30%) |
| 25 | CLA | L | 1503 | - | 45,53,73 | 1.60 | 8 (17%) | 52,89,113 | 2.16 | 15 (28%) |
| 25 | CLA | 7 | 612 | - | 60,68,73 | 1.42 | 8 (13%) | 70,107,113 | 2.01 | 16 (22%) |
| 25 | CLA | 4 | 617 | - | 45,53,73 | 1.62 | 8 (17%) | 52,89,113 | 2.15 | 14 (26%) |
| 25 | CLA | B | 1022 | 54 | 65,73,73 | 1.38 | 9 (13%) | 76,113,113 | 1.92 | 17 (22%) |
| 25 | CLA | A | 1115 | - | 60,68,73 | 1.41 | 8 (13%) | 70,107,113 | 2.01 | 16 (22%) |
| 30 | LHG | A | 5003 | - | 45,45,48 | 0.40 | 0 | 48,51,54 | 1.04 | 3 (6%) |
| 25 | CLA | K | 1403 | 10 | 49,57,73 | 1.56 | 8 (16%) | 55,93,113 | 2.24 | 16 (29%) |
| 25 | CLA | A | 1130 | - | 56,64,73 | 1.46 | 7 (12%) | 65,102,113 | 2.08 | 15 (23%) |
| 31 | LMG | A | 5004 | - | 42,42,55 | 0.78 | 2 (4%) | 50,50,63 | 1.07 | 2 (4%) |
| 45 | OLA | 8 | 809 | - | 19,19,19 | 0.57 | 0 | 19,19,19 | 1.00 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 26 | CHL | 5 | 610 | - | 66,74,74 | 0.83 | 3 (4%) | 73,114,114 | 1.24 | 12 (16%) |
| 25 | CLA | 3 | 612 | 16 | 50,58,73 | 1.52 | 7 (14%) | 58,95,113 | 2.20 | 15 (25%) |
| 32 | SQD | 7 | 805 | - | 38,39,54 | 0.90 | 0 | 47,50,65 | 1.01 | 3 (6%) |
| 25 | CLA | 5 | 605 | - | 46,54,73 | 1.61 | 9 (19%) | 53,90,113 | 2.11 | 14 (26%) |
| 25 | CLA | 5 | 606 | - | 50,58,73 | 1.54 | 9 (18%) | 58,95,113 | 2.23 | 17 (29%) |
| 48 | DGA | 8 | 804 | - | 39,39,43 | 1.16 | 3 (7%) | 41,41,45 | 1.57 | 3 (7%) |
| 25 | CLA | O | 1802 | - | 55,63,73 | 1.47 | 8 (14%) | 64,101,113 | 2.19 | 20 (31%) |
| 25 | CLA | 2 | 606 | - | 46,54,73 | 1.60 | 7 (15%) | 53,90,113 | 2.14 | 15 (28%) |
| 26 | CHL | 6 | 610 | - | 56,64,74 | 0.93 | 3 (5%) | 61,102,114 | 1.34 | 11 (18%) |
| 25 | CLA | A | 1106 | 1 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 2.02 | 17 (22%) |
| 26 | CHL | a | 606 | - | 56,64,74 | 0.93 | 3 (5%) | 61,102,114 | 1.37 | 12 (19%) |
| 32 | SQD | H | 5001 | - | 44,45,54 | 0.85 | 0 | 53,56,65 | 0.97 | 2 (3%) |
| 26 | CHL | 4 | 618 | - | 56,64,74 | 0.93 | 3 (5%) | 61,102,114 | 1.31 | 11 (18%) |
| 25 | CLA | A | 1136 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 2.00 | 15 (19%) |
| 26 | CHL | 3 | 608 | - | 43,51,74 | 1.04 | 3 (6%) | 45,86,114 | 1.48 | 9 (20%) |
| 25 | CLA | B | 1225 | - | 65,73,73 | 1.36 | 7 (10%) | 76,113,113 | 1.91 | 16 (21%) |
| 25 | CLA | 7 | 608 | - | 55,63,73 | 1.48 | 8 (14%) | 64,101,113 | 2.10 | 16 (25%) |
| 25 | CLA | 9 | 605 | - | 60,68,73 | 1.42 | 8 (13%) | 70,107,113 | 2.04 | 18 (25%) |
| 25 | CLA | 9 | 606 | - | 55,63,73 | 1.47 | 6 (10%) | 64,101,113 | 2.06 | 16 (25%) |
| 25 | CLA | A | 1104 | 1 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.95 | 17 (22%) |
| 25 | CLA | A | 1131 | - | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 1.97 | 15 (19%) |
| 25 | CLA | A | 1118 | - | 55,63,73 | 1.48 | 9 (16%) | 64,101,113 | 2.08 | 15 (23%) |
| 48 | DGA | 2 | 803 | - | 36,36,43 | 1.19 | 3 (8%) | 38,38,45 | 1.34 | 3 (7%) |
| 35 | LMT | B | 5006 | - | 36,36,36 | 1.17 | 6 (16%) | 47,47,47 | 0.95 | 1 (2%) |
| 40 | RRX | 3 | 506 | - | 42,42,42 | 4.92 | 24 (57%) | 57,58,58 | 2.81 | 21 (36%) |
| 25 | CLA | 7 | 601 | 20 | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.07 | 17 (24%) |
| 25 | CLA | B | 1223 | - | 65,73,73 | 1.37 | 9 (13%) | 76,113,113 | 2.00 | 17 (22%) |
| 30 | LHG | 7 | 801 | 25 | 36,36,48 | 0.44 | 0 | 39,42,54 | 1.11 | 2 (5%) |
| 25 | CLA | 6 | 602 | - | 52,60,73 | 1.52 | 9 (17%) | 60,97,113 | 2.13 | 17 (28%) |
| 33 | PTY | B | 5005 | - | 41,41,49 | 0.93 | 4 (9%) | 44,46,54 | 1.13 | 2 (4%) |
| 25 | CLA | A | 1113 | - | 60,68,73 | 1.40 | 7 (11%) | 70,107,113 | 2.07 | 19 (27%) |
| 25 | CLA | 4 | 603 | 17 | 56,64,73 | 1.47 | 9 (16%) | 65,102,113 | 2.03 | 16 (24%) |
| 25 | CLA | K | 1404 | 10 | 45,53,73 | 1.62 | 10 (22%) | 52,89,113 | 2.14 | 13 (25%) |
| 26 | CHL | 8 | 604 | 21 | 62,70,74 | 0.97 | 4 (6%) | 68,109,114 | 1.34 | 10 (14%) |
| 26 | CHL | 7 | 611 | - | 56,64,74 | 0.91 | 3 (5%) | 61,102,114 | 1.33 | 10 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 25 | CLA | 4 | 607 | - | 55,63,73 | 1.48 | 8 (14%) | 64,101,113 | 2.11 | 17 (26%) |
| 25 | CLA | 4 | 604 | - | 60,68,73 | 1.40 | 9 (15%) | 70,107,113 | 2.06 | 17 (24%) |
| 26 | CHL | a | 613 | - | 46,54,74 | 0.98 | 3 (6%) | 49,90,114 | 1.38 | 10 (20%) |
| 36 | DGD | 8 | 802 | - | 60,60,67 | 1.08 | 5 (8%) | 74,74,81 | 1.09 | 5 (6%) |
| 25 | CLA | B | 1222 | - | 58,66,73 | 1.42 | 7 (12%) | 67,104,113 | 2.09 | 17 (25%) |
| 29 | BCR | B | 4006 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.24 | 14 (25%) |
| 43 | LUT | 2 | 502 | - | 42,43,43 | 2.37 | 1 (2%) | 51,60,60 | 1.93 | 13 (25%) |
| 25 | CLA | B | 1021 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.95 | 15 (19%) |
| 26 | CHL | 3 | 611 | - | 61,69,74 | 0.96 | 3 (4%) | 67,108,114 | 1.32 | 10 (14%) |
| 47 | PLM | 6 | 804 | - | 17,17,17 | 0.56 | 0 | 17,17,17 | 1.14 | 1 (5%) |
| 25 | CLA | A | 1107 | 1 | 55,63,73 | 1.47 | 8 (14%) | 64,101,113 | 2.11 | 18 (28%) |
| 26 | CHL | 9 | 601 | - | 66,74,74 | 0.81 | 2 (3%) | 73,114,114 | 1.27 | 11 (15%) |
| 25 | CLA | A | 1134 | 1 | 60,68,73 | 1.42 | 9 (15%) | 70,107,113 | 2.09 | 18 (25%) |
| 43 | LUT | 1 | 503 | - | 42,43,43 | 2.38 | 1 (2%) | 51,60,60 | 2.22 | 17 (33%) |
| 25 | CLA | 9 | 602 | - | 46,54,73 | 1.58 | 7 (15%) | 53,90,113 | 2.13 | 16 (30%) |
| 25 | CLA | 6 | 618 | - | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.08 | 13 (24%) |
| 25 | CLA | 3 | 618 | 16 | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.10 | 13 (24%) |
| 30 | LHG | 2 | 802 | - | 48,48,48 | 0.39 | 0 | 51,54,54 | 1.12 | 3 (5%) |
| 47 | PLM | 4 | 803 | - | 16,16,17 | 0.42 | 0 | 15,15,17 | 0.93 | 0 |
| 26 | CHL | 7 | 617 | 20 | 66,74,74 | 0.83 | 3 (4%) | 73,114,114 | 1.20 | 9 (12%) |
| 26 | CHL | 2 | 613 | - | 51,59,74 | 0.96 | 3 (5%) | 55,96,114 | 1.38 | 9 (16%) |
| 25 | CLA | 5 | 615 | 18 | 46,54,73 | 1.61 | 8 (17%) | 53,90,113 | 2.12 | 13 (24%) |
| 30 | LHG | 4 | 802 | - | 31,31,48 | 0.46 | 0 | 34,37,54 | 1.22 | 3 (8%) |
| 25 | CLA | B | 1219 | 2 | 59,67,73 | 1.42 | 8 (13%) | 68,105,113 | 2.07 | 17 (25%) |
| 25 | CLA | 7 | 603 | 20 | 65,73,73 | 1.36 | 9 (13%) | 76,113,113 | 2.00 | 17 (22%) |
| 26 | CHL | 1 | 610 | - | 48,56,74 | 0.90 | 2 (4%) | 51,92,114 | 1.46 | 12 (23%) |
| 43 | LUT | 6 | 501 | - | 42,43,43 | 2.34 | 1 (2%) | 51,60,60 | 1.88 | 14 (27%) |
| 25 | CLA | B | 1226 | - | 65,73,73 | 1.37 | 8 (12%) | 76,113,113 | 1.97 | 17 (22%) |
| 25 | CLA | H | 1701 | - | 55,63,73 | 1.47 | 7 (12%) | 64,101,113 | 2.12 | 15 (23%) |
| 25 | CLA | L | 1501 | 11 | 50,58,73 | 1.55 | 8 (16%) | 58,95,113 | 2.22 | 16 (27%) |
| 25 | CLA | B | 1209 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.98 | 16 (21%) |
| 25 | CLA | O | 1801 | - | 36,46,73 | 1.77 | 8 (22%) | 41,80,113 | 2.17 | 12 (29%) |
| 25 | CLA | 8 | 620 | - | 45,53,73 | 1.62 | 10 (22%) | 52,89,113 | 2.16 | 15 (28%) |
| 29 | BCR | A | 4004 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.31 | 18 (32%) |
| 25 | CLA | 3 | 605 | - | 65,73,73 | 1.34 | 7 (10%) | 76,113,113 | 1.98 | 17 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 29 | BCR | 6 | 503 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.24 | 14 (25%) |
| 29 | BCR | L | 4002 | - | 41,41,41 | 1.83 | 4 (9%) | 56,56,56 | 4.33 | 15 (26%) |
| 26 | CHL | 2 | 610 | - | 48,56,74 | 0.96 | 3 (6%) | 51,92,114 | 1.42 | 10 (19%) |
| 25 | CLA | 6 | 606 | 19 | 65,73,73 | 1.37 | 9 (13%) | 76,113,113 | 2.00 | 18 (23%) |
| 29 | BCR | A | 4003 | - | 41,41,41 | 1.85 | 4 (9%) | 56,56,56 | 4.42 | 17 (30%) |
| 25 | CLA | 6 | 601 | - | 60,68,73 | 1.40 | 8 (13%) | 70,107,113 | 2.05 | 19 (27%) |
| 25 | CLA | A | 1132 | - | 65,73,73 | 1.34 | 8 (12%) | 76,113,113 | 2.00 | 17 (22%) |
| 25 | CLA | 1 | 605 | - | 65,73,73 | 1.33 | 9 (13%) | 76,113,113 | 2.08 | 19 (25%) |
| 26 | CHL | 6 | 617 | 19 | 43,51,74 | 1.02 | 3 (6%) | 45,86,114 | 1.44 | 9 (20%) |
| 25 | CLA | A | 1102 | 25 | 55,63,73 | 1.45 | 6 (10%) | 64,101,113 | 2.20 | 17 (26%) |
| 25 | CLA | 6 | 604 | 19 | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.95 | 19 (25%) |
| 25 | CLA | 6 | 605 | - | 46,54,73 | 1.60 | 9 (19%) | 53,90,113 | 2.15 | 14 (26%) |
| 25 | CLA | 9 | 609 | 23 | 46,54,73 | 1.58 | 7 (15%) | 53,90,113 | 2.18 | 15 (28%) |
| 47 | PLM | a | 804 | - | 16,16,17 | 0.42 | 0 | 15,15,17 | 0.95 | 0 |
| 35 | LMT | A | 5008 | - | 36,36,36 | 1.18 | 6 (16%) | 47,47,47 | 1.00 | 2 (4%) |
| 25 | CLA | 9 | 604 | 23 | 60,68,73 | 1.40 | 7 (11%) | 70,107,113 | 2.06 | 19 (27%) |
| 30 | LHG | 7 | 803 | - | 34,34,48 | 0.44 | 0 | 37,40,54 | 1.15 | 3 (8%) |
| 25 | CLA | 1 | 606 | - | 57,65,73 | 1.42 | 8 (14%) | 66,103,113 | 2.19 | 17 (25%) |
| 29 | BCR | B | 4003 | - | 41,41,41 | 1.86 | 4 (9%) | 56,56,56 | 4.33 | 17 (30%) |
| 26 | CHL | 5 | 618 | - | 51,59,74 | 0.99 | 3 (5%) | 55,96,114 | 1.44 | 11 (20%) |
| 43 | LUT | 9 | 501 | - | 42,43,43 | 2.35 | 1 (2%) | 51,60,60 | 1.92 | 13 (25%) |
| 41 | SPH | 4 | 805 | - | 19,20,20 | 0.64 | 0 | 18,21,21 | 1.08 | 1 (5%) |
| 25 | CLA | B | 1224 | - | 65,73,73 | 1.36 | 8 (12%) | 76,113,113 | 1.98 | 17 (22%) |
| 25 | CLA | 3 | 607 | 30 | 65,73,73 | 1.35 | 8 (12%) | 76,113,113 | 1.92 | 16 (21%) |
| 33 | PTY | 9 | 803 | - | 47,47,49 | 0.89 | 4 (8%) | 50,52,54 | 1.11 | 2 (4%) |
| 25 | CLA | 4 | 608 | - | 51,59,73 | 1.53 | 9 (17%) | 59,96,113 | 2.18 | 16 (27%) |
| 25 | CLA | 9 | 607 | - | 47,55,73 | 1.59 | 9 (19%) | 54,91,113 | 2.16 | 15 (27%) |
| 25 | CLA | 5 | 602 | - | 52,60,73 | 1.51 | 8 (15%) | 60,97,113 | 2.12 | 16 (26%) |
| 25 | CLA | J | 1901 | 9 | 42,50,73 | 1.68 | 8 (19%) | 48,85,113 | 2.20 | 13 (27%) |
| 25 | CLA | A | 1140 | - | 55,63,73 | 1.48 | 8 (14%) | 64,101,113 | 2.11 | 17 (26%) |
| 25 | CLA | 7 | 607 | 30 | 59,67,73 | 1.42 | 8 (13%) | 68,105,113 | 2.04 | 13 (19%) |
| 50 | XAT | 7 | 502 | - | 39,47,47 | 0.70 | 1 (2%) | 54,74,74 | 1.93 | 11 (20%) |
| 41 | SPH | 6 | 806 | - | 19,20,20 | 0.64 | 0 | 18,21,21 | 1.07 | 1 (5%) |
| 28 | SF4 | C | 3003 | 3 | 0,12,12 | - | - | - | | |
| 25 | CLA | 8 | 606 | - | 57,65,73 | 1.42 | 6 (10%) | 66,103,113 | 2.09 | 17 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 25 | CLA | 2 | 621 | 22 | 65,73,73 | 1.37 | 9 (13%) | 76,113,113 | 2.02 | 16 (21%) |
| 50 | XAT | 2 | 501 | - | 39,47,47 | 0.69 | 1 (2%) | 54,74,74 | 1.98 | 14 (25%) |
| 25 | CLA | A | 1129 | - | 50,58,73 | 1.54 | 9 (18%) | 58,95,113 | 2.19 | 17 (29%) |
| 25 | CLA | 5 | 609 | 18 | 51,59,73 | 1.53 | 7 (13%) | 59,96,113 | 2.15 | 17 (28%) |
| 25 | CLA | B | 1228 | - | 65,73,73 | 1.33 | 7 (10%) | 76,113,113 | 2.04 | 19 (25%) |
| 29 | BCR | 7 | 503 | - | 41,41,41 | 1.82 | 4 (9%) | 56,56,56 | 4.31 | 17 (30%) |
| 25 | CLA | A | 1124 | - | 55,63,73 | 1.48 | 8 (14%) | 64,101,113 | 2.09 | 16 (25%) |
| 25 | CLA | O | 1803 | - | 41,49,73 | 1.70 | 9 (21%) | 47,84,113 | 2.24 | 15 (31%) |
| 36 | DGD | B | 5003 | - | 67,67,67 | 1.18 | 7 (10%) | 81,81,81 | 1.02 | 3 (3%) |
| 43 | LUT | 8 | 502 | - | 42,43,43 | 2.33 | 1 (2%) | 51,60,60 | 1.90 | 12 (23%) |
| 43 | LUT | 9 | 502 | - | 42,43,43 | 2.32 | 1 (2%) | 51,60,60 | 1.85 | 12 (23%) |
| 40 | RRX | J | 4002 | - | 42,42,42 | 4.90 | 24 (57%) | 57,58,58 | 2.66 | 21 (36%) |
| 35 | LMT | 2 | 804 | - | 36,36,36 | 1.19 | 6 (16%) | 47,47,47 | 1.06 | 2 (4%) |
| 43 | LUT | 3 | 502 | - | 42,43,43 | 2.39 | 1 (2%) | 51,60,60 | 1.96 | 13 (25%) |
| 45 | OLA | a | 805 | - | 19,19,19 | 0.56 | 0 | 19,19,19 | 1.01 | 0 |
| 25 | CLA | B | 1227 | - | 50,58,73 | 1.55 | 9 (18%) | 58,95,113 | 2.24 | 18 (31%) |
| 35 | LMT | 1 | 804 | - | 36,36,36 | 1.16 | 6 (16%) | 47,47,47 | 1.02 | 3 (6%) |
| 42 | ECH | M | 4001 | - | 42,42,42 | 0.87 | 1 (2%) | 55,58,58 | 2.00 | 14 (25%) |
| 25 | CLA | A | 1127 | - | 65,73,73 | 1.36 | 6 (9%) | 76,113,113 | 1.89 | 15 (19%) |
| 26 | CHL | 8 | 603 | 21 | 66,74,74 | 0.91 | 4 (6%) | 73,114,114 | 1.21 | 9 (12%) |
| 33 | PTY | J | 5001 | - | 27,27,49 | 1.15 | 4 (14%) | 30,32,54 | 1.20 | 2 (6%) |
| 25 | CLA | A | 1138 | - | 65,73,73 | 1.35 | 9 (13%) | 76,113,113 | 1.89 | 16 (21%) |
| 29 | BCR | I | 4001 | - | 41,41,41 | 1.84 | 4 (9%) | 56,56,56 | 4.29 | 16 (28%) |
| 41 | SPH | J | 5002 | - | 19,20,20 | 0.67 | 0 | 18,21,21 | 0.91 | 0 |
| 36 | DGD | 7 | 806 | - | 51,51,67 | 0.92 | 3 (5%) | 65,65,81 | 1.03 | 3 (4%) |
| 25 | CLA | 4 | 616 | - | 50,58,73 | 1.56 | 8 (16%) | 58,95,113 | 2.16 | 16 (27%) |
| 26 | CHL | 6 | 613 | - | 51,59,74 | 0.91 | 2 (3%) | 55,96,114 | 1.42 | 11 (20%) |

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 |
|---|---|---|---|---|---|---|---|
| 25 | CLA | a | 601 | - | 1/1/14/20 | 9/31/109/115 | - |
| 30 | LHG | 9 | 802 | - | - | 27/53/53/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 26 | CHL | 9 | 613 | - | 3/3/15/26 | 0/10/108/137 | - |
| 25 | CLA | B | 1232 | - | 1/1/11/20 | 7/13/91/115 | - |
| 52 | P5S | 8 | 805 | - | - | 23/42/42/59 | - |
| 29 | BCR | L | 4001 | - | - | 12/29/63/63 | 0/2/2/2 |
| 25 | CLA | 2 | 615 | - | 1/1/13/20 | 6/27/105/115 | - |
| 49 | 13X | 6 | 805 | - | - | - | 0/1/1/1 |
| 25 | CLA | H | 1703 | - | 1/1/13/20 | 9/25/103/115 | - |
| 25 | CLA | B | 1217 | - | 1/1/13/20 | 12/27/105/115 | - |
| 47 | PLM | 5 | 804 | - | - | 3/15/15/15 | - |
| 25 | CLA | 2 | 607 | 30 | 1/1/15/20 | 15/37/115/115 | - |
| 25 | CLA | 7 | 606 | - | 1/1/13/20 | 12/23/101/115 | - |
| 25 | CLA | H | 1702 | 8 | 1/1/11/20 | 8/15/93/115 | - |
| 51 | 4RF | 7 | 807 | - | - | 19/39/39/59 | - |
| 48 | DGA | 3 | 803 | - | - | 14/25/25/45 | - |
| 25 | CLA | B | 1210 | - | 1/1/15/20 | 21/37/115/115 | - |
| 43 | LUT | 7 | 501 | - | 1/1/12/27 | 6/29/67/67 | 0/2/2/2 |
| 25 | CLA | 4 | 612 | 17 | 1/1/14/20 | 17/34/112/115 | - |
| 26 | CHL | 7 | 613 | - | 4/4/19/26 | 4/33/131/137 | - |
| 27 | PQN | A | 2001 | - | - | 7/23/43/43 | 0/2/2/2 |
| 29 | BCR | 5 | 504 | - | - | 12/29/63/63 | 0/2/2/2 |
| 25 | CLA | 8 | 612 | - | 1/1/12/20 | 8/19/97/115 | - |
| 25 | CLA | 8 | 605 | - | 1/1/13/20 | 13/25/103/115 | - |
| 25 | CLA | A | 1126 | - | 1/1/15/20 | 22/37/115/115 | - |
| 25 | CLA | 2 | 604 | - | 1/1/13/20 | 13/27/105/115 | - |
| 29 | BCR | O | 4001 | - | - | 13/29/63/63 | 0/2/2/2 |
| 25 | CLA | 2 | 603 | 22 | 1/1/14/20 | 12/31/109/115 | - |
| 29 | BCR | 5 | 503 | - | - | 13/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 1239 | - | 1/1/15/20 | 18/37/115/115 | - |
| 25 | CLA | 3 | 602 | - | 1/1/11/20 | 5/15/93/115 | - |
| 43 | LUT | a | 503 | - | - | 6/29/67/67 | 0/2/2/2 |
| 43 | LUT | 5 | 501 | - | - | 2/29/67/67 | 0/2/2/2 |
| 25 | CLA | L | 1504 | - | 1/1/12/20 | 9/19/97/115 | - |
| 25 | CLA | a | 607 | - | 1/1/13/20 | 14/29/107/115 | - |
| 25 | CLA | A | 1141 | - | 1/1/11/20 | 7/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 5 | 601 | 18 | 1/1/14/20 | 12/31/109/115 | - |
| 30 | LHG | 7 | 802 | - | - | 20/40/40/53 | - |
| 25 | CLA | 7 | 610 | - | 1/1/14/20 | 17/31/109/115 | - |
| 33 | PTY | a | 802 | - | - | 22/41/41/53 | - |
| 25 | CLA | 1 | 603 | - | 1/1/15/20 | 15/37/115/115 | - |
| 38 | LPX | F | 5003 | - | - | 12/31/31/31 | - |
| 25 | CLA | 1 | 607 | 30 | 1/1/15/20 | 18/37/115/115 | - |
| 50 | XAT | 9 | 507 | - | 1/1/12/26 | 8/31/93/93 | 0/4/4/4 |
| 29 | BCR | J | 4001 | - | - | 11/29/63/63 | 0/2/2/2 |
| 24 | CL0 | A | 1011 | - | 3/3/20/25 | 10/37/135/135 | - |
| 25 | CLA | 4 | 601 | - | 1/1/14/20 | 10/31/109/115 | - |
| 25 | CLA | A | 1109 | 25 | 1/1/15/20 | 19/37/115/115 | - |
| 25 | CLA | 6 | 607 | 30 | 1/1/13/20 | 10/25/103/115 | - |
| 25 | CLA | A | 1110 | - | 1/1/12/20 | 9/24/102/115 | - |
| 25 | CLA | 7 | 605 | - | 1/1/11/20 | 4/11/89/115 | - |
| 37 | PCW | B | 5004 | - | - | 24/42/42/57 | - |
| 30 | LHG | a | 801 | - | - | 24/39/39/53 | - |
| 43 | LUT | 5 | 502 | - | - | 3/29/67/67 | 0/2/2/2 |
| 25 | CLA | 1 | 602 | - | 1/1/11/20 | 6/13/91/115 | - |
| 25 | CLA | B | 1229 | - | 1/1/15/20 | 12/37/115/115 | - |
| 25 | CLA | 8 | 602 | - | 1/1/12/20 | 4/22/100/115 | - |
| 25 | CLA | B | 1237 | - | 1/1/15/20 | 20/37/115/115 | - |
| 25 | CLA | 4 | 615 | 17 | 1/1/14/20 | 13/31/109/115 | - |
| 25 | CLA | a | 603 | - | 1/1/15/20 | 18/37/115/115 | - |
| 43 | LUT | 4 | 501 | - | 1/1/12/27 | 6/29/67/67 | 0/2/2/2 |
| 43 | LUT | a | 501 | - | - | 5/29/67/67 | 0/2/2/2 |
| 25 | CLA | 3 | 606 | - | 1/1/15/20 | 16/37/115/115 | - |
| 26 | CHL | 6 | 611 | - | 3/3/17/26 | 5/21/119/137 | - |
| 50 | XAT | 9 | 504 | - | 1/1/12/26 | 13/31/93/93 | 0/4/4/4 |
| 43 | LUT | 5 | 505 | - | - | 10/29/67/67 | 0/2/2/2 |
| 33 | PTY | a | 803 | - | - | 24/41/41/53 | - |
| 26 | CHL | 1 | 604 | - | 4/4/20/26 | 10/39/137/137 | - |
| 25 | CLA | 2 | 608 | - | 1/1/11/20 | 7/13/91/115 | - |
| 25 | CLA | B | 1211 | - | 1/1/13/20 | 11/25/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 25 | CLA | K | 1402 | - | 1/1/14/20 | 10/31/109/115 | - |
| 28 | SF4 | C | 3002 | 3 | - | - | 0/6/5/5 |
| 25 | CLA | A | 1117 | - | 1/1/15/20 | 18/37/115/115 | - |
| 25 | CLA | B | 1238 | - | 1/1/15/20 | 9/37/115/115 | - |
| 25 | CLA | 2 | 601 | - | 1/1/14/20 | 11/31/109/115 | - |
| 25 | CLA | A | 1119 | - | 1/1/15/20 | 20/37/115/115 | - |
| 30 | LHG | 1 | 802 | - | - | 34/53/53/53 | - |
| 26 | CHL | 8 | 601 | 21 | 4/4/19/26 | 4/33/131/137 | - |
| 43 | LUT | 3 | 501 | - | - | 3/29/67/67 | 0/2/2/2 |
| 39 | NEX | F | 4001 | - | 1/1/12/25 | 14/27/83/83 | 0/3/3/3 |
| 30 | LHG | 6 | 802 | - | - | 25/41/41/53 | - |
| 25 | CLA | A | 1108 | - | 1/1/15/20 | 16/37/115/115 | - |
| 25 | CLA | F | 1301 | - | 1/1/12/20 | 11/19/97/115 | - |
| 29 | BCR | 8 | 503 | - | - | 16/29/63/63 | 0/2/2/2 |
| 26 | CHL | 4 | 609 | 17 | 4/4/20/26 | 12/39/137/137 | - |
| 29 | BCR | A | 4002 | - | - | 9/29/63/63 | 0/2/2/2 |
| 25 | CLA | F | 1302 | - | 1/1/13/20 | 10/25/103/115 | - |
| 25 | CLA | G | 1601 | - | 1/1/12/20 | 11/19/97/115 | - |
| 25 | CLA | L | 1502 | - | 1/1/14/20 | 14/31/109/115 | - |
| 25 | CLA | 7 | 602 | - | 1/1/11/20 | 4/11/89/115 | - |
| 25 | CLA | A | 1135 | - | 1/1/12/20 | 7/21/99/115 | - |
| 25 | CLA | B | 1240 | 30 | 1/1/15/20 | 12/37/115/115 | - |
| 32 | SQD | G | 5001 | - | - | 20/41/61/69 | 0/1/1/1 |
| 33 | PTY | G | 5002 | - | - | 10/30/30/53 | - |
| 25 | CLA | B | 1207 | - | 1/1/14/20 | 18/31/109/115 | - |
| 43 | LUT | 2 | 507 | - | 1/1/12/27 | 19/29/67/67 | 0/2/2/2 |
| 30 | LHG | F | 5001 | - | - | 28/47/47/53 | - |
| 25 | CLA | A | 1013 | - | 1/1/15/20 | 18/37/115/115 | - |
| 29 | BCR | A | 4005 | - | - | 16/29/63/63 | 0/2/2/2 |
| 26 | CHL | 6 | 609 | 19 | 4/4/20/26 | 10/39/137/137 | - |
| 36 | DGD | 8 | 803 | - | - | 18/35/75/95 | 0/2/2/2 |
| 25 | CLA | 2 | 612 | - | 1/1/12/20 | 10/19/97/115 | - |
| 30 | LHG | 2 | 801 | 25 | - | 31/53/53/53 | - |
| 25 | CLA | 8 | 615 | 21 | 1/1/11/20 | 9/15/93/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 25 | CLA | B | 1230 | - | 1/1/13/20 | 11/29/107/115 | - |
| 43 | LUT | 8 | 501 | - | - | 3/29/67/67 | 0/2/2/2 |
| 25 | CLA | 3 | 610 | 16 | 1/1/13/20 | 13/28/106/115 | - |
| 44 | AXT | 1 | 502 | - | - | 10/29/71/75 | 0/2/2/2 |
| 25 | CLA | A | 1125 | - | 1/1/15/20 | 25/37/115/115 | - |
| 25 | CLA | B | 1212 | - | 1/1/13/20 | 12/28/106/115 | - |
| 25 | CLA | 4 | 606 | - | 1/1/12/20 | 8/19/97/115 | - |
| 29 | BCR | 3 | 505 | - | - | 11/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 1213 | - | 1/1/13/20 | 14/25/103/115 | - |
| 47 | PLM | 8 | 806 | - | - | 6/13/14/15 | - |
| 25 | CLA | 8 | 608 | - | 1/1/12/20 | 8/22/100/115 | - |
| 29 | BCR | B | 4005 | - | - | 15/29/63/63 | 0/2/2/2 |
| 25 | CLA | 1 | 615 | 15 | 1/1/11/20 | 12/15/93/115 | - |
| 43 | LUT | 1 | 501 | - | - | 3/29/67/67 | 0/2/2/2 |
| 30 | LHG | F | 5002 | - | - | 19/40/40/53 | - |
| 25 | CLA | 1 | 608 | - | 1/1/14/20 | 15/31/109/115 | - |
| 30 | LHG | 4 | 801 | - | - | 30/53/53/53 | - |
| 25 | CLA | B | 1220 | - | 1/1/14/20 | 15/31/109/115 | - |
| 48 | DGA | 5 | 803 | - | - | 14/24/24/45 | - |
| 25 | CLA | A | 1128 | - | 1/1/15/20 | 20/37/115/115 | - |
| 25 | CLA | 4 | 611 | - | 1/1/13/20 | 9/27/105/115 | - |
| 25 | CLA | A | 1012 | - | 1/1/15/20 | 13/37/115/115 | - |
| 45 | OLA | 8 | 808 | - | - | 5/17/17/17 | - |
| 25 | CLA | A | 1101 | - | 1/1/15/20 | 24/37/115/115 | - |
| 26 | CHL | 2 | 609 | 22 | 4/4/20/26 | 11/39/137/137 | - |
| 26 | CHL | 9 | 610 | - | 3/3/17/26 | 2/21/119/137 | - |
| 25 | CLA | B | 1201 | - | 1/1/15/20 | 21/37/115/115 | - |
| 26 | CHL | 8 | 613 | - | 3/3/17/26 | 2/21/119/137 | - |
| 25 | CLA | a | 615 | 15 | 1/1/11/20 | 4/15/93/115 | - |
| 25 | CLA | 5 | 608 | - | 1/1/11/20 | 6/13/91/115 | - |
| 25 | CLA | a | 608 | - | 1/1/13/20 | 10/25/103/115 | - |
| 26 | CHL | 9 | 608 | - | 3/3/16/26 | 5/18/116/137 | - |
| 26 | CHL | 6 | 619 | 19 | 5/5/20/26 | 10/39/137/137 | - |
| 29 | BCR | A | 4001 | - | - | 13/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 5 | 614 | 18 | 1/1/11/20 | 6/15/93/115 | - |
| 29 | BCR | L | 4003 | - | - | 10/29/63/63 | 0/2/2/2 |
| 30 | LHG | 8 | 801 | 25 | - | 28/41/41/53 | - |
| 25 | CLA | B | 1215 | - | 1/1/14/20 | 16/31/109/115 | - |
| 37 | PCW | K | 5001 | - | - | 22/44/44/57 | - |
| 25 | CLA | B | 1231 | - | 1/1/15/20 | 17/37/115/115 | - |
| 25 | CLA | 6 | 612 | - | 1/1/12/20 | 11/19/97/115 | - |
| 26 | CHL | A | 1114 | - | 4/4/20/26 | 9/39/137/137 | - |
| 25 | CLA | 3 | 613 | - | 1/1/14/20 | 12/33/111/115 | - |
| 25 | CLA | A | 1121 | - | 1/1/14/20 | 19/31/109/115 | - |
| 29 | BCR | K | 4002 | - | - | 11/29/63/63 | 0/2/2/2 |
| 25 | CLA | 5 | 607 | - | 1/1/14/20 | 15/31/109/115 | - |
| 33 | PTY | A | 5006 | - | - | 14/37/37/53 | - |
| 25 | CLA | 6 | 603 | - | 1/1/15/20 | 15/37/115/115 | - |
| 32 | SQD | I | 5001 | - | - | 23/49/69/69 | 0/1/1/1 |
| 26 | CHL | 5 | 617 | 18 | 3/3/16/26 | 1/17/115/137 | - |
| 25 | CLA | 7 | 604 | 20 | 1/1/15/20 | 16/37/115/115 | - |
| 32 | SQD | A | 5005 | - | - | 20/49/69/69 | 0/1/1/1 |
| 27 | PQN | B | 2002 | - | - | 8/23/43/43 | 0/2/2/2 |
| 37 | PCW | K | 5002 | - | - | 17/39/39/57 | - |
| 25 | CLA | 8 | 618 | 21 | 1/1/14/20 | 17/31/109/115 | - |
| 25 | CLA | A | 1139 | - | 1/1/13/20 | 11/25/103/115 | - |
| 43 | LUT | 6 | 502 | - | - | 3/29/67/67 | 0/2/2/2 |
| 25 | CLA | A | 1137 | - | 1/1/14/20 | 14/31/109/115 | - |
| 26 | CHL | 1 | 613 | - | 3/3/16/26 | 2/18/116/137 | - |
| 25 | CLA | 1 | 612 | 15 | 1/1/15/20 | 21/37/115/115 | - |
| 30 | LHG | 9 | 801 | - | - | 18/37/37/53 | - |
| 25 | CLA | 5 | 604 | 18 | 1/1/15/20 | 13/37/115/115 | - |
| 25 | CLA | 5 | 603 | 18 | 1/1/13/20 | 16/27/105/115 | - |
| 47 | PLM | 4 | 804 | - | - | 9/15/15/15 | - |
| 26 | CHL | 9 | 603 | - | 4/4/20/26 | 8/39/137/137 | - |
| 25 | CLA | A | 1123 | - | 1/1/15/20 | 11/37/115/115 | - |
| 25 | CLA | 8 | 609 | 21 | 1/1/14/20 | 15/31/109/115 | - |
| 25 | CLA | G | 1603 | - | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 26 | CHL | 3 | 604 | 16 | 4/4/20/26 | 8/39/137/137 | - |
| 29 | BCR | B | 4002 | - | - | 16/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 1221 | - | 1/1/15/20 | 9/37/115/115 | - |
| 26 | CHL | 4 | 613 | - | 3/3/17/26 | 4/23/121/137 | - |
| 25 | CLA | a | 611 | - | 1/1/12/20 | 8/19/97/115 | - |
| 25 | CLA | A | 1103 | - | 1/1/15/20 | 19/37/115/115 | - |
| 25 | CLA | 3 | 616 | - | 1/1/13/20 | 13/27/105/115 | - |
| 25 | CLA | 8 | 607 | 30 | 1/1/11/20 | 6/15/93/115 | - |
| 30 | LHG | B | 5002 | - | - | 29/53/53/53 | - |
| 30 | LHG | B | 5001 | 25 | - | 34/53/53/53 | - |
| 25 | CLA | B | 1214 | - | 1/1/13/20 | 17/30/108/115 | - |
| 41 | SPH | 9 | 804 | - | - | 13/21/21/21 | - |
| 43 | LUT | 4 | 502 | - | - | 4/29/67/67 | 0/2/2/2 |
| 29 | BCR | 3 | 504 | - | - | 11/29/63/63 | 0/2/2/2 |
| 29 | BCR | H | 4001 | - | - | 12/29/63/63 | 0/2/2/2 |
| 29 | BCR | G | 4001 | - | - | 12/29/63/63 | 0/2/2/2 |
| 29 | BCR | 3 | 503 | - | - | 12/29/63/63 | 0/2/2/2 |
| 33 | PTY | G | 5003 | - | - | 13/30/30/53 | - |
| 29 | BCR | B | 4004 | - | - | 9/29/63/63 | 0/2/2/2 |
| 25 | CLA | A | 1133 | - | 1/1/15/20 | 20/37/115/115 | - |
| 25 | CLA | B | 1235 | - | 1/1/15/20 | 21/37/115/115 | - |
| 26 | CHL | 8 | 610 | - | 5/5/18/26 | 4/27/125/137 | - |
| 26 | CHL | a | 610 | - | 3/3/16/26 | 0/18/116/137 | - |
| 33 | PTY | 7 | 804 | - | - | 16/36/36/53 | - |
| 26 | CHL | 5 | 613 | - | 4/4/18/26 | 3/27/125/137 | - |
| 46 | QTB | a | 504 | - | 1/1/5/10 | 1/11/28/28 | 0/1/1/1 |
| 25 | CLA | B | 1206 | 2 | 1/1/15/20 | 23/37/115/115 | - |
| 30 | LHG | A | 5002 | - | - | 37/53/53/53 | - |
| 25 | CLA | a | 612 | 15 | 1/1/13/20 | 10/28/106/115 | - |
| 25 | CLA | a | 605 | - | 1/1/13/20 | 10/25/103/115 | - |
| 26 | CHL | 1 | 611 | - | 4/4/18/26 | 4/27/125/137 | - |
| 25 | CLA | 9 | 612 | - | 1/1/15/20 | 13/37/115/115 | - |
| 25 | CLA | 6 | 615 | 54 | 1/1/15/20 | 15/37/115/115 | - |
| 30 | LHG | 5 | 801 | - | - | 35/53/53/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 26 | CHL | 7 | 609 | 20 | 4/4/19/26 | 10/35/133/137 | - |
| 47 | PLM | 8 | 807 | - | - | 5/15/15/15 | - |
| 25 | CLA | 6 | 608 | - | 1/1/13/20 | 7/25/103/115 | - |
| 25 | CLA | a | 602 | - | 1/1/12/20 | 8/19/97/115 | - |
| 25 | CLA | B | 1236 | - | 1/1/12/20 | 9/23/101/115 | - |
| 25 | CLA | B | 1208 | - | 1/1/13/20 | 11/25/101/115 | - |
| 29 | BCR | 6 | 504 | - | - | 13/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 1023 | - | 1/1/15/20 | 17/37/115/115 | - |
| 26 | CHL | 5 | 611 | - | 3/3/17/26 | 1/21/119/137 | - |
| 33 | PTY | 3 | 802 | - | - | 17/41/41/53 | - |
| 25 | CLA | A | 1112 | - | 1/1/13/20 | 16/25/103/115 | - |
| 26 | CHL | 1 | 609 | 15 | 4/4/20/26 | 12/39/137/137 | - |
| 28 | SF4 | A | 3001 | 1,2 | - | - | 0/6/5/5 |
| 26 | CHL | a | 604 | - | 4/4/19/26 | 7/33/131/137 | - |
| 25 | CLA | B | 1202 | - | 1/1/15/20 | 17/37/115/115 | - |
| 25 | CLA | 2 | 605 | - | 1/1/14/20 | 18/31/109/115 | - |
| 25 | CLA | 3 | 601 | 16 | 1/1/15/20 | 14/37/115/115 | - |
| 29 | BCR | B | 4001 | - | - | 11/29/63/63 | 0/2/2/2 |
| 26 | CHL | 3 | 603 | 16 | 4/4/20/26 | 8/39/137/137 | - |
| 25 | CLA | B | 1205 | - | 1/1/15/20 | 12/37/115/115 | - |
| 25 | CLA | 4 | 605 | - | 1/1/11/20 | 5/15/93/115 | - |
| 25 | CLA | A | 1116 | - | 1/1/14/20 | 13/31/109/115 | - |
| 29 | BCR | 4 | 503 | - | - | 15/29/63/63 | 0/2/2/2 |
| 25 | CLA | B | 1218 | - | 1/1/13/20 | 7/25/103/115 | - |
| 25 | CLA | B | 1234 | - | - | 21/48/87/115 | 0/5/5/9 |
| 25 | CLA | A | 1111 | - | 1/1/15/20 | 21/37/115/115 | - |
| 25 | CLA | G | 1602 | 7 | 1/1/14/20 | 12/31/109/115 | - |
| 30 | LHG | A | 5001 | - | - | 32/53/53/53 | - |
| 25 | CLA | 4 | 602 | - | 1/1/12/20 | 7/22/100/115 | - |
| 26 | CHL | a | 609 | 15 | 3/3/17/26 | 4/24/122/137 | - |
| 29 | BCR | K | 4001 | - | - | 10/29/63/63 | 0/2/2/2 |
| 29 | BCR | B | 4007 | - | - | 7/29/63/63 | 0/2/2/2 |
| 43 | LUT | a | 502 | - | - | 1/29/67/67 | 0/2/2/2 |
| 25 | CLA | B | 1203 | 2 | 1/1/15/20 | 13/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 45 | OLA | 1 | 803 | - | - | 6/17/17/17 | - |
| 25 | CLA | B | 1216 | - | 1/1/15/20 | 20/37/115/115 | - |
| 25 | CLA | B | 1204 | - | 1/1/15/20 | 19/37/115/115 | - |
| 30 | LHG | 6 | 801 | 25 | - | 34/53/53/53 | - |
| 37 | PCW | 6 | 803 | - | - | 22/39/39/57 | - |
| 25 | CLA | 1 | 601 | - | 1/1/14/20 | 14/31/109/115 | - |
| 34 | 3PH | A | 5007 | - | - | 17/34/34/49 | - |
| 30 | LHG | 3 | 801 | 25 | - | 33/53/53/53 | - |
| 25 | CLA | K | 1401 | - | 1/1/11/20 | 6/15/93/115 | - |
| 26 | CHL | 7 | 615 | 20 | 3/3/17/26 | 5/21/119/137 | - |
| 25 | CLA | 2 | 602 | - | 1/1/12/20 | 11/22/100/115 | - |
| 25 | CLA | A | 1105 | - | 1/1/13/20 | 4/28/106/115 | - |
| 25 | CLA | A | 1122 | - | 1/1/14/20 | 19/31/109/115 | - |
| 33 | PTY | 5 | 802 | - | - | 23/41/41/53 | - |
| 25 | CLA | A | 1120 | - | 1/1/11/20 | 7/18/96/115 | - |
| 25 | CLA | 5 | 612 | 18 | 1/1/15/20 | 24/37/115/115 | - |
| 30 | LHG | 1 | 801 | 25 | - | 25/39/39/53 | - |
| 25 | CLA | 4 | 610 | - | 1/1/15/20 | 20/37/115/115 | - |
| 25 | CLA | 8 | 611 | - | 1/1/12/20 | 6/19/97/115 | - |
| 53 | LAP | 8 | 810 | - | - | 15/30/30/30 | - |
| 44 | AXT | 7 | 504 | - | - | 14/29/71/75 | 0/2/2/2 |
| 25 | CLA | L | 1503 | - | 1/1/11/20 | 7/13/91/115 | - |
| 25 | CLA | 7 | 612 | - | 1/1/14/20 | 15/31/109/115 | - |
| 25 | CLA | 4 | 617 | - | 1/1/11/20 | 6/13/91/115 | - |
| 25 | CLA | B | 1022 | 54 | 1/1/15/20 | 13/37/115/115 | - |
| 25 | CLA | A | 1115 | - | 1/1/14/20 | 15/31/109/115 | - |
| 30 | LHG | A | 5003 | - | - | 26/50/50/53 | - |
| 25 | CLA | K | 1403 | 10 | 1/1/11/20 | 11/18/96/115 | - |
| 25 | CLA | A | 1130 | - | 1/1/13/20 | 11/27/105/115 | - |
| 31 | LMG | A | 5004 | - | - | 4/37/57/70 | 0/1/1/1 |
| 45 | OLA | 8 | 809 | - | - | 11/17/17/17 | - |
| 26 | CHL | 5 | 610 | - | 4/4/20/26 | 10/39/137/137 | - |
| 25 | CLA | 3 | 612 | 16 | 1/1/12/20 | 6/19/97/115 | - |
| 32 | SQD | 7 | 805 | - | - | 10/34/54/69 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 5 | 605 | - | 1/1/11/20 | 3/15/93/115 | - |
| 25 | CLA | 5 | 606 | - | 1/1/12/20 | 10/19/97/115 | - |
| 48 | DGA | 8 | 804 | - | - | 23/41/41/45 | - |
| 25 | CLA | O | 1802 | - | 1/1/13/20 | 13/25/103/115 | - |
| 25 | CLA | 2 | 606 | - | 1/1/11/20 | 4/15/93/115 | - |
| 26 | CHL | 6 | 610 | - | 4/4/18/26 | 6/27/125/137 | - |
| 25 | CLA | A | 1106 | 1 | 1/1/15/20 | 19/37/115/115 | - |
| 26 | CHL | a | 606 | - | 4/4/18/26 | 6/27/125/137 | - |
| 32 | SQD | H | 5001 | - | - | 8/40/60/69 | 0/1/1/1 |
| 26 | CHL | 4 | 618 | - | 4/4/18/26 | 4/27/125/137 | - |
| 25 | CLA | A | 1136 | - | 1/1/15/20 | 15/37/115/115 | - |
| 26 | CHL | 3 | 608 | - | 3/3/15/26 | 1/12/110/137 | - |
| 25 | CLA | B | 1225 | - | 1/1/15/20 | 6/37/115/115 | - |
| 25 | CLA | 7 | 608 | - | 1/1/13/20 | 10/25/103/115 | - |
| 25 | CLA | 9 | 605 | - | 1/1/14/20 | 12/31/109/115 | - |
| 25 | CLA | 9 | 606 | - | 1/1/13/20 | 7/25/103/115 | - |
| 25 | CLA | A | 1104 | 1 | 1/1/15/20 | 17/37/115/115 | - |
| 25 | CLA | A | 1131 | - | 1/1/15/20 | 12/37/115/115 | - |
| 25 | CLA | A | 1118 | - | 1/1/13/20 | 13/25/103/115 | - |
| 48 | DGA | 2 | 803 | - | - | 28/38/38/45 | - |
| 35 | LMT | B | 5006 | - | - | 9/21/61/61 | 0/2/2/2 |
| 40 | RRX | 3 | 506 | - | 1/1/11/25 | 11/29/65/65 | 0/2/2/2 |
| 25 | CLA | 7 | 601 | 20 | 1/1/14/20 | 16/31/109/115 | - |
| 25 | CLA | B | 1223 | - | 1/1/15/20 | 13/37/115/115 | - |
| 30 | LHG | 7 | 801 | 25 | - | 26/41/41/53 | - |
| 25 | CLA | 6 | 602 | - | 1/1/12/20 | 8/22/100/115 | - |
| 33 | PTY | B | 5005 | - | - | 20/45/45/53 | - |
| 25 | CLA | A | 1113 | - | 1/1/14/20 | 14/31/109/115 | - |
| 25 | CLA | 4 | 603 | 17 | 1/1/13/20 | 9/27/105/115 | - |
| 25 | CLA | K | 1404 | 10 | 1/1/11/20 | 5/13/91/115 | - |
| 26 | CHL | 8 | 604 | 21 | 4/4/19/26 | 13/35/133/137 | - |
| 26 | CHL | 7 | 611 | - | 4/4/18/26 | 7/27/125/137 | - |
| 25 | CLA | 4 | 607 | - | 1/1/13/20 | 9/25/103/115 | - |
| 25 | CLA | 4 | 604 | - | 1/1/14/20 | 11/31/109/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 26 | CHL | a | 613 | - | 3/3/16/26 | 6/15/113/137 | - |
| 36 | DGD | 8 | 802 | - | - | 18/48/88/95 | 0/2/2/2 |
| 25 | CLA | B | 1222 | - | 1/1/13/20 | 8/29/107/115 | - |
| 29 | BCR | B | 4006 | - | - | 15/29/63/63 | 0/2/2/2 |
| 43 | LUT | 2 | 502 | - | - | 2/29/67/67 | 0/2/2/2 |
| 25 | CLA | B | 1021 | - | 1/1/15/20 | 18/37/115/115 | - |
| 26 | CHL | 3 | 611 | - | 4/4/19/26 | 9/33/131/137 | - |
| 47 | PLM | 6 | 804 | - | - | 8/15/15/15 | - |
| 25 | CLA | A | 1107 | 1 | 1/1/13/20 | 9/25/103/115 | - |
| 26 | CHL | 9 | 601 | - | 4/4/20/26 | 8/39/137/137 | - |
| 25 | CLA | A | 1134 | 1 | 1/1/14/20 | 14/31/109/115 | - |
| 43 | LUT | 1 | 503 | - | - | 8/29/67/67 | 0/2/2/2 |
| 25 | CLA | 9 | 602 | - | 1/1/11/20 | 4/15/93/115 | - |
| 25 | CLA | 6 | 618 | - | 1/1/11/20 | 8/15/93/115 | - |
| 25 | CLA | 3 | 618 | 16 | 1/1/11/20 | 4/15/93/115 | - |
| 30 | LHG | 2 | 802 | - | - | 39/53/53/53 | - |
| 47 | PLM | 4 | 803 | - | - | 5/13/14/15 | - |
| 26 | CHL | 7 | 617 | 20 | 4/4/20/26 | 13/39/137/137 | - |
| 26 | CHL | 2 | 613 | - | 3/3/17/26 | 1/21/119/137 | - |
| 25 | CLA | 5 | 615 | 18 | 1/1/11/20 | 8/15/93/115 | - |
| 30 | LHG | 4 | 802 | - | - | 23/36/36/53 | - |
| 25 | CLA | B | 1219 | 2 | 1/1/13/20 | 14/30/108/115 | - |
| 25 | CLA | 7 | 603 | 20 | 1/1/15/20 | 24/37/115/115 | - |
| 26 | CHL | 1 | 610 | - | 3/3/16/26 | 2/18/116/137 | - |
| 43 | LUT | 6 | 501 | - | - | 3/29/67/67 | 0/2/2/2 |
| 25 | CLA | B | 1226 | - | 1/1/15/20 | 11/37/115/115 | - |
| 25 | CLA | H | 1701 | - | 1/1/13/20 | 10/25/103/115 | - |
| 25 | CLA | L | 1501 | 11 | 1/1/12/20 | 10/19/97/115 | - |
| 25 | CLA | B | 1209 | - | 1/1/15/20 | 16/37/115/115 | - |
| 25 | CLA | O | 1801 | - | 1/1/9/20 | 0/4/78/115 | - |
| 25 | CLA | 8 | 620 | - | 1/1/11/20 | 8/13/91/115 | - |
| 29 | BCR | A | 4004 | - | - | 12/29/63/63 | 0/2/2/2 |
| 25 | CLA | 3 | 605 | - | 1/1/15/20 | 16/37/115/115 | - |
| 29 | BCR | 6 | 503 | - | - | 16/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 29 | BCR | L | 4002 | - | - | 11/29/63/63 | 0/2/2/2 |
| 26 | CHL | 2 | 610 | - | 4/4/16/26 | 0/18/116/137 | - |
| 25 | CLA | 6 | 606 | 19 | 1/1/15/20 | 14/37/115/115 | - |
| 29 | BCR | A | 4003 | - | - | 12/29/63/63 | 0/2/2/2 |
| 25 | CLA | 6 | 601 | - | 1/1/14/20 | 13/31/109/115 | - |
| 25 | CLA | A | 1132 | - | 1/1/15/20 | 15/37/115/115 | - |
| 25 | CLA | 1 | 605 | - | 1/1/15/20 | 20/37/115/115 | - |
| 26 | CHL | 6 | 617 | 19 | 3/3/15/26 | 1/12/110/137 | - |
| 25 | CLA | A | 1102 | 25 | 1/1/13/20 | 10/25/103/115 | - |
| 25 | CLA | 6 | 604 | 19 | 1/1/15/20 | 16/37/115/115 | - |
| 25 | CLA | 6 | 605 | - | 1/1/11/20 | 6/15/93/115 | - |
| 25 | CLA | 9 | 609 | 23 | 1/1/11/20 | 6/15/93/115 | - |
| 47 | PLM | a | 804 | - | - | 4/13/14/15 | - |
| 35 | LMT | A | 5008 | - | - | 10/21/61/61 | 0/2/2/2 |
| 25 | CLA | 9 | 604 | 23 | 1/1/14/20 | 7/31/109/115 | - |
| 30 | LHG | 7 | 803 | - | - | 22/39/39/53 | - |
| 25 | CLA | 1 | 606 | - | 1/1/13/20 | 12/28/106/115 | - |
| 29 | BCR | B | 4003 | - | - | 7/29/63/63 | 0/2/2/2 |
| 26 | CHL | 5 | 618 | - | 3/3/17/26 | 2/21/119/137 | - |
| 43 | LUT | 9 | 501 | - | - | 3/29/67/67 | 0/2/2/2 |
| 41 | SPH | 4 | 805 | - | - | 9/21/21/21 | - |
| 25 | CLA | B | 1224 | - | 1/1/15/20 | 21/37/115/115 | - |
| 25 | CLA | 3 | 607 | 30 | 1/1/15/20 | 18/37/115/115 | - |
| 33 | PTY | 9 | 803 | - | - | 26/51/51/53 | - |
| 25 | CLA | 4 | 608 | - | 1/1/12/20 | 6/21/99/115 | - |
| 25 | CLA | 9 | 607 | - | 1/1/11/20 | 8/16/94/115 | - |
| 25 | CLA | 5 | 602 | - | 1/1/12/20 | 10/22/100/115 | - |
| 25 | CLA | J | 1901 | 9 | 1/1/10/20 | 6/10/88/115 | - |
| 25 | CLA | A | 1140 | - | 1/1/13/20 | 11/25/103/115 | - |
| 25 | CLA | 7 | 607 | 30 | 1/1/13/20 | 11/29/107/115 | - |
| 50 | XAT | 7 | 502 | - | 2/2/12/26 | 0/31/93/93 | 0/4/4/4 |
| 41 | SPH | 6 | 806 | - | - | 9/21/21/21 | - |
| 28 | SF4 | C | 3003 | 3 | - | - | 0/6/5/5 |
| 25 | CLA | 8 | 606 | - | 1/1/13/20 | 15/28/106/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 25 | CLA | 2 | 621 | 22 | 1/1/15/20 | 16/37/115/115 | - |
| 50 | XAT | 2 | 501 | - | 2/2/12/26 | 0/31/93/93 | 0/4/4/4 |
| 25 | CLA | A | 1129 | - | 1/1/12/20 | 9/19/97/115 | - |
| 25 | CLA | 5 | 609 | 18 | 1/1/12/20 | 12/21/99/115 | - |
| 25 | CLA | B | 1228 | - | 1/1/15/20 | 18/37/115/115 | - |
| 29 | BCR | 7 | 503 | - | - | 11/29/63/63 | 0/2/2/2 |
| 25 | CLA | A | 1124 | - | 1/1/13/20 | 7/25/103/115 | - |
| 25 | CLA | O | 1803 | - | 1/1/10/20 | 5/8/86/115 | - |
| 36 | DGD | B | 5003 | - | - | 22/55/95/95 | 0/2/2/2 |
| 43 | LUT | 8 | 502 | - | - | 5/29/67/67 | 0/2/2/2 |
| 43 | LUT | 9 | 502 | - | - | 3/29/67/67 | 0/2/2/2 |
| 40 | RRX | J | 4002 | - | 1/1/11/25 | 13/29/65/65 | 0/2/2/2 |
| 35 | LMT | 2 | 804 | - | - | 6/21/61/61 | 0/2/2/2 |
| 43 | LUT | 3 | 502 | - | - | 2/29/67/67 | 0/2/2/2 |
| 45 | OLA | a | 805 | - | - | 7/17/17/17 | - |
| 25 | CLA | B | 1227 | - | 1/1/12/20 | 13/19/97/115 | - |
| 35 | LMT | 1 | 804 | - | - | 12/21/61/61 | 0/2/2/2 |
| 42 | ECH | M | 4001 | - | - | 5/29/66/66 | 0/2/2/2 |
| 25 | CLA | A | 1127 | - | 1/1/15/20 | 17/37/115/115 | - |
| 26 | CHL | 8 | 603 | 21 | 4/4/20/26 | 8/39/137/137 | - |
| 33 | PTY | J | 5001 | - | - | 21/31/31/53 | - |
| 25 | CLA | A | 1138 | - | 1/1/15/20 | 8/37/115/115 | - |
| 29 | BCR | I | 4001 | - | - | 15/29/63/63 | 0/2/2/2 |
| 41 | SPH | J | 5002 | - | - | 12/21/21/21 | - |
| 36 | DGD | 7 | 806 | - | - | 13/39/79/95 | 0/2/2/2 |
| 25 | CLA | 4 | 616 | - | 1/1/12/20 | 6/19/97/115 | - |
| 26 | CHL | 6 | 613 | - | 3/3/17/26 | 1/21/119/137 | - |

All (2215) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 40 | 3 | 506 | RRX | C26-C25 | 15.50 | 1.61 | 1.34 |
| 40 | J | 4002 | RRX | C26-C25 | 15.46 | 1.61 | 1.34 |
| 40 | 3 | 506 | RRX | C5-C6 | 14.91 | 1.60 | 1.34 |
| 40 | J | 4002 | RRX | C5-C6 | 14.73 | 1.59 | 1.34 |
| 43 | 3 | 502 | LUT | C24-C25 | 14.67 | 1.51 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | 7 | 501 | LUT | C24-C25 | 14.63 | 1.51 | 1.33 |
| 43 | 2 | 507 | LUT | C24-C25 | 14.59 | 1.51 | 1.33 |
| 43 | 2 | 502 | LUT | C24-C25 | 14.57 | 1.51 | 1.33 |
| 43 | 5 | 505 | LUT | C24-C25 | 14.56 | 1.51 | 1.33 |
| 43 | 1 | 503 | LUT | C24-C25 | 14.55 | 1.51 | 1.33 |
| 43 | a | 503 | LUT | C24-C25 | 14.49 | 1.51 | 1.33 |
| 43 | a | 501 | LUT | C24-C25 | 14.47 | 1.51 | 1.33 |
| 43 | 1 | 501 | LUT | C24-C25 | 14.46 | 1.51 | 1.33 |
| 43 | 4 | 501 | LUT | C24-C25 | 14.46 | 1.51 | 1.33 |
| 43 | 3 | 501 | LUT | C24-C25 | 14.45 | 1.51 | 1.33 |
| 43 | a | 502 | LUT | C24-C25 | 14.38 | 1.51 | 1.33 |
| 43 | 8 | 501 | LUT | C24-C25 | 14.37 | 1.51 | 1.33 |
| 43 | 5 | 501 | LUT | C24-C25 | 14.36 | 1.51 | 1.33 |
| 43 | 9 | 501 | LUT | C24-C25 | 14.34 | 1.51 | 1.33 |
| 43 | 6 | 501 | LUT | C24-C25 | 14.29 | 1.50 | 1.33 |
| 43 | 5 | 502 | LUT | C24-C25 | 14.28 | 1.50 | 1.33 |
| 43 | 4 | 502 | LUT | C24-C25 | 14.28 | 1.50 | 1.33 |
| 43 | 8 | 502 | LUT | C24-C25 | 14.26 | 1.50 | 1.33 |
| 43 | 9 | 502 | LUT | C24-C25 | 14.25 | 1.50 | 1.33 |
| 43 | 6 | 502 | LUT | C24-C25 | 14.19 | 1.50 | 1.33 |
| 44 | 1 | 502 | AXT | C5-C6 | 12.77 | 1.56 | 1.34 |
| 40 | J | 4002 | RRX | C29-C28 | -10.25 | 1.37 | 1.52 |
| 40 | 3 | 506 | RRX | C29-C28 | -10.13 | 1.37 | 1.52 |
| 24 | A | 1011 | CL0 | MG-NA | 9.07 | 2.27 | 2.06 |
| 40 | 3 | 506 | RRX | C27-C28 | 8.09 | 1.66 | 1.52 |
| 46 | a | 504 | QTB | C11-C12 | -7.86 | 1.36 | 1.54 |
| 40 | J | 4002 | RRX | C27-C28 | 7.80 | 1.65 | 1.52 |
| 39 | F | 4001 | NEX | C10-C9 | -7.60 | 1.25 | 1.35 |
| 39 | F | 4001 | NEX | C34-C33 | -7.58 | 1.25 | 1.35 |
| 29 | G | 4001 | BCR | C10-C9 | 7.42 | 1.45 | 1.35 |
| 39 | F | 4001 | NEX | C30-C29 | -7.42 | 1.25 | 1.35 |
| 39 | F | 4001 | NEX | C14-C13 | -7.41 | 1.26 | 1.35 |
| 29 | H | 4001 | BCR | C10-C9 | 7.32 | 1.45 | 1.35 |
| 29 | 4 | 503 | BCR | C10-C9 | 7.26 | 1.45 | 1.35 |
| 29 | O | 4001 | BCR | C10-C9 | 7.23 | 1.45 | 1.35 |
| 29 | B | 4002 | BCR | C10-C9 | 7.18 | 1.45 | 1.35 |
| 29 | 3 | 504 | BCR | C10-C9 | 7.15 | 1.45 | 1.35 |
| 29 | L | 4003 | BCR | C10-C9 | 7.14 | 1.45 | 1.35 |
| 29 | 8 | 503 | BCR | C10-C9 | 7.13 | 1.45 | 1.35 |
| 29 | A | 4005 | BCR | C10-C9 | 7.11 | 1.45 | 1.35 |
| 29 | B | 4003 | BCR | C10-C9 | 7.11 | 1.45 | 1.35 |
| 29 | I | 4001 | BCR | C10-C9 | 7.11 | 1.45 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | L | 4001 | BCR | C10-C9 | 7.08 | 1.45 | 1.35 |
| 29 | 3 | 505 | BCR | C10-C9 | 7.08 | 1.45 | 1.35 |
| 29 | B | 4007 | BCR | C10-C9 | 7.04 | 1.45 | 1.35 |
| 29 | K | 4002 | BCR | C10-C9 | 7.03 | 1.45 | 1.35 |
| 29 | K | 4001 | BCR | C10-C9 | 7.02 | 1.45 | 1.35 |
| 29 | L | 4002 | BCR | C10-C9 | 7.01 | 1.45 | 1.35 |
| 29 | 6 | 503 | BCR | C10-C9 | 7.00 | 1.45 | 1.35 |
| 29 | A | 4003 | BCR | C10-C9 | 6.98 | 1.45 | 1.35 |
| 29 | 3 | 503 | BCR | C10-C9 | 6.97 | 1.45 | 1.35 |
| 29 | B | 4005 | BCR | C10-C9 | 6.96 | 1.45 | 1.35 |
| 29 | J | 4001 | BCR | C10-C9 | 6.94 | 1.45 | 1.35 |
| 25 | B | 1234 | CLA | CHC-C1C | 6.92 | 1.40 | 1.35 |
| 29 | 6 | 504 | BCR | C10-C9 | 6.91 | 1.44 | 1.35 |
| 29 | 7 | 503 | BCR | C10-C9 | 6.90 | 1.44 | 1.35 |
| 29 | B | 4004 | BCR | C10-C9 | 6.87 | 1.44 | 1.35 |
| 29 | A | 4001 | BCR | C10-C9 | 6.83 | 1.44 | 1.35 |
| 29 | 5 | 504 | BCR | C10-C9 | 6.83 | 1.44 | 1.35 |
| 29 | 5 | 503 | BCR | C10-C9 | 6.78 | 1.44 | 1.35 |
| 39 | F | 4001 | NEX | C35-C15 | -6.74 | 1.18 | 1.36 |
| 29 | B | 4006 | BCR | C10-C9 | 6.72 | 1.44 | 1.35 |
| 29 | B | 4001 | BCR | C10-C9 | 6.70 | 1.44 | 1.35 |
| 29 | A | 4004 | BCR | C10-C9 | 6.63 | 1.44 | 1.35 |
| 25 | L | 1504 | CLA | MG-NA | 6.47 | 2.21 | 2.06 |
| 25 | 9 | 605 | CLA | MG-NA | 6.45 | 2.21 | 2.06 |
| 40 | 3 | 506 | RRX | C2-C3 | -6.44 | 1.36 | 1.52 |
| 25 | B | 1240 | CLA | MG-NA | 6.44 | 2.21 | 2.06 |
| 25 | 2 | 621 | CLA | MG-NA | 6.43 | 2.21 | 2.06 |
| 25 | A | 1135 | CLA | MG-NA | 6.43 | 2.21 | 2.06 |
| 25 | K | 1402 | CLA | MG-NA | 6.43 | 2.21 | 2.06 |
| 25 | 4 | 617 | CLA | MG-NA | 6.43 | 2.21 | 2.06 |
| 25 | 8 | 605 | CLA | MG-NA | 6.42 | 2.21 | 2.06 |
| 25 | A | 1107 | CLA | MG-NA | 6.42 | 2.21 | 2.06 |
| 25 | O | 1801 | CLA | MG-NA | 6.42 | 2.21 | 2.06 |
| 25 | 5 | 609 | CLA | MG-NA | 6.42 | 2.21 | 2.06 |
| 40 | J | 4002 | RRX | C2-C3 | -6.41 | 1.36 | 1.52 |
| 25 | 2 | 605 | CLA | MG-NA | 6.41 | 2.21 | 2.06 |
| 25 | 4 | 616 | CLA | MG-NA | 6.41 | 2.21 | 2.06 |
| 25 | 2 | 602 | CLA | MG-NA | 6.40 | 2.21 | 2.06 |
| 25 | 3 | 618 | CLA | MG-NA | 6.39 | 2.21 | 2.06 |
| 25 | O | 1803 | CLA | MG-NA | 6.39 | 2.21 | 2.06 |
| 25 | A | 1125 | CLA | MG-NA | 6.39 | 2.21 | 2.06 |
| 25 | A | 1101 | CLA | MG-NA | 6.38 | 2.21 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | G | 1603 | CLA | MG-NA | 6.38 | 2.21 | 2.06 |
| 25 | A | 1123 | CLA | MG-NA | 6.38 | 2.21 | 2.06 |
| 25 | 9 | 612 | CLA | MG-NA | 6.38 | 2.21 | 2.06 |
| 25 | 6 | 602 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | 1 | 602 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | a | 611 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | 4 | 615 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | J | 1901 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | K | 1404 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | 1 | 615 | CLA | MG-NA | 6.37 | 2.21 | 2.06 |
| 25 | 4 | 605 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 25 | 2 | 603 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 25 | 4 | 607 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 25 | B | 1223 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 25 | 6 | 607 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 25 | 6 | 605 | CLA | MG-NA | 6.36 | 2.21 | 2.06 |
| 25 | K | 1403 | CLA | MG-NA | 6.35 | 2.21 | 2.06 |
| 25 | 2 | 615 | CLA | MG-NA | 6.35 | 2.21 | 2.06 |
| 25 | A | 1130 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 9 | 607 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | A | 1136 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | A | 1139 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | O | 1802 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 4 | 602 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 9 | 609 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 9 | 604 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 4 | 610 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 5 | 602 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | G | 1601 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 5 | 615 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | A | 1140 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | 6 | 606 | CLA | MG-NA | 6.34 | 2.21 | 2.06 |
| 25 | F | 1302 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | 6 | 604 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | 7 | 605 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | G | 1602 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | A | 1109 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | A | 1112 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | 7 | 602 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | 9 | 602 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | H | 1701 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | B | 1239 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 7 | 607 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | a | 607 | CLA | MG-NA | 6.33 | 2.21 | 2.06 |
| 25 | 7 | 603 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | A | 1110 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | 1 | 612 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | 5 | 614 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | a | 615 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | L | 1501 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | A | 1134 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | 8 | 620 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 39 | F | 4001 | NEX | C11-C12 | -6.32 | 1.18 | 1.34 |
| 25 | A | 1137 | CLA | MG-NA | 6.32 | 2.21 | 2.06 |
| 25 | a | 602 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | A | 1118 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | 3 | 616 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | 2 | 608 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | K | 1401 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | 5 | 607 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | H | 1702 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | A | 1124 | CLA | MG-NA | 6.31 | 2.21 | 2.06 |
| 25 | 4 | 603 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | 5 | 605 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | 8 | 602 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | 3 | 607 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | B | 1226 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | A | 1122 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | A | 1141 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | A | 1126 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | 3 | 605 | CLA | MG-NA | 6.30 | 2.21 | 2.06 |
| 25 | B | 1209 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 8 | 609 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 3 | 602 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 6 | 618 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | B | 1214 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | B | 1227 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | B | 1229 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 5 | 606 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 5 | 608 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | B | 1237 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 6 | 612 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | B | 1238 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 2 | 606 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | a | 603 | CLA | MG-NA | 6.29 | 2.21 | 2.06 |
| 25 | 9 | 606 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | 7 | 610 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | A | 1127 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | B | 1022 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | 1 | 607 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | A | 1105 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | B | 1218 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | a | 605 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | 2 | 607 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | B | 1225 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | 5 | 603 | CLA | MG-NA | 6.28 | 2.21 | 2.06 |
| 25 | 6 | 615 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | A | 1129 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | A | 1115 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | 5 | 604 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | a | 612 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | B | 1213 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | 4 | 611 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | 8 | 618 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | a | 608 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | 7 | 606 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 39 | F | 4001 | NEX | C31-C32 | -6.27 | 1.18 | 1.34 |
| 25 | B | 1221 | CLA | MG-NA | 6.27 | 2.21 | 2.06 |
| 25 | 7 | 608 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | A | 1108 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | B | 1224 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | A | 1012 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | B | 1219 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | A | 1131 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | 1 | 603 | CLA | MG-NA | 6.26 | 2.21 | 2.06 |
| 25 | 8 | 615 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | A | 1128 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | B | 1201 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | 8 | 607 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | A | 1120 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | B | 1232 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | 3 | 613 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | A | 1116 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | B | 1210 | CLA | MG-NA | 6.25 | 2.21 | 2.06 |
| 25 | B | 1208 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | B | 1217 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 605 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | B | 1235 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | L | 1503 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | 7 | 604 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | A | 1104 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | A | 1117 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | B | 1220 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | 6 | 603 | CLA | MG-NA | 6.24 | 2.21 | 2.06 |
| 25 | 3 | 610 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | B | 1228 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | B | 1236 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | 4 | 604 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | B | 1203 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | 2 | 612 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | F | 1301 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | A | 1121 | CLA | MG-NA | 6.23 | 2.21 | 2.06 |
| 25 | 4 | 601 | CLA | MG-NA | 6.22 | 2.21 | 2.06 |
| 25 | 8 | 608 | CLA | MG-NA | 6.22 | 2.21 | 2.06 |
| 25 | 5 | 612 | CLA | MG-NA | 6.22 | 2.21 | 2.06 |
| 25 | 4 | 608 | CLA | MG-NA | 6.21 | 2.21 | 2.06 |
| 25 | 2 | 601 | CLA | MG-NA | 6.21 | 2.21 | 2.06 |
| 25 | A | 1111 | CLA | MG-NA | 6.21 | 2.21 | 2.06 |
| 29 | A | 4002 | BCR | C10-C9 | 6.21 | 1.44 | 1.35 |
| 25 | B | 1215 | CLA | MG-NA | 6.21 | 2.21 | 2.06 |
| 25 | a | 601 | CLA | MG-NA | 6.21 | 2.21 | 2.06 |
| 25 | B | 1207 | CLA | MG-NA | 6.20 | 2.21 | 2.06 |
| 25 | 4 | 606 | CLA | MG-NA | 6.20 | 2.21 | 2.06 |
| 25 | B | 1206 | CLA | MG-NA | 6.20 | 2.21 | 2.06 |
| 25 | B | 1202 | CLA | MG-NA | 6.20 | 2.21 | 2.06 |
| 25 | 3 | 601 | CLA | MG-NA | 6.20 | 2.21 | 2.06 |
| 25 | A | 1138 | CLA | MG-NA | 6.19 | 2.21 | 2.06 |
| 25 | B | 1230 | CLA | MG-NA | 6.19 | 2.21 | 2.06 |
| 25 | B | 1212 | CLA | MG-NA | 6.19 | 2.21 | 2.06 |
| 25 | 5 | 601 | CLA | MG-NA | 6.18 | 2.21 | 2.06 |
| 25 | 8 | 606 | CLA | MG-NA | 6.18 | 2.21 | 2.06 |
| 25 | A | 1102 | CLA | MG-NA | 6.18 | 2.20 | 2.06 |
| 25 | A | 1113 | CLA | MG-NA | 6.17 | 2.20 | 2.06 |
| 25 | B | 1204 | CLA | MG-NA | 6.17 | 2.20 | 2.06 |
| 25 | 6 | 601 | CLA | MG-NA | 6.17 | 2.20 | 2.06 |
| 25 | B | 1211 | CLA | MG-NA | 6.17 | 2.20 | 2.06 |
| 25 | A | 1106 | CLA | MG-NA | 6.16 | 2.20 | 2.06 |
| 25 | 8 | 611 | CLA | MG-NA | 6.16 | 2.20 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 601 | CLA | MG-NA | 6.15 | 2.20 | 2.06 |
| 25 | 6 | 608 | CLA | MG-NA | 6.15 | 2.20 | 2.06 |
| 25 | 7 | 612 | CLA | MG-NA | 6.15 | 2.20 | 2.06 |
| 25 | A | 1103 | CLA | MG-NA | 6.14 | 2.20 | 2.06 |
| 25 | A | 1133 | CLA | MG-NA | 6.14 | 2.20 | 2.06 |
| 25 | A | 1132 | CLA | MG-NA | 6.14 | 2.20 | 2.06 |
| 25 | B | 1021 | CLA | MG-NA | 6.14 | 2.20 | 2.06 |
| 25 | A | 1119 | CLA | MG-NA | 6.13 | 2.20 | 2.06 |
| 25 | 2 | 604 | CLA | MG-NA | 6.13 | 2.20 | 2.06 |
| 25 | B | 1222 | CLA | MG-NA | 6.13 | 2.20 | 2.06 |
| 25 | H | 1703 | CLA | MG-NA | 6.12 | 2.20 | 2.06 |
| 25 | 7 | 601 | CLA | MG-NA | 6.11 | 2.20 | 2.06 |
| 25 | 4 | 612 | CLA | MG-NA | 6.11 | 2.20 | 2.06 |
| 25 | B | 1231 | CLA | MG-NA | 6.11 | 2.20 | 2.06 |
| 25 | 3 | 606 | CLA | MG-NA | 6.11 | 2.20 | 2.06 |
| 25 | L | 1502 | CLA | MG-NA | 6.11 | 2.20 | 2.06 |
| 25 | 1 | 606 | CLA | MG-NA | 6.11 | 2.20 | 2.06 |
| 25 | B | 1216 | CLA | MG-NA | 6.10 | 2.20 | 2.06 |
| 25 | B | 1023 | CLA | MG-NA | 6.10 | 2.20 | 2.06 |
| 25 | 3 | 612 | CLA | MG-NA | 6.08 | 2.20 | 2.06 |
| 25 | B | 1205 | CLA | MG-NA | 6.07 | 2.20 | 2.06 |
| 25 | A | 1013 | CLA | MG-NA | 6.06 | 2.20 | 2.06 |
| 25 | 1 | 608 | CLA | MG-NA | 6.01 | 2.20 | 2.06 |
| 25 | 8 | 612 | CLA | MG-NA | 6.01 | 2.20 | 2.06 |
| 40 | 3 | 506 | RRX | C1-C6 | -5.91 | 1.45 | 1.53 |
| 40 | J | 4002 | RRX | C1-C6 | -5.90 | 1.45 | 1.53 |
| 29 | G | 4001 | BCR | C24-C23 | 5.85 | 1.50 | 1.33 |
| 29 | B | 4003 | BCR | C24-C23 | 5.83 | 1.50 | 1.33 |
| 29 | L | 4003 | BCR | C24-C23 | 5.79 | 1.50 | 1.33 |
| 29 | 8 | 503 | BCR | C24-C23 | 5.79 | 1.50 | 1.33 |
| 29 | 6 | 503 | BCR | C24-C23 | 5.78 | 1.50 | 1.33 |
| 29 | B | 4002 | BCR | C24-C23 | 5.76 | 1.50 | 1.33 |
| 44 | 7 | 504 | AXT | C26-C25 | 5.75 | 1.43 | 1.35 |
| 29 | K | 4002 | BCR | C24-C23 | 5.74 | 1.50 | 1.33 |
| 29 | 3 | 504 | BCR | C24-C23 | 5.73 | 1.50 | 1.33 |
| 29 | 4 | 503 | BCR | C24-C23 | 5.73 | 1.50 | 1.33 |
| 29 | H | 4001 | BCR | C24-C23 | 5.71 | 1.50 | 1.33 |
| 29 | 6 | 504 | BCR | C24-C23 | 5.71 | 1.50 | 1.33 |
| 29 | O | 4001 | BCR | C24-C23 | 5.71 | 1.50 | 1.33 |
| 29 | B | 4005 | BCR | C24-C23 | 5.69 | 1.50 | 1.33 |
| 29 | B | 4006 | BCR | C24-C23 | 5.69 | 1.50 | 1.33 |
| 29 | 3 | 505 | BCR | C24-C23 | 5.69 | 1.50 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | L | 4001 | BCR | C24-C23 | 5.68 | 1.50 | 1.33 |
| 29 | 5 | 504 | BCR | C24-C23 | 5.67 | 1.50 | 1.33 |
| 29 | A | 4001 | BCR | C24-C23 | 5.65 | 1.50 | 1.33 |
| 29 | K | 4001 | BCR | C24-C23 | 5.65 | 1.50 | 1.33 |
| 29 | A | 4003 | BCR | C24-C23 | 5.63 | 1.50 | 1.33 |
| 29 | J | 4001 | BCR | C24-C23 | 5.63 | 1.50 | 1.33 |
| 29 | B | 4007 | BCR | C24-C23 | 5.60 | 1.50 | 1.33 |
| 29 | L | 4002 | BCR | C24-C23 | 5.60 | 1.50 | 1.33 |
| 29 | B | 4001 | BCR | C24-C23 | 5.59 | 1.50 | 1.33 |
| 29 | 3 | 503 | BCR | C24-C23 | 5.58 | 1.49 | 1.33 |
| 29 | A | 4004 | BCR | C24-C23 | 5.58 | 1.49 | 1.33 |
| 29 | 5 | 503 | BCR | C24-C23 | 5.54 | 1.49 | 1.33 |
| 29 | A | 4002 | BCR | C24-C23 | 5.52 | 1.49 | 1.33 |
| 29 | A | 4005 | BCR | C24-C23 | 5.52 | 1.49 | 1.33 |
| 29 | B | 4004 | BCR | C24-C23 | 5.52 | 1.49 | 1.33 |
| 40 | 3 | 506 | RRX | C30-C25 | -5.50 | 1.46 | 1.53 |
| 29 | A | 4002 | BCR | C11-C12 | -5.49 | 1.20 | 1.34 |
| 39 | F | 4001 | NEX | C7-C8 | 5.48 | 1.41 | 1.32 |
| 29 | I | 4001 | BCR | C24-C23 | 5.47 | 1.49 | 1.33 |
| 29 | 7 | 503 | BCR | C24-C23 | 5.42 | 1.49 | 1.33 |
| 39 | F | 4001 | NEX | C28-C29 | -5.41 | 1.34 | 1.45 |
| 29 | B | 4001 | BCR | C11-C12 | -5.39 | 1.20 | 1.34 |
| 29 | A | 4004 | BCR | C11-C12 | -5.38 | 1.20 | 1.34 |
| 29 | B | 4006 | BCR | C11-C12 | -5.34 | 1.20 | 1.34 |
| 29 | 6 | 504 | BCR | C11-C12 | -5.34 | 1.20 | 1.34 |
| 29 | 5 | 503 | BCR | C11-C12 | -5.30 | 1.20 | 1.34 |
| 29 | A | 4001 | BCR | C11-C12 | -5.29 | 1.21 | 1.34 |
| 29 | 3 | 503 | BCR | C11-C12 | -5.27 | 1.21 | 1.34 |
| 29 | A | 4003 | BCR | C11-C12 | -5.25 | 1.21 | 1.34 |
| 29 | 5 | 504 | BCR | C11-C12 | -5.25 | 1.21 | 1.34 |
| 40 | J | 4002 | RRX | C19-C18 | 5.25 | 1.57 | 1.45 |
| 29 | B | 4005 | BCR | C11-C12 | -5.24 | 1.21 | 1.34 |
| 29 | K | 4001 | BCR | C11-C12 | -5.24 | 1.21 | 1.34 |
| 29 | B | 4004 | BCR | C11-C12 | -5.23 | 1.21 | 1.34 |
| 29 | 7 | 503 | BCR | C11-C12 | -5.22 | 1.21 | 1.34 |
| 29 | J | 4001 | BCR | C11-C12 | -5.22 | 1.21 | 1.34 |
| 29 | B | 4007 | BCR | C11-C12 | -5.18 | 1.21 | 1.34 |
| 29 | 6 | 503 | BCR | C11-C12 | -5.17 | 1.21 | 1.34 |
| 29 | I | 4001 | BCR | C11-C12 | -5.17 | 1.21 | 1.34 |
| 29 | L | 4002 | BCR | C11-C12 | -5.16 | 1.21 | 1.34 |
| 40 | 3 | 506 | RRX | C2-C1 | 5.16 | 1.66 | 1.54 |
| 29 | L | 4003 | BCR | C11-C12 | -5.16 | 1.21 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | K | 4002 | BCR | C11-C12 | -5.15 | 1.21 | 1.34 |
| 46 | a | 504 | QTB | C17-C11 | -5.15 | 1.50 | 1.55 |
| 29 | L | 4001 | BCR | C11-C12 | -5.14 | 1.21 | 1.34 |
| 29 | 8 | 503 | BCR | C11-C12 | -5.13 | 1.21 | 1.34 |
| 29 | B | 4003 | BCR | C11-C12 | -5.13 | 1.21 | 1.34 |
| 29 | 3 | 504 | BCR | C11-C12 | -5.13 | 1.21 | 1.34 |
| 40 | J | 4002 | RRX | C2-C1 | 5.11 | 1.65 | 1.54 |
| 29 | 3 | 505 | BCR | C11-C12 | -5.11 | 1.21 | 1.34 |
| 29 | B | 4002 | BCR | C11-C12 | -5.11 | 1.21 | 1.34 |
| 29 | A | 4005 | BCR | C11-C12 | -5.11 | 1.21 | 1.34 |
| 29 | O | 4001 | BCR | C11-C12 | -5.08 | 1.21 | 1.34 |
| 29 | 4 | 503 | BCR | C11-C12 | -5.07 | 1.21 | 1.34 |
| 24 | A | 1011 | CL0 | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 24 | A | 1011 | CL0 | O2A-C1 | 5.07 | 1.60 | 1.46 |
| 29 | H | 4001 | BCR | C11-C12 | -5.06 | 1.21 | 1.34 |
| 40 | 3 | 506 | RRX | C19-C18 | 5.06 | 1.56 | 1.45 |
| 24 | A | 1011 | CL0 | CHC-C1C | 5.02 | 1.47 | 1.35 |
| 44 | 7 | 504 | AXT | C28-C29 | 4.98 | 1.56 | 1.45 |
| 40 | J | 4002 | RRX | C30-C25 | -4.96 | 1.47 | 1.53 |
| 44 | 7 | 504 | AXT | C32-C33 | 4.95 | 1.56 | 1.45 |
| 29 | G | 4001 | BCR | C11-C12 | -4.91 | 1.21 | 1.34 |
| 40 | 3 | 506 | RRX | C8-C9 | 4.90 | 1.56 | 1.45 |
| 40 | J | 4002 | RRX | C8-C9 | 4.88 | 1.56 | 1.45 |
| 24 | A | 1011 | CL0 | C3B-C2B | 4.84 | 1.47 | 1.40 |
| 44 | 7 | 504 | AXT | C5-C6 | 4.81 | 1.42 | 1.34 |
| 44 | 1 | 502 | AXT | C8-C9 | 4.72 | 1.56 | 1.45 |
| 44 | 1 | 502 | AXT | C28-C29 | 4.71 | 1.56 | 1.45 |
| 24 | A | 1011 | CL0 | CHD-C1D | 4.70 | 1.47 | 1.38 |
| 24 | A | 1011 | CL0 | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 44 | 1 | 502 | AXT | C26-C25 | 4.62 | 1.42 | 1.35 |
| 44 | 1 | 502 | AXT | C12-C13 | 4.50 | 1.55 | 1.45 |
| 44 | 1 | 502 | AXT | C32-C33 | 4.48 | 1.55 | 1.45 |
| 29 | 5 | 503 | BCR | C16-C17 | -4.47 | 1.29 | 1.43 |
| 29 | 7 | 503 | BCR | C16-C17 | -4.47 | 1.29 | 1.43 |
| 40 | J | 4002 | RRX | C27-C26 | -4.44 | 1.44 | 1.51 |
| 29 | B | 4004 | BCR | C16-C17 | -4.44 | 1.29 | 1.43 |
| 29 | B | 4001 | BCR | C16-C17 | -4.44 | 1.29 | 1.43 |
| 29 | A | 4004 | BCR | C16-C17 | -4.43 | 1.29 | 1.43 |
| 40 | 3 | 506 | RRX | C12-C13 | 4.42 | 1.55 | 1.45 |
| 29 | B | 4005 | BCR | C16-C17 | -4.41 | 1.29 | 1.43 |
| 29 | A | 4002 | BCR | C16-C17 | -4.41 | 1.29 | 1.43 |
| 44 | 7 | 504 | AXT | C8-C9 | 4.41 | 1.55 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 29 | B | 4006 | BCR | C16-C17 | -4.41 | 1.29 | 1.43 |
| 29 | I | 4001 | BCR | C16-C17 | -4.40 | 1.29 | 1.43 |
| 24 | A | 1011 | CL0 | C3D-C4D | -4.40 | 1.34 | 1.44 |
| 40 | J | 4002 | RRX | C12-C13 | 4.39 | 1.55 | 1.45 |
| 29 | A | 4003 | BCR | C16-C17 | -4.37 | 1.29 | 1.43 |
| 40 | 3 | 506 | RRX | C27-C26 | -4.37 | 1.44 | 1.51 |
| 29 | A | 4001 | BCR | C16-C17 | -4.37 | 1.29 | 1.43 |
| 29 | 3 | 503 | BCR | C16-C17 | -4.35 | 1.30 | 1.43 |
| 29 | 6 | 503 | BCR | C16-C17 | -4.34 | 1.30 | 1.43 |
| 29 | J | 4001 | BCR | C16-C17 | -4.32 | 1.30 | 1.43 |
| 36 | 8 | 802 | DGD | O1G-C1A | 4.31 | 1.45 | 1.33 |
| 40 | J | 4002 | RRX | C3-C4 | 4.31 | 1.66 | 1.52 |
| 29 | L | 4002 | BCR | C16-C17 | -4.30 | 1.30 | 1.43 |
| 36 | 8 | 803 | DGD | O1G-C1A | 4.30 | 1.45 | 1.33 |
| 44 | 1 | 502 | AXT | C21-C26 | 4.30 | 1.59 | 1.53 |
| 29 | 8 | 503 | BCR | C16-C17 | -4.29 | 1.30 | 1.43 |
| 29 | B | 4007 | BCR | C16-C17 | -4.29 | 1.30 | 1.43 |
| 36 | 7 | 806 | DGD | O1G-C1A | 4.29 | 1.45 | 1.33 |
| 29 | 5 | 504 | BCR | C16-C17 | -4.29 | 1.30 | 1.43 |
| 44 | 7 | 504 | AXT | C12-C13 | 4.28 | 1.55 | 1.45 |
| 29 | K | 4002 | BCR | C16-C17 | -4.28 | 1.30 | 1.43 |
| 29 | B | 4003 | BCR | C16-C17 | -4.27 | 1.30 | 1.43 |
| 29 | B | 4002 | BCR | C16-C17 | -4.26 | 1.30 | 1.43 |
| 46 | a | 504 | QTB | C11-C10 | -4.25 | 1.44 | 1.50 |
| 29 | A | 4005 | BCR | C16-C17 | -4.25 | 1.30 | 1.43 |
| 29 | K | 4001 | BCR | C16-C17 | -4.24 | 1.30 | 1.43 |
| 29 | 3 | 505 | BCR | C16-C17 | -4.24 | 1.30 | 1.43 |
| 40 | 3 | 506 | RRX | C3-C4 | 4.24 | 1.65 | 1.52 |
| 29 | 6 | 504 | BCR | C16-C17 | -4.23 | 1.30 | 1.43 |
| 29 | O | 4001 | BCR | C16-C17 | -4.22 | 1.30 | 1.43 |
| 29 | H | 4001 | BCR | C16-C17 | -4.22 | 1.30 | 1.43 |
| 40 | J | 4002 | RRX | C20-C21 | 4.21 | 1.56 | 1.43 |
| 36 | B | 5003 | DGD | O1G-C1A | 4.21 | 1.45 | 1.33 |
| 29 | L | 4001 | BCR | C16-C17 | -4.20 | 1.30 | 1.43 |
| 29 | 4 | 503 | BCR | C16-C17 | -4.20 | 1.30 | 1.43 |
| 40 | J | 4002 | RRX | C23-C22 | 4.20 | 1.55 | 1.45 |
| 29 | 3 | 504 | BCR | C16-C17 | -4.19 | 1.30 | 1.43 |
| 29 | L | 4003 | BCR | C16-C17 | -4.18 | 1.30 | 1.43 |
| 29 | G | 4001 | BCR | C16-C17 | -4.17 | 1.30 | 1.43 |
| 40 | 3 | 506 | RRX | C23-C22 | 4.08 | 1.54 | 1.45 |
| 25 | A | 1128 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 25 | B | 1226 | CLA | MG-ND | -4.04 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 40 | 3 | 506 | RRX | C20-C21 | 4.02 | 1.55 | 1.43 |
| 25 | 9 | 605 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 25 | A | 1012 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 25 | B | 1022 | CLA | MG-ND | -4.00 | 1.97 | 2.05 |
| 24 | A | 1011 | CL0 | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 25 | B | 1224 | CLA | MG-ND | -3.96 | 1.97 | 2.05 |
| 40 | 3 | 506 | RRX | C15-C14 | 3.95 | 1.55 | 1.43 |
| 25 | A | 1126 | CLA | MG-ND | -3.93 | 1.98 | 2.05 |
| 25 | a | 615 | CLA | MG-ND | -3.92 | 1.98 | 2.05 |
| 25 | 4 | 615 | CLA | MG-ND | -3.91 | 1.98 | 2.05 |
| 25 | A | 1127 | CLA | MG-ND | -3.91 | 1.98 | 2.05 |
| 25 | A | 1123 | CLA | MG-ND | -3.91 | 1.98 | 2.05 |
| 25 | B | 1023 | CLA | MG-ND | -3.90 | 1.98 | 2.05 |
| 25 | 7 | 605 | CLA | MG-ND | -3.90 | 1.98 | 2.05 |
| 25 | 2 | 621 | CLA | MG-ND | -3.90 | 1.98 | 2.05 |
| 25 | A | 1131 | CLA | MG-ND | -3.90 | 1.98 | 2.05 |
| 25 | B | 1021 | CLA | MG-ND | -3.89 | 1.98 | 2.05 |
| 25 | B | 1221 | CLA | MG-ND | -3.88 | 1.98 | 2.05 |
| 25 | A | 1112 | CLA | MG-ND | -3.87 | 1.98 | 2.05 |
| 25 | A | 1133 | CLA | MG-ND | -3.87 | 1.98 | 2.05 |
| 25 | J | 1901 | CLA | MG-ND | -3.86 | 1.98 | 2.05 |
| 25 | K | 1402 | CLA | MG-ND | -3.86 | 1.98 | 2.05 |
| 25 | A | 1129 | CLA | MG-ND | -3.85 | 1.98 | 2.05 |
| 40 | J | 4002 | RRX | C15-C14 | 3.85 | 1.55 | 1.43 |
| 25 | 6 | 607 | CLA | MG-ND | -3.85 | 1.98 | 2.05 |
| 25 | A | 1141 | CLA | MG-ND | -3.85 | 1.98 | 2.05 |
| 25 | 5 | 608 | CLA | MG-ND | -3.85 | 1.98 | 2.05 |
| 25 | 2 | 615 | CLA | MG-ND | -3.84 | 1.98 | 2.05 |
| 25 | 8 | 620 | CLA | MG-ND | -3.84 | 1.98 | 2.05 |
| 25 | 6 | 615 | CLA | MG-ND | -3.84 | 1.98 | 2.05 |
| 25 | 1 | 615 | CLA | MG-ND | -3.83 | 1.98 | 2.05 |
| 25 | B | 1206 | CLA | MG-ND | -3.83 | 1.98 | 2.05 |
| 25 | 5 | 605 | CLA | MG-ND | -3.83 | 1.98 | 2.05 |
| 25 | A | 1013 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | B | 1211 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | A | 1107 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | A | 1115 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | B | 1223 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | 7 | 612 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | 5 | 614 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | 8 | 611 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |
| 25 | A | 1102 | CLA | MG-ND | -3.82 | 1.98 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 612 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | B | 1214 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | B | 1210 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | B | 1232 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | 6 | 608 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | B | 1219 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | 3 | 607 | CLA | MG-ND | -3.81 | 1.98 | 2.05 |
| 25 | 2 | 607 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | A | 1113 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | 9 | 612 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | A | 1134 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | a | 612 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | K | 1401 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | B | 1225 | CLA | MG-ND | -3.80 | 1.98 | 2.05 |
| 25 | 1 | 602 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 5 | 609 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 6 | 612 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 8 | 607 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 2 | 606 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | A | 1117 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 9 | 602 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | A | 1121 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | B | 1212 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | A | 1119 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | F | 1302 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | a | 601 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 9 | 604 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | A | 1104 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 4 | 607 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | 6 | 606 | CLA | MG-ND | -3.79 | 1.98 | 2.05 |
| 25 | B | 1240 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | 3 | 606 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | B | 1201 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | A | 1118 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | 2 | 604 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | A | 1135 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | 3 | 605 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | 9 | 609 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | 8 | 615 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | H | 1703 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | L | 1503 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | 6 | 605 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1228 | CLA | MG-ND | -3.78 | 1.98 | 2.05 |
| 25 | O | 1802 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | 9 | 607 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | 5 | 615 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | A | 1103 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | F | 1301 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | B | 1227 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | B | 1235 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | 5 | 602 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | 2 | 605 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | A | 1124 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | B | 1239 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | 7 | 607 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | A | 1132 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | A | 1139 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | B | 1208 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | A | 1136 | CLA | MG-ND | -3.77 | 1.98 | 2.05 |
| 25 | 2 | 608 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 6 | 618 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | K | 1404 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 4 | 605 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | L | 1502 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | A | 1109 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | A | 1138 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 7 | 608 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | A | 1125 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 7 | 603 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | A | 1140 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | a | 611 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 3 | 601 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 8 | 602 | CLA | MG-ND | -3.76 | 1.98 | 2.05 |
| 25 | 8 | 605 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 3 | 610 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 6 | 602 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 7 | 610 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 3 | 616 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 7 | 602 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 4 | 608 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 2 | 602 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | A | 1130 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | B | 1230 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 1 | 601 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 610 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | L | 1501 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | B | 1204 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | A | 1116 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | B | 1220 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 7 | 604 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | 2 | 603 | CLA | MG-ND | -3.75 | 1.98 | 2.05 |
| 25 | H | 1702 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | G | 1602 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | 8 | 606 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | 8 | 618 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | A | 1120 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | B | 1213 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | 2 | 601 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | B | 1205 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | 1 | 606 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | G | 1601 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | a | 607 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | 6 | 603 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | B | 1207 | CLA | MG-ND | -3.74 | 1.98 | 2.05 |
| 25 | 4 | 602 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | 7 | 606 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | B | 1238 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | B | 1218 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | K | 1403 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | 2 | 612 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | a | 603 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 24 | A | 1011 | CL0 | C1D-ND | -3.73 | 1.33 | 1.37 |
| 25 | A | 1111 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | 3 | 613 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | B | 1203 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | 4 | 604 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | 5 | 606 | CLA | MG-ND | -3.73 | 1.98 | 2.05 |
| 25 | 4 | 601 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | L | 1504 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | 5 | 601 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | B | 1237 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | O | 1801 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | B | 1216 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | a | 602 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | 4 | 611 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | 4 | 617 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 9 | 606 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | a | 605 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | 5 | 607 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | 1 | 608 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | B | 1217 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | O | 1803 | CLA | MG-ND | -3.72 | 1.98 | 2.05 |
| 25 | 3 | 602 | CLA | MG-ND | -3.71 | 1.98 | 2.05 |
| 25 | 7 | 601 | CLA | MG-ND | -3.71 | 1.98 | 2.05 |
| 25 | B | 1202 | CLA | MG-ND | -3.71 | 1.98 | 2.05 |
| 25 | 1 | 603 | CLA | MG-ND | -3.71 | 1.98 | 2.05 |
| 25 | 4 | 612 | CLA | MG-ND | -3.71 | 1.98 | 2.05 |
| 25 | H | 1701 | CLA | MG-ND | -3.71 | 1.98 | 2.05 |
| 25 | 4 | 616 | CLA | MG-ND | -3.70 | 1.98 | 2.05 |
| 25 | B | 1215 | CLA | MG-ND | -3.70 | 1.98 | 2.05 |
| 25 | A | 1122 | CLA | MG-ND | -3.70 | 1.98 | 2.05 |
| 25 | 8 | 609 | CLA | MG-ND | -3.70 | 1.98 | 2.05 |
| 25 | 5 | 603 | CLA | MG-ND | -3.70 | 1.98 | 2.05 |
| 25 | A | 1137 | CLA | MG-ND | -3.70 | 1.98 | 2.05 |
| 25 | 1 | 607 | CLA | MG-ND | -3.69 | 1.98 | 2.05 |
| 25 | 3 | 618 | CLA | MG-ND | -3.69 | 1.98 | 2.05 |
| 25 | 4 | 603 | CLA | MG-ND | -3.69 | 1.98 | 2.05 |
| 25 | 8 | 612 | CLA | MG-ND | -3.69 | 1.98 | 2.05 |
| 25 | B | 1236 | CLA | MG-ND | -3.69 | 1.98 | 2.05 |
| 25 | A | 1108 | CLA | MG-ND | -3.68 | 1.98 | 2.05 |
| 25 | 6 | 601 | CLA | MG-ND | -3.68 | 1.98 | 2.05 |
| 25 | B | 1222 | CLA | MG-ND | -3.68 | 1.98 | 2.05 |
| 25 | G | 1603 | CLA | MG-ND | -3.68 | 1.98 | 2.05 |
| 24 | A | 1011 | CL0 | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 25 | 5 | 612 | CLA | MG-ND | -3.67 | 1.98 | 2.05 |
| 25 | A | 1110 | CLA | MG-ND | -3.67 | 1.98 | 2.05 |
| 25 | 4 | 606 | CLA | MG-ND | -3.66 | 1.98 | 2.05 |
| 25 | 5 | 604 | CLA | MG-ND | -3.66 | 1.98 | 2.05 |
| 25 | A | 1105 | CLA | MG-ND | -3.65 | 1.98 | 2.05 |
| 25 | 1 | 605 | CLA | MG-ND | -3.65 | 1.98 | 2.05 |
| 25 | a | 608 | CLA | MG-ND | -3.64 | 1.98 | 2.05 |
| 25 | A | 1106 | CLA | MG-ND | -3.63 | 1.98 | 2.05 |
| 25 | A | 1101 | CLA | MG-ND | -3.63 | 1.98 | 2.05 |
| 25 | 8 | 608 | CLA | MG-ND | -3.62 | 1.98 | 2.05 |
| 25 | B | 1209 | CLA | MG-ND | -3.62 | 1.98 | 2.05 |
| 25 | B | 1231 | CLA | MG-ND | -3.62 | 1.98 | 2.05 |
| 25 | 6 | 604 | CLA | MG-ND | -3.61 | 1.98 | 2.05 |
| 25 | B | 1229 | CLA | MG-ND | -3.61 | 1.98 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 53 | 8 | 810 | LAP | P9-O6 | 3.60 | 1.73 | 1.59 |
| 40 | 3 | 506 | RRX | C11-C10 | 3.59 | 1.54 | 1.43 |
| 25 | 3 | 612 | CLA | MG-ND | -3.58 | 1.98 | 2.05 |
| 26 | 9 | 613 | CHL | C3A-C2A | -3.56 | 1.51 | 1.54 |
| 25 | B | 1230 | CLA | C1C-NC | -3.54 | 1.32 | 1.37 |
| 40 | J | 4002 | RRX | C11-C10 | 3.50 | 1.54 | 1.43 |
| 40 | J | 4002 | RRX | C24-C25 | 3.49 | 1.57 | 1.45 |
| 26 | 3 | 611 | CHL | C3B-C2B | -3.49 | 1.35 | 1.40 |
| 48 | 5 | 803 | DGA | OG2-CB1 | 3.49 | 1.44 | 1.34 |
| 25 | A | 1128 | CLA | C1C-NC | -3.48 | 1.32 | 1.37 |
| 44 | 7 | 504 | AXT | C31-C30 | 3.48 | 1.54 | 1.43 |
| 25 | B | 1212 | CLA | C1C-NC | -3.47 | 1.32 | 1.37 |
| 25 | B | 1206 | CLA | C1C-NC | -3.46 | 1.32 | 1.37 |
| 25 | 4 | 611 | CLA | C1C-NC | -3.44 | 1.32 | 1.37 |
| 25 | B | 1215 | CLA | C1C-NC | -3.44 | 1.32 | 1.37 |
| 48 | 8 | 804 | DGA | OG2-CB1 | 3.44 | 1.44 | 1.34 |
| 25 | B | 1210 | CLA | C1C-NC | -3.44 | 1.32 | 1.37 |
| 25 | 4 | 605 | CLA | C1C-NC | -3.43 | 1.32 | 1.37 |
| 25 | 3 | 606 | CLA | C1C-NC | -3.42 | 1.32 | 1.37 |
| 40 | J | 4002 | RRX | C16-C17 | 3.42 | 1.54 | 1.43 |
| 25 | 7 | 601 | CLA | C1C-NC | -3.41 | 1.32 | 1.37 |
| 25 | B | 1204 | CLA | C1C-NC | -3.41 | 1.32 | 1.37 |
| 25 | A | 1133 | CLA | C1C-NC | -3.41 | 1.32 | 1.37 |
| 48 | 3 | 803 | DGA | OG2-CB1 | 3.41 | 1.43 | 1.34 |
| 37 | K | 5002 | PCW | O3-C11 | 3.41 | 1.43 | 1.33 |
| 25 | B | 1023 | CLA | C1C-NC | -3.41 | 1.32 | 1.37 |
| 44 | 7 | 504 | AXT | C21-C26 | 3.41 | 1.58 | 1.53 |
| 25 | A | 1106 | CLA | C1C-NC | -3.41 | 1.32 | 1.37 |
| 25 | B | 1223 | CLA | C1C-NC | -3.41 | 1.32 | 1.37 |
| 37 | B | 5004 | PCW | O3-C11 | 3.40 | 1.43 | 1.33 |
| 25 | A | 1111 | CLA | C1C-NC | -3.40 | 1.32 | 1.37 |
| 25 | A | 1124 | CLA | C1C-NC | -3.40 | 1.32 | 1.37 |
| 40 | 3 | 506 | RRX | C16-C17 | 3.40 | 1.54 | 1.43 |
| 25 | A | 1101 | CLA | C1C-NC | -3.40 | 1.32 | 1.37 |
| 26 | 8 | 603 | CHL | C4B-NB | 3.40 | 1.38 | 1.35 |
| 25 | 8 | 612 | CLA | C1C-NC | -3.40 | 1.32 | 1.37 |
| 25 | A | 1105 | CLA | C1C-NC | -3.40 | 1.32 | 1.37 |
| 25 | K | 1401 | CLA | C1C-NC | -3.39 | 1.32 | 1.37 |
| 25 | A | 1113 | CLA | C1C-NC | -3.39 | 1.32 | 1.37 |
| 26 | 3 | 604 | CHL | C4B-NB | 3.39 | 1.38 | 1.35 |
| 26 | a | 604 | CHL | C4B-NB | 3.39 | 1.38 | 1.35 |
| 37 | K | 5001 | PCW | O3-C11 | 3.39 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 26 | 8 | 604 | CHL | C4B-NB | 3.39 | 1.38 | 1.35 |
| 25 | B | 1226 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 25 | 5 | 605 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 25 | B | 1225 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 25 | F | 1301 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 25 | B | 1207 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 48 | 2 | 803 | DGA | OG2-CB1 | 3.38 | 1.43 | 1.34 |
| 25 | 8 | 620 | CLA | CBB-CAB | 3.38 | 1.51 | 1.29 |
| 25 | A | 1122 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 26 | 8 | 601 | CHL | C4B-NB | 3.38 | 1.38 | 1.35 |
| 25 | A | 1112 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 25 | B | 1227 | CLA | C1C-NC | -3.38 | 1.32 | 1.37 |
| 37 | 6 | 803 | PCW | O3-C11 | 3.38 | 1.43 | 1.33 |
| 25 | L | 1504 | CLA | CBB-CAB | 3.38 | 1.51 | 1.29 |
| 25 | B | 1205 | CLA | C1C-NC | -3.37 | 1.32 | 1.37 |
| 24 | A | 1011 | CL0 | MG-NC | 3.37 | 2.14 | 2.06 |
| 25 | B | 1214 | CLA | C1C-NC | -3.37 | 1.32 | 1.37 |
| 25 | 1 | 602 | CLA | CBB-CAB | 3.37 | 1.51 | 1.29 |
| 25 | A | 1140 | CLA | C1C-NC | -3.37 | 1.32 | 1.37 |
| 25 | J | 1901 | CLA | CBB-CAB | 3.37 | 1.51 | 1.29 |
| 25 | a | 607 | CLA | CBB-CAB | 3.37 | 1.51 | 1.29 |
| 25 | a | 602 | CLA | CBB-CAB | 3.37 | 1.51 | 1.29 |
| 48 | 3 | 803 | DGA | OG1-CA1 | 3.37 | 1.43 | 1.33 |
| 25 | A | 1102 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 7 | 612 | CLA | C1C-NC | -3.36 | 1.32 | 1.37 |
| 25 | L | 1501 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 5 | 607 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | L | 1502 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 26 | 9 | 601 | CHL | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | B | 1218 | CLA | C1C-NC | -3.36 | 1.32 | 1.37 |
| 25 | O | 1803 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 1 | 615 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 48 | 5 | 803 | DGA | OG1-CA1 | 3.36 | 1.43 | 1.33 |
| 25 | 5 | 602 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 2 | 621 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | L | 1503 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | A | 1128 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 5 | 608 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 26 | a | 609 | CHL | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 26 | 6 | 619 | CHL | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | G | 1602 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 4 | 617 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 6 | 603 | CLA | C1C-NC | -3.36 | 1.32 | 1.37 |
| 25 | 2 | 604 | CLA | C1C-NC | -3.36 | 1.32 | 1.37 |
| 25 | 2 | 606 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | A | 1111 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | B | 1210 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | B | 1207 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 7 | 610 | CLA | C1C-NC | -3.36 | 1.32 | 1.37 |
| 25 | a | 605 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 7 | 612 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 26 | 5 | 611 | CHL | C3B-C2B | -3.36 | 1.35 | 1.40 |
| 25 | B | 1230 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | G | 1601 | CLA | CBB-CAB | 3.36 | 1.51 | 1.29 |
| 25 | 4 | 611 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | a | 615 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 4 | 605 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 8 | 605 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | L | 1502 | CLA | C1C-NC | -3.35 | 1.32 | 1.37 |
| 25 | 3 | 618 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 6 | 607 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 2 | 612 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 9 | 606 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 48 | 8 | 804 | DGA | OG1-CA1 | 3.35 | 1.43 | 1.33 |
| 25 | B | 1221 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | A | 1127 | CLA | C1C-NC | -3.35 | 1.32 | 1.37 |
| 25 | 5 | 606 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | K | 1401 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 4 | 610 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 4 | 615 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | B | 1222 | CLA | C1C-NC | -3.35 | 1.32 | 1.37 |
| 25 | B | 1219 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 1 | 606 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | a | 608 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 7 | 610 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | B | 1227 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 7 | 606 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | B | 1217 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | O | 1802 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 9 | 602 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 2 | 605 | CLA | C1C-NC | -3.35 | 1.32 | 1.37 |
| 48 | 2 | 803 | DGA | OG1-CA1 | 3.35 | 1.43 | 1.33 |
| 25 | 3 | 602 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 6 | 601 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 608 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | B | 1206 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 6 | 608 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | A | 1123 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 6 | 615 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | B | 1203 | CLA | C1C-NC | -3.35 | 1.32 | 1.37 |
| 25 | 2 | 608 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | A | 1117 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 9 | 607 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | 5 | 604 | CLA | CBB-CAB | 3.35 | 1.51 | 1.29 |
| 25 | A | 1124 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 602 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 608 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | a | 612 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | K | 1402 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 5 | 605 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 40 | 3 | 506 | RRX | C24-C25 | 3.34 | 1.57 | 1.45 |
| 25 | B | 1224 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 612 | CLA | C1C-NC | -3.34 | 1.32 | 1.37 |
| 25 | B | 1201 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 8 | 615 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 26 | 1 | 613 | CHL | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1220 | CLA | C1C-NC | -3.34 | 1.32 | 1.37 |
| 25 | 1 | 603 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1223 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | A | 1107 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1240 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | a | 603 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 601 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1238 | CLA | C1C-NC | -3.34 | 1.32 | 1.37 |
| 25 | 7 | 601 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1235 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 3 | 610 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 606 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 5 | 603 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1228 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 6 | 618 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | F | 1302 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1229 | CLA | C1C-NC | -3.34 | 1.32 | 1.37 |
| 25 | O | 1801 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | A | 1109 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 3 | 613 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 6 | 602 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | F | 1301 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 1 | 605 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 2 | 602 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 26 | 6 | 617 | CHL | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 1 | 612 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | a | 601 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 40 | J | 4002 | RRX | C29-C30 | 3.34 | 1.65 | 1.54 |
| 25 | B | 1226 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | K | 1404 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 3 | 607 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | K | 1403 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 7 | 607 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 8 | 605 | CLA | C1C-NC | -3.34 | 1.32 | 1.37 |
| 25 | A | 1013 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 7 | 603 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1215 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 604 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | A | 1012 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 4 | 612 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 9 | 605 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 5 | 612 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | 2 | 603 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | B | 1212 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | G | 1603 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | a | 611 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | A | 1110 | CLA | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 26 | 5 | 613 | CHL | CBB-CAB | 3.34 | 1.51 | 1.29 |
| 25 | A | 1121 | CLA | C1C-NC | -3.34 | 1.32 | 1.37 |
| 25 | 3 | 601 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 8 | 606 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1138 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 6 | 605 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1209 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 6 | 612 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1239 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 26 | 3 | 611 | CHL | C4B-NB | 3.33 | 1.38 | 1.35 |
| 25 | 8 | 618 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1211 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1213 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 1 | 607 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 26 | 6 | 609 | CHL | CBB-CAB | 3.33 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 602 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 5 | 614 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1119 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 8 | 611 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1103 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1134 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 5 | 609 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | H | 1701 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1126 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1231 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 4 | 616 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1023 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1232 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 3 | 606 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 2 | 604 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1109 | CLA | C1C-NC | -3.33 | 1.32 | 1.37 |
| 25 | 4 | 607 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1132 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1139 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1108 | CLA | C1C-NC | -3.33 | 1.32 | 1.37 |
| 25 | 7 | 602 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1222 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1138 | CLA | C1C-NC | -3.33 | 1.32 | 1.37 |
| 25 | 7 | 608 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 8 | 607 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 9 | 612 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 26 | 3 | 608 | CHL | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 5 | 601 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 8 | 612 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 2 | 607 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1121 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 8 | 609 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1118 | CLA | C1C-NC | -3.33 | 1.32 | 1.37 |
| 25 | A | 1140 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | B | 1203 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 26 | 7 | 615 | CHL | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 6 | 606 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 7 | 605 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | A | 1118 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 3 | 605 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |
| 25 | 7 | 604 | CLA | C1C-NC | -3.33 | 1.32 | 1.37 |
| 25 | A | 1141 | CLA | CBB-CAB | 3.33 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 601 | CLA | C1C-NC | -3.32 | 1.32 | 1.37 |
| 25 | B | 1229 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | H | 1703 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | A | 1106 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | H | 1702 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | A | 1113 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | 9 | 604 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 26 | 3 | 603 | CHL | C4B-NB | 3.32 | 1.38 | 1.35 |
| 25 | A | 1107 | CLA | C1C-NC | -3.32 | 1.32 | 1.37 |
| 25 | 1 | 608 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1204 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1236 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | A | 1108 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1021 | CLA | C1C-NC | -3.32 | 1.32 | 1.37 |
| 25 | A | 1136 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 26 | 1 | 611 | CHL | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | A | 1101 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 26 | 1 | 604 | CHL | C4B-NB | 3.32 | 1.38 | 1.35 |
| 25 | 1 | 601 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1216 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1219 | CLA | C1C-NC | -3.32 | 1.32 | 1.37 |
| 25 | B | 1238 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 26 | 2 | 610 | CHL | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | 6 | 603 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | K | 1403 | CLA | C1C-NC | -3.32 | 1.32 | 1.37 |
| 25 | A | 1105 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 26 | 9 | 608 | CHL | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | A | 1120 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1205 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | 5 | 615 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | 3 | 618 | CLA | C1C-NC | -3.32 | 1.32 | 1.37 |
| 25 | B | 1022 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | A | 1129 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | 7 | 604 | CLA | CBB-CAB | 3.32 | 1.51 | 1.29 |
| 25 | B | 1232 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | A | 1116 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | A | 1122 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | A | 1137 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | B | 1236 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | A | 1131 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | B | 1237 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | 3 | 612 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 9 | 609 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | A | 1013 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | A | 1137 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | 3 | 616 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | 2 | 605 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | A | 1135 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | 1 | 602 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | B | 1209 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | 2 | 615 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 26 | 7 | 617 | CHL | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | 4 | 608 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | 7 | 603 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | B | 1214 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | B | 1220 | CLA | CBB-CAB | 3.31 | 1.51 | 1.29 |
| 25 | 3 | 612 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | H | 1701 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 25 | 5 | 602 | CLA | C1C-NC | -3.31 | 1.32 | 1.37 |
| 44 | 7 | 504 | AXT | C35-C34 | 3.31 | 1.53 | 1.43 |
| 25 | 4 | 601 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | 5 | 615 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | B | 1237 | CLA | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 26 | 9 | 610 | CHL | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 25 | B | 1225 | CLA | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 25 | B | 1218 | CLA | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 25 | G | 1601 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | B | 1231 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | 2 | 601 | CLA | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 25 | A | 1115 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | A | 1132 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | a | 602 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | B | 1202 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | 6 | 608 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | A | 1133 | CLA | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 25 | B | 1202 | CLA | CBB-CAB | 3.30 | 1.51 | 1.29 |
| 25 | 5 | 601 | CLA | C1C-NC | -3.30 | 1.32 | 1.37 |
| 25 | A | 1104 | CLA | CBB-CAB | 3.29 | 1.51 | 1.29 |
| 25 | B | 1021 | CLA | CBB-CAB | 3.29 | 1.51 | 1.29 |
| 26 | 4 | 609 | CHL | CBB-CAB | 3.29 | 1.51 | 1.29 |
| 36 | B | 5003 | DGD | CAA-C9A | -3.29 | 1.33 | 1.51 |
| 25 | 4 | 607 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 26 | 7 | 617 | CHL | C4B-NB | 3.29 | 1.38 | 1.35 |
| 26 | 9 | 613 | CHL | C4B-NB | 3.29 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 616 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | 7 | 608 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | 2 | 608 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | A | 1112 | CLA | CBB-CAB | 3.29 | 1.51 | 1.29 |
| 25 | A | 1139 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | 6 | 618 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | B | 1208 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | L | 1501 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | A | 1120 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | J | 1901 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | a | 608 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 25 | 6 | 606 | CLA | C1C-NC | -3.29 | 1.32 | 1.37 |
| 26 | 6 | 617 | CHL | C4B-NB | 3.28 | 1.38 | 1.35 |
| 25 | A | 1130 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | 3 | 607 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | a | 601 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | 4 | 603 | CLA | CBB-CAB | 3.28 | 1.51 | 1.29 |
| 25 | 6 | 602 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | 3 | 605 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 26 | 8 | 610 | CHL | CBB-CAB | 3.28 | 1.51 | 1.29 |
| 25 | B | 1228 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | a | 603 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 26 | 1 | 610 | CHL | CBB-CAB | 3.28 | 1.51 | 1.29 |
| 25 | A | 1116 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | 1 | 607 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | 2 | 612 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | B | 1234 | CLA | CBB-CAB | 3.28 | 1.51 | 1.29 |
| 25 | 8 | 602 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | 2 | 615 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | B | 1211 | CLA | C1C-NC | -3.28 | 1.32 | 1.37 |
| 25 | A | 1130 | CLA | CBB-CAB | 3.27 | 1.51 | 1.29 |
| 26 | a | 613 | CHL | CBB-CAB | 3.27 | 1.51 | 1.29 |
| 25 | A | 1117 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | A | 1110 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | A | 1115 | CLA | CBB-CAB | 3.27 | 1.51 | 1.29 |
| 25 | B | 1239 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | a | 607 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | B | 1224 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | 3 | 610 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | 3 | 613 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | A | 1127 | CLA | CBB-CAB | 3.27 | 1.51 | 1.29 |
| 26 | 7 | 611 | CHL | CBB-CAB | 3.27 | 1.51 | 1.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | G | 1603 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 26 | a | 610 | CHL | CBB-CAB | 3.27 | 1.51 | 1.29 |
| 26 | 9 | 603 | CHL | C4B-NB | 3.27 | 1.38 | 1.35 |
| 25 | A | 1103 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | 2 | 601 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 26 | a | 610 | CHL | C4B-NB | 3.27 | 1.38 | 1.35 |
| 25 | B | 1216 | CLA | C1C-NC | -3.27 | 1.32 | 1.37 |
| 25 | 8 | 609 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 25 | 8 | 611 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 26 | 4 | 613 | CHL | C4B-NB | 3.26 | 1.38 | 1.35 |
| 25 | 7 | 605 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 25 | 1 | 612 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 26 | 5 | 617 | CHL | CBB-CAB | 3.26 | 1.50 | 1.29 |
| 36 | B | 5003 | DGD | CDB-CCB | -3.26 | 1.33 | 1.51 |
| 25 | 6 | 607 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 25 | 1 | 608 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 36 | B | 5003 | DGD | CGB-CFB | -3.26 | 1.33 | 1.51 |
| 25 | 6 | 604 | CLA | CBB-CAB | 3.26 | 1.50 | 1.29 |
| 25 | 5 | 609 | CLA | C1C-NC | -3.26 | 1.32 | 1.37 |
| 31 | A | 5004 | LMG | C37-C36 | -3.25 | 1.33 | 1.51 |
| 25 | B | 1217 | CLA | C1C-NC | -3.25 | 1.32 | 1.37 |
| 25 | L | 1504 | CLA | C1C-NC | -3.25 | 1.32 | 1.37 |
| 26 | 4 | 613 | CHL | CBB-CAB | 3.25 | 1.50 | 1.29 |
| 26 | A | 1114 | CHL | CBB-CAB | 3.25 | 1.50 | 1.29 |
| 25 | A | 1135 | CLA | CBB-CAB | 3.25 | 1.50 | 1.29 |
| 25 | 1 | 601 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 36 | 8 | 802 | DGD | CDA-CCA | -3.25 | 1.33 | 1.51 |
| 36 | 8 | 802 | DGD | CAB-C9B | -3.25 | 1.33 | 1.51 |
| 26 | 4 | 618 | CHL | CBB-CAB | 3.25 | 1.50 | 1.29 |
| 25 | A | 1129 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 25 | 8 | 615 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 26 | A | 1114 | CHL | C4B-NB | 3.25 | 1.38 | 1.35 |
| 25 | a | 615 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 25 | 4 | 610 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 26 | 9 | 613 | CHL | CBB-CAB | 3.25 | 1.50 | 1.29 |
| 44 | 1 | 502 | AXT | C15-C14 | 3.25 | 1.53 | 1.43 |
| 25 | A | 1104 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 25 | 4 | 604 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 26 | 6 | 613 | CHL | CBB-CAB | 3.25 | 1.50 | 1.29 |
| 25 | B | 1240 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 25 | 8 | 608 | CLA | C1C-NC | -3.25 | 1.33 | 1.37 |
| 40 | 3 | 506 | RRX | C29-C30 | 3.24 | 1.65 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1136 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 25 | 4 | 602 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 26 | 5 | 611 | CHL | C4B-NB | 3.24 | 1.38 | 1.35 |
| 26 | 7 | 611 | CHL | C4B-NB | 3.24 | 1.38 | 1.35 |
| 36 | 8 | 802 | DGD | CAA-C9A | -3.24 | 1.33 | 1.51 |
| 25 | 1 | 606 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 25 | L | 1503 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 25 | 7 | 606 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 26 | 5 | 610 | CHL | CBB-CAB | 3.24 | 1.50 | 1.29 |
| 25 | 5 | 603 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 26 | 8 | 613 | CHL | C4B-NB | 3.24 | 1.38 | 1.35 |
| 25 | A | 1125 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 25 | 5 | 612 | CLA | C1C-NC | -3.24 | 1.33 | 1.37 |
| 44 | 1 | 502 | AXT | C31-C30 | 3.23 | 1.53 | 1.43 |
| 25 | 4 | 606 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | 2 | 603 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | 5 | 608 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | 8 | 606 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 26 | 6 | 610 | CHL | CBB-CAB | 3.23 | 1.50 | 1.29 |
| 25 | A | 1102 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 26 | 1 | 611 | CHL | C4B-NB | 3.23 | 1.38 | 1.35 |
| 26 | 2 | 613 | CHL | C4B-NB | 3.23 | 1.38 | 1.35 |
| 25 | H | 1702 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | a | 611 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 36 | B | 5003 | DGD | CAB-C9B | -3.23 | 1.33 | 1.51 |
| 36 | B | 5003 | DGD | CGA-CFA | -3.23 | 1.33 | 1.51 |
| 25 | 5 | 607 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | B | 1235 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | 2 | 606 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | 6 | 615 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 25 | 7 | 607 | CLA | C1C-NC | -3.23 | 1.33 | 1.37 |
| 26 | 3 | 608 | CHL | C4B-NB | 3.23 | 1.38 | 1.35 |
| 25 | B | 1201 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | 2 | 607 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 26 | 7 | 615 | CHL | C4B-NB | 3.22 | 1.38 | 1.35 |
| 25 | 9 | 602 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | 9 | 604 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | A | 1141 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | O | 1803 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | a | 605 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | 4 | 603 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |
| 25 | 8 | 618 | CLA | C1C-NC | -3.22 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 26 | 8 | 601 | CHL | C3B-C2B | -3.22 | 1.35 | 1.40 |
| 26 | 8 | 613 | CHL | CBB-CAB | 3.22 | 1.50 | 1.29 |
| 26 | 4 | 609 | CHL | C4B-NB | 3.22 | 1.38 | 1.35 |
| 25 | G | 1602 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | 2 | 621 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 44 | 7 | 504 | AXT | C15-C14 | 3.21 | 1.53 | 1.43 |
| 25 | H | 1703 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | 6 | 601 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | A | 1012 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | F | 1302 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 26 | 7 | 609 | CHL | C4B-NB | 3.21 | 1.38 | 1.35 |
| 25 | 7 | 602 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 26 | 1 | 609 | CHL | C4B-NB | 3.21 | 1.38 | 1.35 |
| 25 | a | 612 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | 4 | 615 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | A | 1131 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | 4 | 616 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 26 | 7 | 609 | CHL | CBB-CAB | 3.21 | 1.50 | 1.29 |
| 25 | 9 | 612 | CLA | C1C-NC | -3.21 | 1.33 | 1.37 |
| 25 | 1 | 605 | CLA | C1C-NC | -3.20 | 1.33 | 1.37 |
| 26 | 5 | 617 | CHL | C4B-NB | 3.20 | 1.38 | 1.35 |
| 26 | 1 | 609 | CHL | CBB-CAB | 3.20 | 1.50 | 1.29 |
| 25 | K | 1402 | CLA | C1C-NC | -3.20 | 1.33 | 1.37 |
| 26 | 4 | 618 | CHL | C4B-NB | 3.20 | 1.38 | 1.35 |
| 26 | 2 | 610 | CHL | C4B-NB | 3.20 | 1.38 | 1.35 |
| 36 | 7 | 806 | DGD | CAA-C9A | -3.20 | 1.33 | 1.51 |
| 26 | 5 | 618 | CHL | CBB-CAB | 3.20 | 1.50 | 1.29 |
| 36 | B | 5003 | DGD | CDA-CCA | -3.19 | 1.33 | 1.51 |
| 25 | A | 1119 | CLA | C1C-NC | -3.19 | 1.33 | 1.37 |
| 25 | 1 | 603 | CLA | C1C-NC | -3.19 | 1.33 | 1.37 |
| 26 | 2 | 613 | CHL | CBB-CAB | 3.19 | 1.50 | 1.29 |
| 25 | 5 | 614 | CLA | C1C-NC | -3.19 | 1.33 | 1.37 |
| 25 | 9 | 609 | CLA | C1C-NC | -3.19 | 1.33 | 1.37 |
| 26 | 9 | 603 | CHL | CBB-CAB | 3.19 | 1.50 | 1.29 |
| 25 | A | 1134 | CLA | C1C-NC | -3.19 | 1.33 | 1.37 |
| 25 | O | 1802 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | 5 | 606 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | 9 | 605 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 44 | 1 | 502 | AXT | C35-C34 | 3.18 | 1.53 | 1.43 |
| 25 | A | 1123 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | A | 1126 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | 9 | 607 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 617 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 44 | 1 | 502 | AXT | C11-C10 | 3.18 | 1.53 | 1.43 |
| 25 | 6 | 612 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | A | 1125 | CLA | CBB-CAB | 3.18 | 1.50 | 1.29 |
| 26 | 7 | 613 | CHL | C4B-NB | 3.18 | 1.38 | 1.35 |
| 26 | 9 | 608 | CHL | C4B-NB | 3.18 | 1.38 | 1.35 |
| 25 | K | 1404 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | 5 | 604 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 26 | a | 613 | CHL | C4B-NB | 3.18 | 1.38 | 1.35 |
| 25 | 6 | 605 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 25 | 8 | 620 | CLA | C1C-NC | -3.18 | 1.33 | 1.37 |
| 26 | 8 | 604 | CHL | C3B-C2B | -3.17 | 1.36 | 1.40 |
| 25 | 2 | 602 | CLA | C1C-NC | -3.17 | 1.33 | 1.37 |
| 25 | O | 1801 | CLA | C1C-NC | -3.17 | 1.33 | 1.37 |
| 26 | a | 604 | CHL | CBB-CAB | 3.17 | 1.50 | 1.29 |
| 26 | 6 | 611 | CHL | CBB-CAB | 3.16 | 1.50 | 1.29 |
| 25 | 1 | 615 | CLA | C1C-NC | -3.16 | 1.33 | 1.37 |
| 26 | a | 606 | CHL | C4B-NB | 3.16 | 1.38 | 1.35 |
| 26 | 7 | 613 | CHL | CBB-CAB | 3.16 | 1.50 | 1.29 |
| 26 | 1 | 604 | CHL | CBB-CAB | 3.15 | 1.50 | 1.29 |
| 26 | a | 606 | CHL | CBB-CAB | 3.15 | 1.50 | 1.29 |
| 25 | B | 1022 | CLA | C1C-NC | -3.15 | 1.33 | 1.37 |
| 25 | 8 | 607 | CLA | C1C-NC | -3.14 | 1.33 | 1.37 |
| 26 | 6 | 611 | CHL | C4B-NB | 3.14 | 1.38 | 1.35 |
| 26 | 6 | 619 | CHL | C4B-NB | 3.14 | 1.38 | 1.35 |
| 25 | 9 | 606 | CLA | C1C-NC | -3.14 | 1.33 | 1.37 |
| 26 | 5 | 618 | CHL | C4B-NB | 3.14 | 1.38 | 1.35 |
| 26 | 8 | 610 | CHL | C4B-NB | 3.13 | 1.38 | 1.35 |
| 25 | B | 1221 | CLA | C1C-NC | -3.13 | 1.33 | 1.37 |
| 25 | 3 | 602 | CLA | C1C-NC | -3.13 | 1.33 | 1.37 |
| 26 | 3 | 603 | CHL | CBB-CAB | 3.12 | 1.50 | 1.29 |
| 25 | B | 1213 | CLA | C1C-NC | -3.12 | 1.33 | 1.37 |
| 26 | 9 | 610 | CHL | C4B-NB | 3.12 | 1.38 | 1.35 |
| 26 | 2 | 609 | CHL | C4B-NB | 3.11 | 1.38 | 1.35 |
| 26 | 8 | 603 | CHL | CBB-CAB | 3.11 | 1.49 | 1.29 |
| 26 | 6 | 610 | CHL | C4B-NB | 3.09 | 1.38 | 1.35 |
| 26 | 2 | 609 | CHL | C3B-C2B | -3.08 | 1.36 | 1.40 |
| 26 | 3 | 604 | CHL | CBB-CAB | 3.08 | 1.49 | 1.29 |
| 26 | 8 | 604 | CHL | CBB-CAB | 3.08 | 1.49 | 1.29 |
| 40 | J | 4002 | RRX | C4-C5 | -3.07 | 1.44 | 1.51 |
| 25 | A | 1125 | CLA | C3B-C2B | -3.07 | 1.36 | 1.40 |
| 26 | 5 | 610 | CHL | C4B-NB | 3.07 | 1.37 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 6 | 604 | CLA | C1C-NC | -3.07 | 1.33 | 1.37 |
| 26 | 3 | 611 | CHL | CBB-CAB | 3.07 | 1.49 | 1.29 |
| 26 | 5 | 611 | CHL | CBB-CAB | 3.06 | 1.49 | 1.29 |
| 26 | 1 | 613 | CHL | C4B-NB | 3.05 | 1.37 | 1.35 |
| 26 | 6 | 609 | CHL | C4B-NB | 3.05 | 1.37 | 1.35 |
| 24 | A | 1011 | CL0 | C3D-C2D | 3.05 | 1.47 | 1.39 |
| 40 | 3 | 506 | RRX | C7-C6 | 3.04 | 1.55 | 1.45 |
| 26 | 5 | 618 | CHL | C3B-C2B | -3.01 | 1.36 | 1.40 |
| 26 | 8 | 603 | CHL | C3B-C2B | -3.01 | 1.36 | 1.40 |
| 26 | 8 | 601 | CHL | CBB-CAB | 3.01 | 1.49 | 1.29 |
| 26 | 2 | 609 | CHL | CBB-CAB | 3.00 | 1.49 | 1.29 |
| 40 | J | 4002 | RRX | C7-C6 | 3.00 | 1.55 | 1.45 |
| 26 | A | 1114 | CHL | C3B-C2B | -2.98 | 1.36 | 1.40 |
| 40 | 3 | 506 | RRX | C4-C5 | -2.97 | 1.45 | 1.51 |
| 52 | 8 | 805 | P5S | O37-C38 | 2.97 | 1.42 | 1.34 |
| 26 | 1 | 610 | CHL | C4B-NB | 2.95 | 1.37 | 1.35 |
| 26 | a | 606 | CHL | C3B-C2B | -2.94 | 1.36 | 1.40 |
| 26 | 5 | 613 | CHL | C4B-NB | 2.94 | 1.37 | 1.35 |
| 25 | B | 1234 | CLA | C3B-C2B | -2.93 | 1.36 | 1.40 |
| 44 | 7 | 504 | AXT | C11-C10 | 2.92 | 1.52 | 1.43 |
| 26 | 6 | 613 | CHL | C4B-NB | 2.92 | 1.37 | 1.35 |
| 26 | 9 | 601 | CHL | C4B-NB | 2.91 | 1.37 | 1.35 |
| 25 | 6 | 604 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 25 | B | 1021 | CLA | C3B-C2B | -2.90 | 1.36 | 1.40 |
| 26 | 3 | 604 | CHL | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 24 | A | 1011 | CL0 | C4D-CHA | 2.87 | 1.48 | 1.38 |
| 25 | A | 1125 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 25 | A | 1127 | CLA | C3B-C2B | -2.86 | 1.36 | 1.40 |
| 26 | 3 | 603 | CHL | C3B-C2B | -2.86 | 1.36 | 1.40 |
| 25 | A | 1135 | CLA | C3B-C2B | -2.85 | 1.36 | 1.40 |
| 25 | A | 1137 | CLA | C3B-C2B | -2.84 | 1.36 | 1.40 |
| 26 | a | 609 | CHL | C4B-NB | 2.84 | 1.37 | 1.35 |
| 53 | 8 | 810 | LAP | P9-O4 | 2.84 | 1.70 | 1.59 |
| 26 | 2 | 613 | CHL | C3B-C2B | -2.81 | 1.36 | 1.40 |
| 26 | a | 604 | CHL | C3B-C2B | -2.80 | 1.36 | 1.40 |
| 25 | B | 1229 | CLA | C3B-C2B | -2.80 | 1.36 | 1.40 |
| 25 | B | 1231 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 25 | 4 | 603 | CLA | C3B-C2B | -2.76 | 1.36 | 1.40 |
| 40 | 3 | 506 | RRX | C32-C1 | 2.76 | 1.59 | 1.53 |
| 40 | J | 4002 | RRX | C32-C1 | 2.76 | 1.59 | 1.53 |
| 25 | 5 | 601 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 25 | F | 1301 | CLA | C3B-C2B | -2.75 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 603 | CLA | CHC-C1C | 2.75 | 1.42 | 1.35 |
| 25 | 8 | 607 | CLA | C3B-C2B | -2.74 | 1.36 | 1.40 |
| 25 | 7 | 601 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 25 | B | 1214 | CLA | C3B-C2B | -2.73 | 1.36 | 1.40 |
| 25 | A | 1116 | CLA | CHC-C1C | 2.73 | 1.42 | 1.35 |
| 25 | B | 1022 | CLA | C3B-C2B | -2.73 | 1.36 | 1.40 |
| 25 | 6 | 601 | CLA | CHC-C1C | 2.73 | 1.42 | 1.35 |
| 25 | B | 1211 | CLA | CHC-C1C | 2.73 | 1.42 | 1.35 |
| 25 | 9 | 606 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 25 | A | 1013 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 25 | A | 1130 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 25 | 5 | 604 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 38 | F | 5003 | LPX | P1-O1 | 2.72 | 1.70 | 1.59 |
| 25 | A | 1133 | CLA | C3B-C2B | -2.72 | 1.36 | 1.40 |
| 25 | A | 1119 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 25 | B | 1202 | CLA | C3B-C2B | -2.72 | 1.36 | 1.40 |
| 25 | B | 1215 | CLA | C3B-C2B | -2.72 | 1.36 | 1.40 |
| 25 | B | 1213 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 25 | O | 1802 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 25 | 6 | 604 | CLA | C3B-C2B | -2.71 | 1.36 | 1.40 |
| 25 | A | 1115 | CLA | C3B-C2B | -2.71 | 1.36 | 1.40 |
| 25 | A | 1139 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 25 | 4 | 611 | CLA | C3B-C2B | -2.71 | 1.36 | 1.40 |
| 25 | B | 1208 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 25 | G | 1602 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 25 | B | 1237 | CLA | C3B-C2B | -2.71 | 1.36 | 1.40 |
| 25 | O | 1803 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 25 | B | 1229 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 25 | B | 1235 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 25 | B | 1225 | CLA | C3B-C2B | -2.70 | 1.36 | 1.40 |
| 25 | B | 1222 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 25 | A | 1127 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 25 | B | 1238 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 25 | A | 1012 | CLA | C3B-C2B | -2.69 | 1.36 | 1.40 |
| 25 | B | 1239 | CLA | C3B-C2B | -2.69 | 1.36 | 1.40 |
| 24 | A | 1011 | CL0 | C1C-NC | -2.69 | 1.33 | 1.37 |
| 25 | B | 1209 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 25 | A | 1124 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 25 | 6 | 605 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 44 | 7 | 504 | AXT | C27-C26 | 2.69 | 1.54 | 1.45 |
| 25 | B | 1023 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 25 | A | 1106 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1115 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 25 | A | 1108 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | A | 1138 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | 4 | 606 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | 8 | 620 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | 3 | 613 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | A | 1130 | CLA | C3B-C2B | -2.68 | 1.36 | 1.40 |
| 44 | 7 | 504 | AXT | C24-C25 | 2.68 | 1.53 | 1.47 |
| 25 | 8 | 609 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 26 | 6 | 611 | CHL | C3B-C2B | -2.68 | 1.36 | 1.40 |
| 35 | B | 5006 | LMT | O3'-C3' | -2.68 | 1.36 | 1.43 |
| 25 | B | 1223 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | B | 1205 | CLA | C3B-C2B | -2.68 | 1.36 | 1.40 |
| 26 | 8 | 601 | CHL | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | H | 1703 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | 3 | 602 | CLA | CHC-C1C | 2.68 | 1.41 | 1.35 |
| 25 | 3 | 612 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | B | 1201 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | 5 | 614 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | 8 | 606 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | 4 | 616 | CLA | C3B-C2B | -2.67 | 1.36 | 1.40 |
| 25 | L | 1502 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | L | 1503 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | B | 1209 | CLA | C3B-C2B | -2.67 | 1.36 | 1.40 |
| 25 | a | 605 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | 9 | 602 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | 4 | 604 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | 8 | 612 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | A | 1136 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 25 | A | 1012 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | A | 1110 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 1 | 601 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | a | 608 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | B | 1234 | CLA | C1C-NC | -2.66 | 1.32 | 1.38 |
| 25 | 2 | 612 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | A | 1102 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | G | 1603 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 5 | 609 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 7 | 606 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 9 | 604 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 9 | 609 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 4 | 610 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 602 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | B | 1022 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 25 | 5 | 605 | CLA | CHC-C1C | 2.66 | 1.41 | 1.35 |
| 26 | 6 | 610 | CHL | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 25 | B | 1217 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | A | 1106 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 25 | B | 1236 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 2 | 605 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 2 | 615 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 4 | 603 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 4 | 615 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | G | 1603 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 25 | 1 | 606 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | A | 1129 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | B | 1202 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | A | 1140 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | F | 1302 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 3 | 612 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 25 | B | 1210 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | B | 1224 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 8 | 608 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | K | 1402 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | 1 | 605 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 25 | L | 1501 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | A | 1110 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 25 | A | 1120 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | a | 602 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | 7 | 608 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 25 | a | 601 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 35 | 2 | 804 | LMT | O3'-C3' | -2.64 | 1.36 | 1.43 |
| 25 | A | 1136 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 25 | B | 1232 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | 9 | 607 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | a | 615 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | 8 | 615 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | A | 1108 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 25 | A | 1135 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 44 | 1 | 502 | AXT | C1-C6 | 2.64 | 1.57 | 1.53 |
| 25 | 7 | 602 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | 7 | 604 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | 1 | 608 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | A | 1126 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 606 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 25 | 2 | 602 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | A | 1105 | CLA | C3B-C2B | -2.63 | 1.36 | 1.40 |
| 25 | A | 1104 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | A | 1137 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | O | 1801 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | a | 607 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 52 | 8 | 805 | P5S | O19-C17 | 2.63 | 1.41 | 1.33 |
| 25 | A | 1122 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 35 | A | 5008 | LMT | O3'-C3' | -2.63 | 1.36 | 1.43 |
| 25 | 7 | 605 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | A | 1122 | CLA | C3B-C2B | -2.63 | 1.36 | 1.40 |
| 25 | 4 | 601 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | A | 1103 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | 1 | 607 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | B | 1219 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | 3 | 601 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | 4 | 607 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | A | 1134 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 25 | 2 | 604 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | K | 1404 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 5 | 602 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | A | 1101 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 3 | 618 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | A | 1101 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |
| 25 | B | 1216 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 6 | 602 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 2 | 606 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | B | 1203 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 1 | 603 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 7 | 603 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |
| 25 | B | 1228 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 4 | 608 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | A | 1118 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |
| 25 | 9 | 605 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 5 | 607 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 5 | 608 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 2 | 608 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 2 | 612 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |
| 25 | A | 1121 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 3 | 605 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | B | 1223 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1105 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | B | 1212 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | B | 1237 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | B | 1230 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | B | 1240 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 6 | 618 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | 8 | 618 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 25 | A | 1116 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |
| 25 | A | 1113 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 6 | 607 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 6 | 615 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 26 | 8 | 613 | CHL | C3B-C2B | -2.61 | 1.36 | 1.40 |
| 25 | 4 | 602 | CLA | C3B-C2B | -2.61 | 1.36 | 1.40 |
| 37 | K | 5002 | PCW | O2-C2 | -2.61 | 1.40 | 1.46 |
| 25 | 1 | 615 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | a | 612 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 7 | 607 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 5 | 612 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 4 | 612 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 6 | 603 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | 8 | 607 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 25 | B | 1207 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | A | 1107 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | 4 | 616 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 50 | 2 | 501 | XAT | O24-C25 | -2.60 | 1.42 | 1.46 |
| 25 | B | 1218 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | B | 1225 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | G | 1601 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | 5 | 615 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 26 | 1 | 604 | CHL | C3B-C2B | -2.60 | 1.36 | 1.40 |
| 25 | 8 | 605 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | 6 | 612 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | A | 1134 | CLA | C3B-C2B | -2.60 | 1.36 | 1.40 |
| 25 | B | 1232 | CLA | C3B-C2B | -2.60 | 1.36 | 1.40 |
| 25 | J | 1901 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | a | 611 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | a | 603 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | 1 | 602 | CLA | C3B-C2B | -2.60 | 1.36 | 1.40 |
| 25 | 3 | 607 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | B | 1231 | CLA | C3B-C2B | -2.60 | 1.36 | 1.40 |
| 25 | B | 1227 | CLA | CHC-C1C | 2.60 | 1.41 | 1.35 |
| 25 | B | 1239 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 9 | 612 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 25 | B | 1204 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 25 | K | 1401 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 25 | B | 1021 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 25 | H | 1702 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 25 | 6 | 608 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 31 | A | 5004 | LMG | C19-C18 | -2.59 | 1.33 | 1.51 |
| 25 | L | 1504 | CLA | CHC-C1C | 2.59 | 1.41 | 1.35 |
| 35 | 1 | 804 | LMT | O3'-C3' | -2.59 | 1.36 | 1.43 |
| 25 | A | 1109 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | A | 1133 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | K | 1403 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | A | 1141 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | 4 | 602 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | 7 | 610 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | A | 1117 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | 6 | 606 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 26 | 9 | 603 | CHL | C3B-C2B | -2.58 | 1.36 | 1.40 |
| 25 | 7 | 602 | CLA | C3B-C2B | -2.58 | 1.36 | 1.40 |
| 25 | 7 | 612 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | A | 1104 | CLA | C3B-C2B | -2.58 | 1.36 | 1.40 |
| 25 | 1 | 602 | CLA | CHC-C1C | 2.58 | 1.41 | 1.35 |
| 25 | 7 | 603 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | A | 1132 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | 3 | 610 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | B | 1220 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | A | 1139 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 25 | 8 | 608 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 25 | 2 | 601 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | 7 | 608 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | 6 | 606 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 25 | 8 | 611 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | 4 | 617 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 33 | G | 5003 | PTY | O7-C6 | -2.57 | 1.40 | 1.46 |
| 25 | B | 1205 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | B | 1221 | CLA | CHC-C1C | 2.57 | 1.41 | 1.35 |
| 25 | 2 | 605 | CLA | C3B-C2B | -2.56 | 1.36 | 1.40 |
| 25 | 2 | 603 | CLA | CHC-C1C | 2.56 | 1.41 | 1.35 |
| 25 | 3 | 616 | CLA | CHC-C1C | 2.56 | 1.41 | 1.35 |
| 25 | A | 1140 | CLA | C3B-C2B | -2.56 | 1.36 | 1.40 |
| 25 | 8 | 602 | CLA | C3B-C2B | -2.56 | 1.36 | 1.40 |
| 25 | 8 | 615 | CLA | C3B-C2B | -2.56 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1111 | CLA | CHC-C1C | 2.56 | 1.41 | 1.35 |
| 26 | 5 | 610 | CHL | C3B-C2B | -2.56 | 1.36 | 1.40 |
| 25 | 1 | 607 | CLA | C3B-C2B | -2.56 | 1.36 | 1.40 |
| 37 | 6 | 803 | PCW | O2-C2 | -2.55 | 1.40 | 1.46 |
| 37 | K | 5001 | PCW | O2-C2 | -2.55 | 1.40 | 1.46 |
| 25 | 2 | 607 | CLA | CHC-C1C | 2.55 | 1.41 | 1.35 |
| 25 | B | 1238 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 33 | B | 5005 | PTY | O7-C6 | -2.55 | 1.40 | 1.46 |
| 25 | A | 1120 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 33 | A | 5006 | PTY | O7-C6 | -2.55 | 1.40 | 1.46 |
| 25 | F | 1301 | CLA | CHC-C1C | 2.55 | 1.41 | 1.35 |
| 25 | B | 1203 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 25 | 3 | 618 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 25 | A | 1123 | CLA | CHC-C1C | 2.54 | 1.41 | 1.35 |
| 25 | A | 1131 | CLA | CHC-C1C | 2.54 | 1.41 | 1.35 |
| 25 | B | 1236 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 24 | A | 1011 | CL0 | C1B-CHB | 2.54 | 1.48 | 1.41 |
| 25 | H | 1701 | CLA | CHC-C1C | 2.54 | 1.41 | 1.35 |
| 25 | B | 1214 | CLA | CHC-C1C | 2.54 | 1.41 | 1.35 |
| 25 | B | 1207 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 25 | 1 | 612 | CLA | CHC-C1C | 2.54 | 1.41 | 1.35 |
| 25 | 5 | 602 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 26 | 7 | 609 | CHL | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 25 | A | 1112 | CLA | CHC-C1C | 2.54 | 1.41 | 1.35 |
| 25 | 6 | 602 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 25 | B | 1217 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 25 | A | 1118 | CLA | CHC-C1C | 2.53 | 1.41 | 1.35 |
| 25 | 2 | 621 | CLA | CHC-C1C | 2.53 | 1.41 | 1.35 |
| 25 | H | 1703 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 25 | G | 1601 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 33 | a | 802 | PTY | O7-C6 | -2.52 | 1.40 | 1.46 |
| 25 | 8 | 605 | CLA | C3B-C2B | -2.52 | 1.36 | 1.40 |
| 25 | A | 1126 | CLA | C3B-C2B | -2.52 | 1.36 | 1.40 |
| 33 | a | 803 | PTY | O7-C6 | -2.51 | 1.40 | 1.46 |
| 25 | 4 | 611 | CLA | CHC-C1C | 2.51 | 1.41 | 1.35 |
| 25 | 3 | 606 | CLA | CHC-C1C | 2.51 | 1.41 | 1.35 |
| 25 | 4 | 610 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |
| 25 | K | 1403 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |
| 25 | B | 1215 | CLA | CHC-C1C | 2.51 | 1.41 | 1.35 |
| 24 | A | 1011 | CL0 | C4B-CHC | 2.51 | 1.48 | 1.41 |
| 37 | B | 5004 | PCW | O2-C2 | -2.51 | 1.40 | 1.46 |
| 34 | A | 5007 | 3PH | O21-C2 | -2.51 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 605 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |
| 25 | 6 | 618 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |
| 33 | J | 5001 | PTY | O7-C6 | -2.50 | 1.40 | 1.46 |
| 51 | 7 | 807 | 4RF | O21-C20 | -2.50 | 1.40 | 1.46 |
| 25 | 5 | 605 | CLA | C3B-C2B | -2.50 | 1.36 | 1.40 |
| 25 | a | 608 | CLA | C3B-C2B | -2.50 | 1.36 | 1.40 |
| 33 | G | 5002 | PTY | O7-C6 | -2.50 | 1.40 | 1.46 |
| 25 | 2 | 602 | CLA | C3B-C2B | -2.49 | 1.36 | 1.40 |
| 25 | a | 602 | CLA | C3B-C2B | -2.49 | 1.36 | 1.40 |
| 25 | 4 | 605 | CLA | CHC-C1C | 2.48 | 1.41 | 1.35 |
| 26 | 8 | 604 | CHL | CHC-C1C | 2.48 | 1.41 | 1.35 |
| 25 | J | 1901 | CLA | C3B-C2B | -2.47 | 1.36 | 1.40 |
| 25 | 8 | 609 | CLA | C3B-C2B | -2.47 | 1.36 | 1.40 |
| 25 | 1 | 608 | CLA | C3B-C2B | -2.47 | 1.36 | 1.40 |
| 26 | 7 | 613 | CHL | C3B-C2B | -2.47 | 1.36 | 1.40 |
| 26 | 3 | 604 | CHL | CHC-C1C | 2.47 | 1.41 | 1.35 |
| 25 | 6 | 607 | CLA | C3B-C2B | -2.46 | 1.37 | 1.40 |
| 35 | 1 | 804 | LMT | O2B-C2B | -2.45 | 1.37 | 1.43 |
| 26 | a | 604 | CHL | CHC-C1C | 2.44 | 1.41 | 1.35 |
| 44 | 1 | 502 | AXT | C27-C26 | 2.44 | 1.53 | 1.45 |
| 35 | 1 | 804 | LMT | O2'-C2' | -2.44 | 1.37 | 1.43 |
| 25 | K | 1401 | CLA | C3B-C2B | -2.44 | 1.37 | 1.40 |
| 26 | 1 | 609 | CHL | C3B-C2B | -2.43 | 1.37 | 1.40 |
| 40 | 3 | 506 | RRX | C35-C13 | 2.43 | 1.55 | 1.50 |
| 33 | 9 | 803 | PTY | O7-C6 | -2.42 | 1.40 | 1.46 |
| 25 | A | 1128 | CLA | CHC-C1C | 2.42 | 1.41 | 1.35 |
| 25 | B | 1226 | CLA | CHC-C1C | 2.42 | 1.41 | 1.35 |
| 33 | 3 | 802 | PTY | O4-C30 | 2.42 | 1.40 | 1.33 |
| 33 | 9 | 803 | PTY | O4-C30 | 2.42 | 1.40 | 1.33 |
| 25 | 4 | 617 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 25 | L | 1504 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 25 | B | 1224 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 35 | 2 | 804 | LMT | O2B-C2B | -2.41 | 1.37 | 1.43 |
| 50 | 7 | 502 | XAT | O24-C25 | -2.40 | 1.42 | 1.46 |
| 33 | a | 802 | PTY | O4-C30 | 2.40 | 1.40 | 1.33 |
| 33 | J | 5001 | PTY | O4-C30 | 2.40 | 1.40 | 1.33 |
| 37 | K | 5001 | PCW | O2-C31 | 2.40 | 1.41 | 1.34 |
| 33 | A | 5006 | PTY | O4-C30 | 2.39 | 1.40 | 1.33 |
| 25 | A | 1131 | CLA | C3B-C2B | -2.39 | 1.37 | 1.40 |
| 25 | A | 1132 | CLA | C3B-C2B | -2.39 | 1.37 | 1.40 |
| 35 | 2 | 804 | LMT | O2'-C2' | -2.39 | 1.37 | 1.43 |
| 25 | B | 1023 | CLA | C3B-C2B | -2.39 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 26 | 9 | 610 | CHL | C3B-C2B | -2.38 | 1.37 | 1.40 |
| 25 | 4 | 612 | CLA | C3B-C2B | -2.38 | 1.37 | 1.40 |
| 33 | 7 | 804 | PTY | O4-C30 | 2.38 | 1.40 | 1.33 |
| 51 | 7 | 807 | 4RF | O40-C41 | 2.38 | 1.40 | 1.33 |
| 25 | 1 | 612 | CLA | C3B-C2B | -2.38 | 1.37 | 1.40 |
| 50 | 9 | 507 | XAT | O24-C25 | -2.38 | 1.42 | 1.46 |
| 35 | 2 | 804 | LMT | O3B-C3B | -2.37 | 1.37 | 1.43 |
| 25 | 2 | 608 | CLA | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 40 | J | 4002 | RRX | C35-C13 | 2.37 | 1.55 | 1.50 |
| 25 | 5 | 615 | CLA | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 26 | 4 | 618 | CHL | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 25 | 2 | 621 | CLA | C3B-C2B | -2.37 | 1.37 | 1.40 |
| 33 | a | 803 | PTY | O4-C30 | 2.36 | 1.40 | 1.33 |
| 33 | 5 | 802 | PTY | O4-C30 | 2.36 | 1.40 | 1.33 |
| 37 | B | 5004 | PCW | O2-C31 | 2.36 | 1.41 | 1.34 |
| 25 | B | 1226 | CLA | C3B-C2B | -2.36 | 1.37 | 1.40 |
| 25 | 2 | 615 | CLA | C3B-C2B | -2.35 | 1.37 | 1.40 |
| 25 | B | 1206 | CLA | CHC-C1C | 2.35 | 1.41 | 1.35 |
| 25 | 9 | 612 | CLA | C3B-C2B | -2.35 | 1.37 | 1.40 |
| 35 | A | 5008 | LMT | O2B-C2B | -2.35 | 1.37 | 1.43 |
| 26 | 1 | 604 | CHL | CHC-C1C | 2.35 | 1.41 | 1.35 |
| 33 | B | 5005 | PTY | O4-C30 | 2.34 | 1.40 | 1.33 |
| 25 | a | 612 | CLA | C3B-C2B | -2.34 | 1.37 | 1.40 |
| 38 | F | 5003 | LPX | P1-O2 | 2.34 | 1.68 | 1.59 |
| 51 | 7 | 807 | 4RF | O18-C16 | 2.34 | 1.40 | 1.33 |
| 37 | K | 5002 | PCW | O2-C31 | 2.33 | 1.40 | 1.34 |
| 25 | 5 | 607 | CLA | C3B-C2B | -2.33 | 1.37 | 1.40 |
| 35 | A | 5008 | LMT | O3B-C3B | -2.33 | 1.37 | 1.43 |
| 26 | 3 | 603 | CHL | CHC-C1C | 2.32 | 1.40 | 1.35 |
| 26 | 4 | 613 | CHL | C3B-C2B | -2.32 | 1.37 | 1.40 |
| 33 | 7 | 804 | PTY | O7-C8 | 2.31 | 1.40 | 1.34 |
| 25 | A | 1125 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 35 | 1 | 804 | LMT | O3B-C3B | -2.31 | 1.37 | 1.43 |
| 25 | 4 | 615 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 26 | 8 | 610 | CHL | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 25 | 4 | 607 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 37 | 6 | 803 | PCW | O2-C31 | 2.30 | 1.40 | 1.34 |
| 26 | a | 613 | CHL | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 35 | B | 5006 | LMT | O2B-C2B | -2.30 | 1.37 | 1.43 |
| 34 | A | 5007 | 3PH | O31-C31 | 2.30 | 1.40 | 1.33 |
| 33 | 3 | 802 | PTY | O7-C6 | -2.30 | 1.40 | 1.46 |
| 25 | 5 | 603 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1220 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 46 | a | 504 | QTB | C14-C12 | -2.28 | 1.48 | 1.53 |
| 25 | 6 | 604 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 25 | L | 1501 | CLA | C3B-C2B | -2.28 | 1.37 | 1.40 |
| 25 | 8 | 618 | CLA | C3B-C2B | -2.28 | 1.37 | 1.40 |
| 33 | 5 | 802 | PTY | O7-C8 | 2.28 | 1.40 | 1.34 |
| 25 | A | 1129 | CLA | C3B-C2B | -2.28 | 1.37 | 1.40 |
| 35 | B | 5006 | LMT | O3B-C3B | -2.27 | 1.37 | 1.43 |
| 25 | 6 | 612 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 25 | H | 1701 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 25 | 3 | 616 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 25 | 8 | 612 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 25 | 7 | 610 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 25 | A | 1109 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 33 | 3 | 802 | PTY | O7-C8 | 2.26 | 1.40 | 1.34 |
| 35 | A | 5008 | LMT | O2'-C2' | -2.26 | 1.37 | 1.43 |
| 35 | B | 5006 | LMT | O2'-C2' | -2.26 | 1.37 | 1.43 |
| 26 | 1 | 611 | CHL | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 25 | A | 1128 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 25 | B | 1234 | CLA | C3D-C4D | -2.24 | 1.39 | 1.43 |
| 26 | 9 | 613 | CHL | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 25 | 2 | 603 | CLA | C1A-CHA | 2.24 | 1.52 | 1.43 |
| 25 | 2 | 607 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 44 | 7 | 504 | AXT | C1-C6 | 2.24 | 1.56 | 1.53 |
| 25 | H | 1702 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 25 | K | 1402 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 52 | 8 | 805 | P5S | O37-C2 | -2.24 | 1.41 | 1.46 |
| 25 | 6 | 608 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 25 | 2 | 615 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 25 | 8 | 609 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 25 | B | 1204 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 25 | A | 1013 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 25 | 6 | 601 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 25 | 5 | 614 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 44 | 7 | 504 | AXT | C37-C21 | 2.23 | 1.58 | 1.53 |
| 25 | K | 1404 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 44 | 1 | 502 | AXT | C37-C21 | 2.22 | 1.58 | 1.53 |
| 26 | 8 | 603 | CHL | CHC-C1C | 2.22 | 1.40 | 1.35 |
| 51 | 7 | 807 | 4RF | O18-C19 | -2.22 | 1.40 | 1.45 |
| 25 | B | 1240 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 25 | 7 | 612 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 25 | A | 1119 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 9 | 607 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 25 | A | 1116 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 25 | B | 1235 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 25 | 9 | 605 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 33 | 7 | 804 | PTY | O7-C6 | -2.20 | 1.41 | 1.46 |
| 51 | 7 | 807 | 4RF | O40-C39 | -2.20 | 1.40 | 1.45 |
| 25 | 4 | 606 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 25 | B | 1227 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 25 | G | 1602 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 33 | 5 | 802 | PTY | O7-C6 | -2.19 | 1.41 | 1.46 |
| 25 | 2 | 607 | CLA | C1A-CHA | 2.19 | 1.52 | 1.43 |
| 25 | 5 | 612 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 25 | 5 | 605 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 25 | 5 | 601 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 25 | B | 1229 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 25 | a | 615 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 25 | B | 1208 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 25 | A | 1140 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 25 | O | 1803 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 33 | a | 803 | PTY | O7-C8 | 2.18 | 1.40 | 1.34 |
| 25 | A | 1124 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 25 | A | 1012 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 25 | 6 | 607 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 33 | a | 802 | PTY | O7-C8 | 2.18 | 1.40 | 1.34 |
| 25 | A | 1138 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 25 | A | 1121 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 25 | 9 | 605 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 25 | 6 | 603 | CLA | C1B-NB | 2.17 | 1.37 | 1.35 |
| 25 | B | 1022 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 25 | A | 1141 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 25 | 4 | 612 | CLA | C1A-CHA | 2.17 | 1.52 | 1.43 |
| 25 | A | 1134 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 25 | 2 | 602 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 25 | 5 | 614 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 25 | A | 1120 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 25 | A | 1139 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 42 | M | 4001 | ECH | C1-C6 | -2.17 | 1.50 | 1.53 |
| 25 | 8 | 611 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 25 | 3 | 613 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 25 | O | 1803 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 25 | B | 1217 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 25 | B | 1231 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1212 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 25 | 4 | 603 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 25 | A | 1109 | CLA | C1A-CHA | 2.16 | 1.52 | 1.43 |
| 25 | A | 1141 | CLA | C1A-CHA | 2.16 | 1.52 | 1.43 |
| 33 | A | 5006 | PTY | O7-C8 | 2.16 | 1.40 | 1.34 |
| 25 | A | 1134 | CLA | C1A-CHA | 2.16 | 1.52 | 1.43 |
| 25 | O | 1803 | CLA | C1B-NB | 2.16 | 1.37 | 1.35 |
| 25 | 2 | 604 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 25 | 4 | 615 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 25 | 8 | 620 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 26 | 4 | 609 | CHL | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 25 | 5 | 608 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 25 | K | 1404 | CLA | C1A-CHA | 2.16 | 1.52 | 1.43 |
| 25 | 6 | 615 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 26 | 9 | 608 | CHL | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 35 | 1 | 804 | LMT | O4'-C4B | -2.16 | 1.37 | 1.43 |
| 35 | B | 5006 | LMT | O4'-C4B | -2.16 | 1.37 | 1.43 |
| 25 | A | 1130 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 51 | 7 | 807 | 4RF | O21-C22 | 2.15 | 1.40 | 1.34 |
| 25 | B | 1204 | CLA | C1B-NB | 2.15 | 1.37 | 1.35 |
| 25 | B | 1205 | CLA | C1B-NB | 2.15 | 1.37 | 1.35 |
| 25 | 2 | 601 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | 8 | 607 | CLA | C1A-CHA | 2.15 | 1.52 | 1.43 |
| 25 | B | 1201 | CLA | C1A-CHA | 2.15 | 1.52 | 1.43 |
| 25 | a | 607 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | a | 615 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | 3 | 601 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | 4 | 608 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | L | 1504 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 34 | A | 5007 | 3PH | O21-C21 | 2.15 | 1.40 | 1.34 |
| 25 | 7 | 604 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 25 | 7 | 607 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | B | 1206 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 25 | H | 1703 | CLA | C1B-NB | 2.15 | 1.37 | 1.35 |
| 25 | O | 1801 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 25 | 2 | 605 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 35 | 2 | 804 | LMT | O4'-C4B | -2.15 | 1.37 | 1.43 |
| 33 | 9 | 803 | PTY | O7-C8 | 2.15 | 1.40 | 1.34 |
| 25 | 5 | 615 | CLA | C1A-CHA | 2.14 | 1.52 | 1.43 |
| 25 | A | 1117 | CLA | C1A-CHA | 2.14 | 1.52 | 1.43 |
| 25 | B | 1211 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | B | 1235 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1236 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | 2 | 605 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | 4 | 610 | CLA | C1A-CHA | 2.14 | 1.52 | 1.43 |
| 25 | B | 1213 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | B | 1226 | CLA | C3D-C4D | -2.14 | 1.39 | 1.44 |
| 25 | B | 1202 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | a | 612 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | a | 607 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 25 | 4 | 617 | CLA | C1A-CHA | 2.14 | 1.52 | 1.43 |
| 34 | A | 5007 | 3PH | O31-C3 | -2.13 | 1.40 | 1.45 |
| 25 | L | 1502 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 37 | K | 5001 | PCW | P-O4P | 2.13 | 1.67 | 1.59 |
| 25 | 7 | 605 | CLA | C3D-C4D | -2.13 | 1.39 | 1.44 |
| 25 | A | 1123 | CLA | C1A-CHA | 2.13 | 1.52 | 1.43 |
| 25 | H | 1702 | CLA | C1A-CHA | 2.13 | 1.52 | 1.43 |
| 48 | 2 | 803 | DGA | OG2-CG2 | -2.13 | 1.41 | 1.46 |
| 25 | 1 | 605 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 25 | A | 1112 | CLA | C1A-CHA | 2.13 | 1.51 | 1.43 |
| 25 | A | 1101 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 5 | 608 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 44 | 7 | 504 | AXT | C17-C1 | 2.13 | 1.58 | 1.53 |
| 25 | B | 1201 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 5 | 606 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | A | 1124 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 33 | 9 | 803 | PTY | O4-C1 | -2.13 | 1.40 | 1.45 |
| 25 | H | 1701 | CLA | C1A-CHA | 2.13 | 1.51 | 1.43 |
| 25 | A | 1126 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 4 | 607 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 5 | 607 | CLA | C1A-CHA | 2.13 | 1.51 | 1.43 |
| 25 | B | 1221 | CLA | C1A-CHA | 2.13 | 1.51 | 1.43 |
| 25 | G | 1602 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 25 | A | 1102 | CLA | C1A-CHA | 2.13 | 1.51 | 1.43 |
| 25 | 3 | 607 | CLA | C1A-CHA | 2.13 | 1.51 | 1.43 |
| 25 | A | 1115 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 5 | 601 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 6 | 605 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 25 | 4 | 604 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 25 | B | 1223 | CLA | C3D-C4D | -2.12 | 1.39 | 1.44 |
| 25 | 9 | 607 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 25 | 5 | 607 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 25 | 7 | 601 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 37 | K | 5002 | PCW | P-O4P | 2.12 | 1.67 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1123 | CLA | MG-NC | 2.12 | 2.11 | 2.06 |
| 25 | 8 | 618 | CLA | C3D-C4D | -2.12 | 1.39 | 1.44 |
| 33 | G | 5002 | PTY | O7-C8 | 2.12 | 1.40 | 1.34 |
| 25 | a | 608 | CLA | C1A-CHA | 2.12 | 1.51 | 1.43 |
| 35 | A | 5008 | LMT | O1'-C1' | -2.12 | 1.36 | 1.40 |
| 25 | 6 | 615 | CLA | C1A-CHA | 2.12 | 1.51 | 1.43 |
| 25 | 7 | 607 | CLA | C1A-CHA | 2.12 | 1.51 | 1.43 |
| 25 | 2 | 612 | CLA | C1B-NB | 2.12 | 1.37 | 1.35 |
| 25 | 6 | 612 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 25 | 6 | 601 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 25 | 9 | 606 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 25 | a | 601 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 33 | J | 5001 | PTY | O7-C8 | 2.12 | 1.40 | 1.34 |
| 25 | 1 | 601 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 25 | B | 1216 | CLA | C3D-C4D | -2.12 | 1.39 | 1.44 |
| 25 | A | 1141 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 25 | 9 | 607 | CLA | C1A-CHA | 2.12 | 1.51 | 1.43 |
| 25 | 8 | 615 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | 2 | 603 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 25 | L | 1501 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | 9 | 612 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | L | 1503 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | K | 1403 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | a | 605 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 25 | 6 | 603 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 25 | B | 1235 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | 1 | 615 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | A | 1135 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | A | 1113 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 25 | 8 | 620 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 25 | B | 1209 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | 1 | 608 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | B | 1224 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | B | 1208 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 25 | a | 612 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | K | 1404 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | A | 1108 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | B | 1209 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 25 | a | 615 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | B | 1240 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 25 | 7 | 610 | CLA | C1A-CHA | 2.11 | 1.51 | 1.43 |
| 25 | B | 1223 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 605 | CLA | C3D-C4D | -2.10 | 1.39 | 1.44 |
| 25 | B | 1238 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | O | 1802 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 37 | 6 | 803 | PCW | P-O4P | 2.10 | 1.67 | 1.59 |
| 25 | A | 1137 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 35 | A | 5008 | LMT | O4'-C4B | -2.10 | 1.38 | 1.43 |
| 25 | G | 1601 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 33 | B | 5005 | PTY | O4-C1 | -2.10 | 1.40 | 1.45 |
| 25 | a | 603 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 25 | A | 1106 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | A | 1123 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 25 | 8 | 605 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | B | 1216 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 25 | 4 | 615 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 25 | F | 1302 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | B | 1223 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 25 | B | 1239 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | 5 | 605 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | A | 1122 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 33 | 5 | 802 | PTY | O4-C1 | -2.10 | 1.40 | 1.45 |
| 25 | 4 | 601 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 25 | 4 | 616 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 25 | K | 1402 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 37 | B | 5004 | PCW | P-O4P | 2.10 | 1.67 | 1.59 |
| 25 | 3 | 606 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 25 | 6 | 607 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 26 | 6 | 617 | CHL | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 25 | 4 | 608 | CLA | C1B-NB | 2.10 | 1.37 | 1.35 |
| 25 | A | 1110 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | B | 1226 | CLA | CHD-C1D | 2.09 | 1.42 | 1.38 |
| 25 | B | 1224 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | 5 | 609 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | 1 | 612 | CLA | C1B-NB | 2.09 | 1.37 | 1.35 |
| 25 | 3 | 602 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 26 | a | 610 | CHL | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 25 | 2 | 606 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | A | 1140 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | B | 1206 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | 4 | 608 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | 1 | 612 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | 9 | 605 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | 3 | 618 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 9 | 602 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | A | 1133 | CLA | C1B-NB | 2.09 | 1.37 | 1.35 |
| 35 | B | 5006 | LMT | O1'-C1' | -2.09 | 1.36 | 1.40 |
| 25 | a | 602 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | 5 | 604 | CLA | C3D-C4D | -2.09 | 1.39 | 1.44 |
| 25 | G | 1601 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 26 | 2 | 610 | CHL | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 25 | 1 | 606 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | O | 1802 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | 9 | 609 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | 8 | 611 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | F | 1302 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | L | 1504 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | 3 | 607 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 25 | a | 608 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 33 | J | 5001 | PTY | O4-C1 | -2.09 | 1.40 | 1.45 |
| 25 | 7 | 608 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | B | 1219 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 26 | 7 | 611 | CHL | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 48 | 8 | 804 | DGA | OG2-CG2 | -2.09 | 1.41 | 1.46 |
| 25 | 5 | 604 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 25 | B | 1219 | CLA | C1A-CHA | 2.09 | 1.51 | 1.43 |
| 25 | a | 608 | CLA | C1B-NB | 2.09 | 1.37 | 1.35 |
| 25 | 8 | 615 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | 7 | 607 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 25 | O | 1803 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | 7 | 604 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 25 | a | 603 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 33 | 7 | 804 | PTY | O4-C1 | -2.08 | 1.40 | 1.45 |
| 25 | 3 | 618 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | A | 1104 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 25 | B | 1218 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 25 | B | 1222 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 25 | 1 | 603 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 25 | L | 1502 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 33 | a | 802 | PTY | O4-C1 | -2.08 | 1.40 | 1.45 |
| 25 | 4 | 611 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | A | 1113 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | B | 1220 | CLA | C1B-NB | 2.08 | 1.37 | 1.35 |
| 25 | B | 1214 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 24 | A | 1011 | CL0 | C1D-C2D | 2.08 | 1.49 | 1.45 |
| 25 | 8 | 605 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1217 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 25 | K | 1401 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | B | 1214 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | 5 | 614 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | 5 | 608 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | 6 | 605 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 25 | 2 | 608 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 25 | 7 | 601 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 25 | a | 607 | CLA | C1B-NB | 2.08 | 1.37 | 1.35 |
| 25 | B | 1240 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | 3 | 616 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | a | 607 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 25 | H | 1703 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 25 | 4 | 610 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 25 | A | 1119 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 25 | B | 1218 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 25 | F | 1301 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 2 | 615 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | B | 1023 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 2 | 621 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 8 | 620 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | B | 1222 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | B | 1232 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | H | 1702 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | B | 1217 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 6 | 612 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 4 | 606 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 25 | A | 1122 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | B | 1203 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 26 | 7 | 613 | CHL | CHC-C1C | 2.07 | 1.40 | 1.35 |
| 25 | 7 | 606 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | A | 1126 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 25 | 1 | 601 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 25 | A | 1118 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | 7 | 605 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | 9 | 604 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 48 | 3 | 803 | DGA | OG2-CG2 | -2.07 | 1.41 | 1.46 |
| 25 | 1 | 607 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 33 | G | 5003 | PTY | O7-C8 | 2.07 | 1.40 | 1.34 |
| 25 | 7 | 601 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 25 | B | 1022 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | 4 | 604 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 602 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 3 | 610 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 2 | 608 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | B | 1210 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 6 | 606 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 25 | 6 | 618 | CLA | C1B-NB | 2.07 | 1.37 | 1.35 |
| 25 | K | 1403 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | 7 | 610 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 25 | B | 1231 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 50 | 9 | 504 | XAT | O24-C25 | -2.07 | 1.43 | 1.46 |
| 46 | a | 504 | QTB | C03-C02 | -2.07 | 1.33 | 1.35 |
| 25 | A | 1103 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 25 | B | 1207 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | 4 | 603 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | B | 1220 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 25 | B | 1228 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | 1 | 603 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | 5 | 603 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | A | 1109 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | 3 | 605 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | A | 1107 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | 4 | 605 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | 6 | 608 | CLA | C1B-NB | 2.06 | 1.37 | 1.35 |
| 25 | A | 1012 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | 1 | 615 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 25 | A | 1121 | CLA | C1B-NB | 2.06 | 1.37 | 1.35 |
| 25 | B | 1204 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | a | 612 | CLA | C1B-NB | 2.06 | 1.37 | 1.35 |
| 25 | a | 601 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 25 | A | 1139 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | 5 | 601 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 33 | a | 803 | PTY | O4-C1 | -2.06 | 1.40 | 1.45 |
| 25 | B | 1021 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 25 | 6 | 615 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 36 | 7 | 806 | DGD | O3G-C1D | 2.06 | 1.43 | 1.40 |
| 25 | B | 1211 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 25 | J | 1901 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | a | 605 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 25 | 1 | 605 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | 7 | 612 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 25 | 4 | 607 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 26 | 2 | 609 | CHL | CHC-C1C | 2.05 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 613 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | A | 1133 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | 5 | 602 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 2 | 601 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | O | 1801 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | K | 1402 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | 7 | 603 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | A | 1105 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 6 | 608 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | A | 1101 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | 2 | 603 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 1 | 607 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | B | 1228 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | 3 | 605 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | A | 1108 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | B | 1202 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | 4 | 604 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 9 | 612 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 48 | 5 | 803 | DGA | OG2-CG2 | -2.05 | 1.41 | 1.46 |
| 25 | A | 1118 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | B | 1239 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | A | 1121 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 25 | A | 1125 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | a | 602 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | 8 | 608 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | B | 1227 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | 2 | 607 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 2 | 604 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | A | 1013 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 7 | 606 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | a | 611 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 25 | 4 | 616 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | A | 1136 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | 1 | 608 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | a | 601 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 26 | 3 | 608 | CHL | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 25 | A | 1115 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 44 | 7 | 504 | AXT | C22-C23 | 2.05 | 1.56 | 1.52 |
| 25 | 4 | 606 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | A | 1111 | CLA | C1A-CHA | 2.05 | 1.51 | 1.43 |
| 25 | 2 | 621 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 25 | 9 | 604 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 612 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 25 | G | 1602 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 3 | 601 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | 6 | 618 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | B | 1221 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 25 | B | 1221 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 26 | 7 | 615 | CHL | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 25 | B | 1203 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | O | 1801 | CLA | C1B-NB | 2.04 | 1.37 | 1.35 |
| 25 | B | 1232 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | A | 1124 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 35 | 1 | 804 | LMT | O1'-C1' | -2.04 | 1.36 | 1.40 |
| 25 | A | 1126 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | A | 1122 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 25 | B | 1212 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 3 | 602 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 25 | B | 1231 | CLA | C1B-NB | 2.04 | 1.37 | 1.35 |
| 25 | 5 | 603 | CLA | C1B-NB | 2.04 | 1.37 | 1.35 |
| 25 | 1 | 606 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | 2 | 621 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 25 | A | 1107 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | a | 611 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 7 | 605 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 5 | 603 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | A | 1120 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | A | 1132 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 25 | 8 | 605 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 3 | 610 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 25 | 6 | 605 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 6 | 606 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | 5 | 612 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 9 | 609 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 5 | 615 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | B | 1213 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | A | 1132 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 7 | 603 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | 6 | 604 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 25 | L | 1503 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 25 | 2 | 612 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 25 | A | 1103 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 26 | 7 | 617 | CHL | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 25 | A | 1125 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1220 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 25 | B | 1225 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | A | 1125 | CLA | C1B-NB | 2.03 | 1.37 | 1.35 |
| 25 | H | 1702 | CLA | C1B-NB | 2.03 | 1.37 | 1.35 |
| 26 | 5 | 611 | CHL | CHC-C1C | 2.03 | 1.40 | 1.35 |
| 25 | 1 | 605 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | B | 1237 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | B | 1205 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | B | 1227 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | A | 1138 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | G | 1603 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | 1 | 607 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | 6 | 608 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | 6 | 602 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | G | 1603 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 25 | B | 1236 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | 3 | 606 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | 4 | 602 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 25 | 4 | 617 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | A | 1104 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | K | 1402 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | 5 | 606 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 33 | A | 5006 | PTY | O4-C1 | -2.03 | 1.40 | 1.45 |
| 25 | 1 | 601 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | 6 | 608 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | A | 1110 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 25 | 9 | 607 | CLA | C1B-NB | 2.03 | 1.37 | 1.35 |
| 25 | 8 | 607 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | B | 1204 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | A | 1134 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | B | 1227 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | 8 | 618 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | B | 1208 | CLA | C1B-NB | 2.03 | 1.37 | 1.35 |
| 25 | A | 1129 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 25 | 9 | 602 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 25 | K | 1404 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | A | 1110 | CLA | C1B-NB | 2.03 | 1.37 | 1.35 |
| 25 | 7 | 602 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 25 | L | 1501 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | 1 | 606 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 6 | 603 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | A | 1129 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 606 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | A | 1129 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | A | 1128 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | 5 | 609 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | O | 1802 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 25 | A | 1116 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | A | 1135 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 8 | 620 | CLA | C1B-NB | 2.02 | 1.37 | 1.35 |
| 25 | 8 | 620 | CLA | MG-NC | 2.02 | 2.11 | 2.06 |
| 25 | A | 1123 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | B | 1205 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | B | 1221 | CLA | MG-NC | 2.02 | 2.11 | 2.06 |
| 25 | 4 | 602 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | B | 1229 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | A | 1111 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 25 | A | 1131 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 3 | 612 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | A | 1138 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | L | 1502 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | A | 1107 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | B | 1215 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 5 | 602 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | B | 1219 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | 1 | 605 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 5 | 606 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 7 | 612 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | B | 1202 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | 6 | 606 | CLA | C1B-NB | 2.02 | 1.37 | 1.35 |
| 25 | 4 | 604 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | 1 | 602 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | 7 | 603 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 2 | 612 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | A | 1118 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | A | 1136 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | 8 | 602 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | 2 | 601 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | B | 1217 | CLA | MG-NC | 2.02 | 2.11 | 2.06 |
| 25 | B | 1021 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | a | 605 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | A | 1110 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 25 | 7 | 604 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 25 | 5 | 605 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1236 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | 3 | 613 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 25 | 5 | 603 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 5 | 604 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 25 | B | 1230 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 33 | B | 5005 | PTY | O7-C8 | 2.01 | 1.40 | 1.34 |
| 25 | 4 | 608 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | a | 611 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 25 | 7 | 608 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 25 | 4 | 603 | CLA | C1B-NB | 2.01 | 1.37 | 1.35 |
| 25 | 7 | 610 | CLA | C1B-NB | 2.01 | 1.37 | 1.35 |
| 25 | B | 1205 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 25 | A | 1128 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | 3 | 610 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | 5 | 612 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 33 | 3 | 802 | PTY | O4-C1 | -2.01 | 1.40 | 1.45 |
| 25 | A | 1137 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | 6 | 602 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 36 | 8 | 802 | DGD | CDB-CCB | -2.01 | 1.33 | 1.49 |
| 25 | B | 1237 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 44 | 1 | 502 | AXT | C17-C1 | 2.01 | 1.57 | 1.53 |
| 25 | A | 1123 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | B | 1237 | CLA | C1B-NB | 2.01 | 1.37 | 1.35 |
| 25 | K | 1404 | CLA | C1B-NB | 2.01 | 1.37 | 1.35 |
| 25 | a | 611 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | A | 1117 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 35 | 2 | 804 | LMT | O1'-C1' | -2.01 | 1.36 | 1.40 |
| 25 | 1 | 602 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 25 | 2 | 606 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | B | 1221 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 25 | B | 1210 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 25 | A | 1131 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | B | 1211 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 1 | 608 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 6 | 603 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 26 | 5 | 617 | CHL | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 25 | A | 1133 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 25 | A | 1106 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 8 | 606 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 2 | 602 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 6 | 603 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 8 | 602 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 602 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 25 | 4 | 601 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 25 | B | 1238 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | A | 1105 | CLA | C1B-NB | 2.00 | 1.37 | 1.35 |
| 25 | 6 | 601 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | A | 1105 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | A | 1141 | CLA | MG-NC | 2.00 | 2.11 | 2.06 |
| 25 | 6 | 605 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 25 | A | 1119 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 25 | a | 601 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | 3 | 607 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | 5 | 612 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | J | 1901 | CLA | C1B-NB | 2.00 | 1.37 | 1.35 |
| 25 | B | 1022 | CLA | MG-NC | 2.00 | 2.11 | 2.06 |
| 25 | 9 | 612 | CLA | MG-NC | 2.00 | 2.11 | 2.06 |
| 25 | A | 1139 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | B | 1210 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | A | 1135 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | A | 1116 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | L | 1503 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 25 | A | 1131 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 25 | A | 1138 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | 8 | 609 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | 2 | 605 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | B | 1238 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 25 | 6 | 602 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |

All (4958) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 9 | 504 | XAT | C20-C13-C14 | -30.45 | 80.27 | 122.92 |
| 29 | H | 4001 | BCR | C37-C22-C21 | -30.28 | 80.51 | 122.92 |
| 29 | H | 4001 | BCR | C23-C22-C21 | 27.27 | 160.78 | 118.94 |
| 50 | 9 | 504 | XAT | C12-C13-C14 | 26.86 | 160.15 | 118.94 |
| 39 | F | 4001 | NEX | C17-C1-C6 | -26.13 | 87.08 | 110.47 |
| 50 | 9 | 504 | XAT | C20-C13-C12 | -24.21 | 79.93 | 118.08 |
| 29 | H | 4001 | BCR | C37-C22-C23 | -23.83 | 80.53 | 118.08 |
| 25 | B | 1201 | CLA | C4-C3-C5 | -22.47 | 77.46 | 115.27 |
| 25 | B | 1201 | CLA | C5-C3-C2 | 18.88 | 159.33 | 121.12 |
| 29 | 6 | 504 | BCR | C10-C11-C12 | 18.18 | 179.95 | 123.22 |
| 29 | H | 4001 | BCR | C10-C11-C12 | 17.71 | 178.50 | 123.22 |
| 29 | L | 4003 | BCR | C10-C11-C12 | 17.61 | 178.18 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | B | 4005 | BCR | C10-C11-C12 | 17.58 | 178.07 | 123.22 |
| 29 | O | 4001 | BCR | C10-C11-C12 | 17.56 | 178.00 | 123.22 |
| 29 | 4 | 503 | BCR | C10-C11-C12 | 17.54 | 177.96 | 123.22 |
| 29 | 5 | 503 | BCR | C10-C11-C12 | 17.54 | 177.96 | 123.22 |
| 29 | L | 4001 | BCR | C10-C11-C12 | 17.52 | 177.90 | 123.22 |
| 29 | O | 4001 | BCR | C16-C15-C14 | 17.48 | 159.29 | 123.47 |
| 29 | 3 | 504 | BCR | C10-C11-C12 | 17.48 | 177.77 | 123.22 |
| 29 | 3 | 503 | BCR | C10-C11-C12 | 17.47 | 177.73 | 123.22 |
| 29 | 5 | 504 | BCR | C10-C11-C12 | 17.45 | 177.67 | 123.22 |
| 29 | K | 4002 | BCR | C10-C11-C12 | 17.40 | 177.52 | 123.22 |
| 29 | K | 4001 | BCR | C10-C11-C12 | 17.38 | 177.46 | 123.22 |
| 29 | A | 4003 | BCR | C10-C11-C12 | 17.34 | 177.34 | 123.22 |
| 29 | B | 4007 | BCR | C10-C11-C12 | 17.33 | 177.31 | 123.22 |
| 29 | 6 | 503 | BCR | C10-C11-C12 | 17.30 | 177.20 | 123.22 |
| 29 | B | 4002 | BCR | C10-C11-C12 | 17.28 | 177.14 | 123.22 |
| 29 | 7 | 503 | BCR | C10-C11-C12 | 17.26 | 177.09 | 123.22 |
| 29 | 3 | 505 | BCR | C10-C11-C12 | 17.25 | 177.04 | 123.22 |
| 29 | G | 4001 | BCR | C10-C11-C12 | 17.22 | 176.94 | 123.22 |
| 29 | 8 | 503 | BCR | C10-C11-C12 | 17.08 | 176.53 | 123.22 |
| 29 | B | 4004 | BCR | C10-C11-C12 | 17.03 | 176.37 | 123.22 |
| 29 | J | 4001 | BCR | C10-C11-C12 | 16.96 | 176.15 | 123.22 |
| 29 | I | 4001 | BCR | C10-C11-C12 | 16.94 | 176.09 | 123.22 |
| 29 | A | 4004 | BCR | C10-C11-C12 | 16.94 | 176.07 | 123.22 |
| 29 | B | 4006 | BCR | C10-C11-C12 | 16.87 | 175.87 | 123.22 |
| 29 | 5 | 504 | BCR | C16-C15-C14 | 16.82 | 157.93 | 123.47 |
| 29 | A | 4001 | BCR | C10-C11-C12 | 16.60 | 175.03 | 123.22 |
| 29 | L | 4002 | BCR | C10-C11-C12 | 16.58 | 174.95 | 123.22 |
| 29 | B | 4001 | BCR | C10-C11-C12 | 16.51 | 174.74 | 123.22 |
| 29 | B | 4003 | BCR | C10-C11-C12 | 16.38 | 174.33 | 123.22 |
| 25 | B | 1201 | CLA | C4-C3-C2 | -16.30 | 81.87 | 123.68 |
| 29 | A | 4005 | BCR | C10-C11-C12 | 16.25 | 173.93 | 123.22 |
| 29 | A | 4002 | BCR | C10-C11-C12 | 16.11 | 173.48 | 123.22 |
| 29 | G | 4001 | BCR | C16-C15-C14 | 14.63 | 153.45 | 123.47 |
| 29 | B | 4003 | BCR | C11-C10-C9 | 14.30 | 147.72 | 127.31 |
| 29 | 4 | 503 | BCR | C16-C15-C14 | 14.24 | 152.64 | 123.47 |
| 29 | 5 | 503 | BCR | C16-C15-C14 | 13.90 | 151.95 | 123.47 |
| 29 | A | 4005 | BCR | C11-C10-C9 | 13.72 | 146.90 | 127.31 |
| 29 | B | 4002 | BCR | C11-C10-C9 | 13.61 | 146.74 | 127.31 |
| 29 | L | 4002 | BCR | C11-C10-C9 | 13.61 | 146.73 | 127.31 |
| 29 | B | 4007 | BCR | C16-C15-C14 | 13.47 | 151.06 | 123.47 |
| 29 | I | 4001 | BCR | C11-C10-C9 | 13.47 | 146.53 | 127.31 |
| 29 | A | 4003 | BCR | C21-C20-C19 | 13.46 | 165.23 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | L | 4001 | BCR | C16-C15-C14 | 13.27 | 150.65 | 123.47 |
| 29 | 3 | 503 | BCR | C16-C15-C14 | 13.26 | 150.64 | 123.47 |
| 29 | L | 4003 | BCR | C11-C10-C9 | 13.26 | 146.23 | 127.31 |
| 29 | J | 4001 | BCR | C11-C10-C9 | 13.24 | 146.21 | 127.31 |
| 29 | 3 | 505 | BCR | C11-C10-C9 | 13.22 | 146.18 | 127.31 |
| 29 | 6 | 504 | BCR | C16-C15-C14 | 13.17 | 150.45 | 123.47 |
| 29 | A | 4002 | BCR | C16-C15-C14 | 13.15 | 150.42 | 123.47 |
| 29 | 8 | 503 | BCR | C11-C10-C9 | 13.15 | 146.08 | 127.31 |
| 29 | B | 4001 | BCR | C11-C10-C9 | 13.13 | 146.05 | 127.31 |
| 29 | A | 4001 | BCR | C11-C10-C9 | 13.11 | 146.02 | 127.31 |
| 29 | 3 | 504 | BCR | C11-C10-C9 | 13.10 | 146.01 | 127.31 |
| 29 | L | 4003 | BCR | C16-C15-C14 | 13.06 | 150.23 | 123.47 |
| 29 | K | 4001 | BCR | C11-C10-C9 | 13.05 | 145.94 | 127.31 |
| 29 | 4 | 503 | BCR | C11-C10-C9 | 13.03 | 145.90 | 127.31 |
| 29 | A | 4003 | BCR | C16-C15-C14 | 13.01 | 150.12 | 123.47 |
| 29 | B | 4006 | BCR | C16-C15-C14 | 12.98 | 150.07 | 123.47 |
| 29 | B | 4006 | BCR | C11-C10-C9 | 12.95 | 145.80 | 127.31 |
| 29 | A | 4003 | BCR | C11-C10-C9 | 12.95 | 145.79 | 127.31 |
| 29 | O | 4001 | BCR | C11-C10-C9 | 12.89 | 145.71 | 127.31 |
| 29 | B | 4005 | BCR | C16-C15-C14 | 12.89 | 149.88 | 123.47 |
| 29 | H | 4001 | BCR | C16-C15-C14 | 12.83 | 149.75 | 123.47 |
| 29 | B | 4005 | BCR | C11-C10-C9 | 12.79 | 145.56 | 127.31 |
| 29 | B | 4007 | BCR | C11-C10-C9 | 12.78 | 145.56 | 127.31 |
| 29 | K | 4002 | BCR | C21-C20-C19 | 12.76 | 163.05 | 123.22 |
| 29 | K | 4001 | BCR | C21-C20-C19 | 12.73 | 162.93 | 123.22 |
| 29 | 6 | 503 | BCR | C11-C10-C9 | 12.65 | 145.36 | 127.31 |
| 29 | A | 4004 | BCR | C11-C10-C9 | 12.64 | 145.36 | 127.31 |
| 29 | B | 4004 | BCR | C11-C10-C9 | 12.60 | 145.29 | 127.31 |
| 29 | 3 | 504 | BCR | C21-C20-C19 | 12.58 | 162.49 | 123.22 |
| 29 | G | 4001 | BCR | C21-C20-C19 | 12.58 | 162.46 | 123.22 |
| 29 | H | 4001 | BCR | C11-C10-C9 | 12.58 | 145.26 | 127.31 |
| 29 | 6 | 503 | BCR | C16-C15-C14 | 12.47 | 149.01 | 123.47 |
| 29 | B | 4002 | BCR | C16-C15-C14 | 12.42 | 148.91 | 123.47 |
| 29 | 7 | 503 | BCR | C11-C10-C9 | 12.41 | 145.03 | 127.31 |
| 29 | A | 4001 | BCR | C21-C20-C19 | 12.33 | 161.70 | 123.22 |
| 29 | L | 4001 | BCR | C11-C10-C9 | 12.33 | 144.91 | 127.31 |
| 29 | 3 | 505 | BCR | C21-C20-C19 | 12.29 | 161.57 | 123.22 |
| 29 | B | 4001 | BCR | C21-C20-C19 | 12.24 | 161.41 | 123.22 |
| 29 | B | 4001 | BCR | C11-C12-C13 | 12.16 | 160.56 | 126.42 |
| 29 | K | 4002 | BCR | C11-C10-C9 | 12.08 | 144.56 | 127.31 |
| 29 | K | 4001 | BCR | C16-C15-C14 | 12.08 | 148.23 | 123.47 |
| 29 | A | 4005 | BCR | C11-C12-C13 | 12.06 | 160.29 | 126.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | L | 4002 | BCR | C21-C20-C19 | 12.02 | 160.72 | 123.22 |
| 29 | 6 | 504 | BCR | C11-C10-C9 | 12.01 | 144.46 | 127.31 |
| 29 | 3 | 505 | BCR | C16-C15-C14 | 12.00 | 148.06 | 123.47 |
| 29 | L | 4002 | BCR | C11-C12-C13 | 12.00 | 160.13 | 126.42 |
| 29 | B | 4003 | BCR | C11-C12-C13 | 11.97 | 160.05 | 126.42 |
| 29 | B | 4006 | BCR | C21-C20-C19 | 11.97 | 160.57 | 123.22 |
| 29 | 6 | 504 | BCR | C21-C20-C19 | 11.94 | 160.47 | 123.22 |
| 29 | 7 | 503 | BCR | C16-C15-C14 | 11.92 | 147.89 | 123.47 |
| 29 | K | 4002 | BCR | C16-C15-C14 | 11.91 | 147.88 | 123.47 |
| 29 | 3 | 503 | BCR | C11-C10-C9 | 11.89 | 144.28 | 127.31 |
| 29 | 3 | 504 | BCR | C16-C15-C14 | 11.80 | 147.65 | 123.47 |
| 29 | O | 4001 | BCR | C21-C20-C19 | 11.80 | 160.05 | 123.22 |
| 29 | J | 4001 | BCR | C21-C20-C19 | 11.78 | 159.98 | 123.22 |
| 29 | 5 | 503 | BCR | C11-C10-C9 | 11.77 | 144.10 | 127.31 |
| 29 | B | 4004 | BCR | C16-C15-C14 | 11.76 | 147.56 | 123.47 |
| 29 | 5 | 504 | BCR | C11-C10-C9 | 11.75 | 144.08 | 127.31 |
| 29 | I | 4001 | BCR | C16-C15-C14 | 11.75 | 147.55 | 123.47 |
| 29 | 8 | 503 | BCR | C16-C15-C14 | 11.66 | 147.36 | 123.47 |
| 29 | L | 4001 | BCR | C21-C20-C19 | 11.66 | 159.60 | 123.22 |
| 29 | A | 4004 | BCR | C16-C15-C14 | 11.62 | 147.27 | 123.47 |
| 29 | A | 4004 | BCR | C11-C12-C13 | 11.52 | 158.78 | 126.42 |
| 29 | B | 4004 | BCR | C11-C12-C13 | 11.50 | 158.72 | 126.42 |
| 29 | L | 4002 | BCR | C16-C15-C14 | 11.48 | 147.00 | 123.47 |
| 29 | L | 4003 | BCR | C21-C20-C19 | 11.47 | 159.02 | 123.22 |
| 29 | J | 4001 | BCR | C16-C15-C14 | 11.46 | 146.95 | 123.47 |
| 29 | A | 4001 | BCR | C11-C12-C13 | 11.45 | 158.57 | 126.42 |
| 29 | H | 4001 | BCR | C21-C20-C19 | 11.44 | 158.93 | 123.22 |
| 29 | A | 4002 | BCR | C21-C20-C19 | 11.42 | 158.84 | 123.22 |
| 29 | A | 4004 | BCR | C21-C20-C19 | 11.41 | 158.81 | 123.22 |
| 29 | B | 4003 | BCR | C21-C20-C19 | 11.33 | 158.58 | 123.22 |
| 29 | G | 4001 | BCR | C11-C10-C9 | 11.23 | 143.34 | 127.31 |
| 29 | B | 4007 | BCR | C21-C20-C19 | 11.20 | 158.18 | 123.22 |
| 29 | B | 4005 | BCR | C21-C20-C19 | 11.14 | 157.97 | 123.22 |
| 29 | B | 4001 | BCR | C16-C15-C14 | 11.12 | 146.25 | 123.47 |
| 29 | B | 4002 | BCR | C21-C20-C19 | 11.10 | 157.85 | 123.22 |
| 29 | 6 | 503 | BCR | C21-C20-C19 | 11.08 | 157.79 | 123.22 |
| 39 | F | 4001 | NEX | C16-C1-C6 | 11.04 | 120.36 | 110.47 |
| 29 | 8 | 503 | BCR | C21-C20-C19 | 11.03 | 157.63 | 123.22 |
| 29 | 3 | 503 | BCR | C11-C12-C13 | 10.99 | 157.30 | 126.42 |
| 29 | K | 4002 | BCR | C11-C12-C13 | 10.98 | 157.26 | 126.42 |
| 29 | J | 4001 | BCR | C11-C12-C13 | 10.97 | 157.24 | 126.42 |
| 29 | B | 4003 | BCR | C16-C15-C14 | 10.96 | 145.92 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | B | 4004 | BCR | C21-C20-C19 | 10.90 | 157.24 | 123.22 |
| 29 | 5 | 504 | BCR | C11-C12-C13 | 10.82 | 156.82 | 126.42 |
| 29 | 4 | 503 | BCR | C21-C20-C19 | 10.81 | 156.96 | 123.22 |
| 29 | 8 | 503 | BCR | C11-C12-C13 | 10.80 | 156.75 | 126.42 |
| 29 | B | 4007 | BCR | C11-C12-C13 | 10.75 | 156.62 | 126.42 |
| 29 | K | 4001 | BCR | C11-C12-C13 | 10.71 | 156.50 | 126.42 |
| 29 | 7 | 503 | BCR | C11-C12-C13 | 10.71 | 156.49 | 126.42 |
| 29 | I | 4001 | BCR | C11-C12-C13 | 10.69 | 156.44 | 126.42 |
| 29 | A | 4005 | BCR | C16-C15-C14 | 10.63 | 145.24 | 123.47 |
| 29 | A | 4001 | BCR | C16-C15-C14 | 10.60 | 145.20 | 123.47 |
| 29 | 6 | 504 | BCR | C11-C12-C13 | 10.60 | 156.19 | 126.42 |
| 29 | 3 | 504 | BCR | C11-C12-C13 | 10.53 | 156.00 | 126.42 |
| 29 | 5 | 503 | BCR | C21-C20-C19 | 10.52 | 156.04 | 123.22 |
| 29 | H | 4001 | BCR | C11-C12-C13 | 10.51 | 155.93 | 126.42 |
| 29 | A | 4002 | BCR | C11-C10-C9 | 10.51 | 142.31 | 127.31 |
| 29 | 5 | 504 | BCR | C21-C20-C19 | 10.49 | 155.95 | 123.22 |
| 29 | 3 | 503 | BCR | C21-C20-C19 | 10.47 | 155.90 | 123.22 |
| 29 | B | 4002 | BCR | C11-C12-C13 | 10.36 | 155.53 | 126.42 |
| 29 | A | 4005 | BCR | C21-C20-C19 | 10.33 | 155.45 | 123.22 |
| 29 | L | 4001 | BCR | C11-C12-C13 | 10.27 | 155.26 | 126.42 |
| 29 | 3 | 505 | BCR | C11-C12-C13 | 10.22 | 155.14 | 126.42 |
| 29 | 6 | 503 | BCR | C11-C12-C13 | 10.22 | 155.13 | 126.42 |
| 29 | A | 4002 | BCR | C11-C12-C13 | 10.17 | 154.97 | 126.42 |
| 29 | 5 | 503 | BCR | C11-C12-C13 | 10.11 | 154.80 | 126.42 |
| 29 | I | 4001 | BCR | C21-C20-C19 | 10.10 | 154.74 | 123.22 |
| 29 | A | 4003 | BCR | C11-C12-C13 | 9.99 | 154.47 | 126.42 |
| 29 | O | 4001 | BCR | C11-C12-C13 | 9.88 | 154.18 | 126.42 |
| 29 | 4 | 503 | BCR | C11-C12-C13 | 9.85 | 154.09 | 126.42 |
| 29 | B | 4005 | BCR | C11-C12-C13 | 9.82 | 154.00 | 126.42 |
| 29 | L | 4003 | BCR | C11-C12-C13 | 9.77 | 153.86 | 126.42 |
| 29 | B | 4006 | BCR | C11-C12-C13 | 9.64 | 153.49 | 126.42 |
| 25 | B | 1206 | CLA | C4A-NA-C1A | 9.50 | 110.98 | 106.71 |
| 29 | 7 | 503 | BCR | C20-C19-C18 | 9.48 | 153.06 | 126.42 |
| 25 | B | 1205 | CLA | C4A-NA-C1A | 9.47 | 110.96 | 106.71 |
| 40 | J | 4002 | RRX | C15-C14-C13 | -9.43 | 113.86 | 127.31 |
| 29 | 5 | 504 | BCR | C20-C19-C18 | 9.38 | 152.76 | 126.42 |
| 29 | A | 4005 | BCR | C20-C19-C18 | 9.35 | 152.69 | 126.42 |
| 25 | A | 1141 | CLA | C4A-NA-C1A | 9.30 | 110.89 | 106.71 |
| 25 | 2 | 603 | CLA | C4A-NA-C1A | 9.28 | 110.88 | 106.71 |
| 25 | B | 1221 | CLA | C4A-NA-C1A | 9.27 | 110.87 | 106.71 |
| 25 | A | 1123 | CLA | C4A-NA-C1A | 9.26 | 110.87 | 106.71 |
| 25 | 4 | 612 | CLA | C4A-NA-C1A | 9.26 | 110.87 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 2 | 615 | CLA | C4A-NA-C1A | 9.19 | 110.84 | 106.71 |
| 29 | 4 | 503 | BCR | C20-C19-C18 | 9.17 | 152.19 | 126.42 |
| 25 | 5 | 615 | CLA | C4A-NA-C1A | 9.16 | 110.83 | 106.71 |
| 25 | B | 1235 | CLA | C4A-NA-C1A | 9.16 | 110.82 | 106.71 |
| 25 | 8 | 615 | CLA | C4A-NA-C1A | 9.15 | 110.82 | 106.71 |
| 40 | 3 | 506 | RRX | C15-C14-C13 | -9.14 | 114.26 | 127.31 |
| 25 | B | 1228 | CLA | C4A-NA-C1A | 9.14 | 110.81 | 106.71 |
| 29 | G | 4001 | BCR | C11-C12-C13 | 9.13 | 152.06 | 126.42 |
| 25 | A | 1103 | CLA | C4A-NA-C1A | 9.11 | 110.80 | 106.71 |
| 25 | B | 1201 | CLA | C4A-NA-C1A | 9.11 | 110.80 | 106.71 |
| 29 | I | 4001 | BCR | C20-C19-C18 | 9.08 | 151.92 | 126.42 |
| 25 | 5 | 612 | CLA | C4A-NA-C1A | 9.08 | 110.79 | 106.71 |
| 25 | A | 1118 | CLA | C4A-NA-C1A | 9.06 | 110.78 | 106.71 |
| 25 | A | 1109 | CLA | C4A-NA-C1A | 9.06 | 110.78 | 106.71 |
| 25 | A | 1102 | CLA | C4A-NA-C1A | 9.04 | 110.77 | 106.71 |
| 25 | 1 | 606 | CLA | C4A-NA-C1A | 9.02 | 110.76 | 106.71 |
| 25 | 6 | 612 | CLA | C4A-NA-C1A | 9.02 | 110.76 | 106.71 |
| 25 | 2 | 607 | CLA | C4A-NA-C1A | 9.02 | 110.76 | 106.71 |
| 25 | 8 | 609 | CLA | C4A-NA-C1A | 9.00 | 110.75 | 106.71 |
| 25 | A | 1117 | CLA | C4A-NA-C1A | 8.98 | 110.74 | 106.71 |
| 25 | a | 615 | CLA | C4A-NA-C1A | 8.98 | 110.74 | 106.71 |
| 29 | 3 | 503 | BCR | C20-C19-C18 | 8.97 | 151.62 | 126.42 |
| 25 | B | 1230 | CLA | C4A-NA-C1A | 8.97 | 110.74 | 106.71 |
| 29 | 7 | 503 | BCR | C21-C20-C19 | 8.96 | 151.19 | 123.22 |
| 25 | B | 1212 | CLA | C4A-NA-C1A | 8.96 | 110.73 | 106.71 |
| 25 | 1 | 608 | CLA | C4A-NA-C1A | 8.96 | 110.73 | 106.71 |
| 25 | 5 | 607 | CLA | C4A-NA-C1A | 8.95 | 110.73 | 106.71 |
| 25 | B | 1021 | CLA | C4A-NA-C1A | 8.95 | 110.73 | 106.71 |
| 25 | B | 1222 | CLA | C4A-NA-C1A | 8.94 | 110.72 | 106.71 |
| 25 | 9 | 612 | CLA | C4A-NA-C1A | 8.93 | 110.72 | 106.71 |
| 25 | A | 1106 | CLA | C4A-NA-C1A | 8.92 | 110.72 | 106.71 |
| 25 | H | 1701 | CLA | C4A-NA-C1A | 8.92 | 110.72 | 106.71 |
| 29 | 5 | 503 | BCR | C20-C19-C18 | 8.91 | 151.46 | 126.42 |
| 25 | H | 1702 | CLA | C4A-NA-C1A | 8.91 | 110.71 | 106.71 |
| 25 | a | 603 | CLA | C4A-NA-C1A | 8.91 | 110.71 | 106.71 |
| 25 | 8 | 607 | CLA | C4A-NA-C1A | 8.91 | 110.71 | 106.71 |
| 25 | F | 1301 | CLA | C4A-NA-C1A | 8.90 | 110.71 | 106.71 |
| 25 | A | 1111 | CLA | C4A-NA-C1A | 8.87 | 110.70 | 106.71 |
| 25 | 1 | 612 | CLA | C4A-NA-C1A | 8.87 | 110.69 | 106.71 |
| 25 | B | 1217 | CLA | C4A-NA-C1A | 8.86 | 110.69 | 106.71 |
| 25 | K | 1404 | CLA | C4A-NA-C1A | 8.86 | 110.69 | 106.71 |
| 25 | 3 | 606 | CLA | C4A-NA-C1A | 8.85 | 110.69 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 616 | CLA | C4A-NA-C1A | 8.85 | 110.69 | 106.71 |
| 25 | J | 1901 | CLA | C4A-NA-C1A | 8.84 | 110.68 | 106.71 |
| 25 | 6 | 615 | CLA | C4A-NA-C1A | 8.84 | 110.68 | 106.71 |
| 25 | A | 1112 | CLA | C4A-NA-C1A | 8.82 | 110.67 | 106.71 |
| 25 | a | 608 | CLA | C4A-NA-C1A | 8.82 | 110.67 | 106.71 |
| 25 | 6 | 608 | CLA | C4A-NA-C1A | 8.82 | 110.67 | 106.71 |
| 25 | 1 | 615 | CLA | C4A-NA-C1A | 8.81 | 110.67 | 106.71 |
| 25 | A | 1131 | CLA | C4A-NA-C1A | 8.81 | 110.67 | 106.71 |
| 25 | 4 | 610 | CLA | C4A-NA-C1A | 8.81 | 110.67 | 106.71 |
| 25 | A | 1136 | CLA | C4A-NA-C1A | 8.80 | 110.66 | 106.71 |
| 25 | 8 | 611 | CLA | C4A-NA-C1A | 8.80 | 110.66 | 106.71 |
| 25 | L | 1502 | CLA | C4A-NA-C1A | 8.80 | 110.66 | 106.71 |
| 29 | B | 4005 | BCR | C20-C19-C18 | 8.80 | 151.13 | 126.42 |
| 25 | 9 | 607 | CLA | C4A-NA-C1A | 8.79 | 110.66 | 106.71 |
| 25 | 1 | 603 | CLA | C4A-NA-C1A | 8.78 | 110.66 | 106.71 |
| 25 | 3 | 613 | CLA | C4A-NA-C1A | 8.78 | 110.65 | 106.71 |
| 25 | L | 1501 | CLA | C4A-NA-C1A | 8.77 | 110.65 | 106.71 |
| 25 | 7 | 612 | CLA | C4A-NA-C1A | 8.77 | 110.65 | 106.71 |
| 25 | 7 | 608 | CLA | C4A-NA-C1A | 8.76 | 110.65 | 106.71 |
| 25 | B | 1214 | CLA | C4A-NA-C1A | 8.75 | 110.64 | 106.71 |
| 25 | 8 | 612 | CLA | C4A-NA-C1A | 8.75 | 110.64 | 106.71 |
| 25 | B | 1023 | CLA | C4A-NA-C1A | 8.75 | 110.64 | 106.71 |
| 25 | 7 | 610 | CLA | C4A-NA-C1A | 8.75 | 110.64 | 106.71 |
| 25 | B | 1224 | CLA | C4A-NA-C1A | 8.75 | 110.64 | 106.71 |
| 25 | F | 1302 | CLA | C4A-NA-C1A | 8.74 | 110.64 | 106.71 |
| 25 | 7 | 607 | CLA | C4A-NA-C1A | 8.74 | 110.64 | 106.71 |
| 25 | B | 1239 | CLA | C4A-NA-C1A | 8.74 | 110.64 | 106.71 |
| 25 | 4 | 617 | CLA | C4A-NA-C1A | 8.73 | 110.63 | 106.71 |
| 25 | 3 | 610 | CLA | C4A-NA-C1A | 8.73 | 110.63 | 106.71 |
| 25 | 3 | 618 | CLA | C4A-NA-C1A | 8.72 | 110.63 | 106.71 |
| 29 | O | 4001 | BCR | C20-C19-C18 | 8.71 | 150.89 | 126.42 |
| 25 | 6 | 603 | CLA | C4A-NA-C1A | 8.71 | 110.62 | 106.71 |
| 25 | a | 612 | CLA | C4A-NA-C1A | 8.70 | 110.62 | 106.71 |
| 25 | 1 | 605 | CLA | C4A-NA-C1A | 8.70 | 110.62 | 106.71 |
| 25 | 5 | 601 | CLA | C4A-NA-C1A | 8.70 | 110.62 | 106.71 |
| 25 | 8 | 618 | CLA | C4A-NA-C1A | 8.69 | 110.61 | 106.71 |
| 25 | A | 1139 | CLA | C4A-NA-C1A | 8.68 | 110.61 | 106.71 |
| 25 | 7 | 603 | CLA | C4A-NA-C1A | 8.67 | 110.61 | 106.71 |
| 25 | 4 | 601 | CLA | C4A-NA-C1A | 8.66 | 110.60 | 106.71 |
| 25 | 2 | 608 | CLA | C4A-NA-C1A | 8.66 | 110.60 | 106.71 |
| 25 | K | 1401 | CLA | C4A-NA-C1A | 8.65 | 110.60 | 106.71 |
| 25 | 3 | 612 | CLA | C4A-NA-C1A | 8.65 | 110.60 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 608 | CLA | C4A-NA-C1A | 8.65 | 110.60 | 106.71 |
| 25 | 2 | 601 | CLA | C4A-NA-C1A | 8.65 | 110.59 | 106.71 |
| 25 | L | 1503 | CLA | C4A-NA-C1A | 8.64 | 110.59 | 106.71 |
| 25 | A | 1120 | CLA | C4A-NA-C1A | 8.63 | 110.59 | 106.71 |
| 25 | K | 1403 | CLA | C4A-NA-C1A | 8.63 | 110.58 | 106.71 |
| 25 | 9 | 602 | CLA | C4A-NA-C1A | 8.62 | 110.58 | 106.71 |
| 25 | A | 1134 | CLA | C4A-NA-C1A | 8.62 | 110.58 | 106.71 |
| 25 | O | 1803 | CLA | C4A-NA-C1A | 8.62 | 110.58 | 106.71 |
| 25 | A | 1132 | CLA | C4A-NA-C1A | 8.62 | 110.58 | 106.71 |
| 25 | A | 1126 | CLA | C4A-NA-C1A | 8.61 | 110.58 | 106.71 |
| 25 | 8 | 620 | CLA | C4A-NA-C1A | 8.61 | 110.58 | 106.71 |
| 25 | B | 1202 | CLA | C4A-NA-C1A | 8.60 | 110.57 | 106.71 |
| 25 | 4 | 611 | CLA | C4A-NA-C1A | 8.60 | 110.57 | 106.71 |
| 25 | B | 1223 | CLA | C4A-NA-C1A | 8.59 | 110.57 | 106.71 |
| 25 | 3 | 607 | CLA | C4A-NA-C1A | 8.59 | 110.57 | 106.71 |
| 25 | a | 602 | CLA | C4A-NA-C1A | 8.59 | 110.57 | 106.71 |
| 25 | 4 | 606 | CLA | C4A-NA-C1A | 8.59 | 110.57 | 106.71 |
| 25 | B | 1213 | CLA | C4A-NA-C1A | 8.57 | 110.56 | 106.71 |
| 25 | 3 | 602 | CLA | C4A-NA-C1A | 8.57 | 110.56 | 106.71 |
| 25 | A | 1128 | CLA | C4A-NA-C1A | 8.57 | 110.56 | 106.71 |
| 25 | B | 1219 | CLA | C4A-NA-C1A | 8.57 | 110.56 | 106.71 |
| 25 | 5 | 606 | CLA | C4A-NA-C1A | 8.57 | 110.56 | 106.71 |
| 25 | 5 | 608 | CLA | C4A-NA-C1A | 8.56 | 110.56 | 106.71 |
| 25 | B | 1232 | CLA | C4A-NA-C1A | 8.56 | 110.56 | 106.71 |
| 25 | 2 | 621 | CLA | C4A-NA-C1A | 8.56 | 110.55 | 106.71 |
| 25 | B | 1237 | CLA | C4A-NA-C1A | 8.55 | 110.55 | 106.71 |
| 25 | G | 1601 | CLA | C4A-NA-C1A | 8.55 | 110.55 | 106.71 |
| 25 | A | 1140 | CLA | C4A-NA-C1A | 8.55 | 110.55 | 106.71 |
| 25 | B | 1227 | CLA | C4A-NA-C1A | 8.55 | 110.55 | 106.71 |
| 25 | B | 1215 | CLA | C4A-NA-C1A | 8.55 | 110.55 | 106.71 |
| 25 | A | 1115 | CLA | C4A-NA-C1A | 8.55 | 110.55 | 106.71 |
| 25 | 4 | 607 | CLA | C4A-NA-C1A | 8.54 | 110.55 | 106.71 |
| 29 | B | 4004 | BCR | C20-C19-C18 | 8.54 | 150.40 | 126.42 |
| 29 | L | 4003 | BCR | C20-C19-C18 | 8.54 | 150.40 | 126.42 |
| 25 | B | 1204 | CLA | C4A-NA-C1A | 8.53 | 110.54 | 106.71 |
| 25 | O | 1802 | CLA | C4A-NA-C1A | 8.53 | 110.54 | 106.71 |
| 25 | G | 1602 | CLA | C4A-NA-C1A | 8.52 | 110.54 | 106.71 |
| 25 | a | 611 | CLA | C4A-NA-C1A | 8.52 | 110.54 | 106.71 |
| 25 | 7 | 601 | CLA | C4A-NA-C1A | 8.52 | 110.54 | 106.71 |
| 25 | A | 1122 | CLA | C4A-NA-C1A | 8.52 | 110.53 | 106.71 |
| 25 | B | 1210 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |
| 25 | 8 | 606 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | a | 607 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |
| 25 | 6 | 606 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |
| 25 | A | 1012 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |
| 25 | A | 1137 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |
| 25 | O | 1801 | CLA | C4A-NA-C1A | 8.51 | 110.53 | 106.71 |
| 29 | B | 4002 | BCR | C20-C19-C18 | 8.50 | 150.31 | 126.42 |
| 25 | B | 1220 | CLA | C4A-NA-C1A | 8.50 | 110.53 | 106.71 |
| 25 | 4 | 604 | CLA | C4A-NA-C1A | 8.49 | 110.52 | 106.71 |
| 25 | 3 | 601 | CLA | C4A-NA-C1A | 8.49 | 110.52 | 106.71 |
| 25 | K | 1402 | CLA | C4A-NA-C1A | 8.49 | 110.52 | 106.71 |
| 25 | 9 | 609 | CLA | C4A-NA-C1A | 8.49 | 110.52 | 106.71 |
| 25 | 2 | 612 | CLA | C4A-NA-C1A | 8.46 | 110.51 | 106.71 |
| 25 | B | 1234 | CLA | CMD-C2D-C1D | 8.46 | 134.73 | 124.17 |
| 25 | 6 | 607 | CLA | C4A-NA-C1A | 8.45 | 110.51 | 106.71 |
| 25 | a | 601 | CLA | C4A-NA-C1A | 8.45 | 110.51 | 106.71 |
| 25 | B | 1236 | CLA | C4A-NA-C1A | 8.44 | 110.50 | 106.71 |
| 25 | A | 1013 | CLA | C4A-NA-C1A | 8.44 | 110.50 | 106.71 |
| 25 | A | 1127 | CLA | C4A-NA-C1A | 8.43 | 110.50 | 106.71 |
| 25 | 5 | 614 | CLA | C4A-NA-C1A | 8.43 | 110.50 | 106.71 |
| 39 | F | 4001 | NEX | C17-C1-C16 | -8.43 | 82.65 | 108.53 |
| 25 | A | 1133 | CLA | C4A-NA-C1A | 8.43 | 110.50 | 106.71 |
| 25 | 7 | 605 | CLA | C4A-NA-C1A | 8.41 | 110.49 | 106.71 |
| 25 | 5 | 609 | CLA | C4A-NA-C1A | 8.40 | 110.48 | 106.71 |
| 25 | 1 | 602 | CLA | C4A-NA-C1A | 8.39 | 110.48 | 106.71 |
| 25 | A | 1101 | CLA | C4A-NA-C1A | 8.39 | 110.48 | 106.71 |
| 25 | 3 | 605 | CLA | C4A-NA-C1A | 8.38 | 110.47 | 106.71 |
| 25 | 5 | 604 | CLA | C4A-NA-C1A | 8.37 | 110.47 | 106.71 |
| 25 | a | 605 | CLA | C4A-NA-C1A | 8.37 | 110.47 | 106.71 |
| 25 | 9 | 604 | CLA | C4A-NA-C1A | 8.36 | 110.47 | 106.71 |
| 29 | 6 | 503 | BCR | C20-C19-C18 | 8.36 | 149.91 | 126.42 |
| 25 | B | 1238 | CLA | C4A-NA-C1A | 8.36 | 110.47 | 106.71 |
| 25 | 2 | 606 | CLA | C4A-NA-C1A | 8.35 | 110.46 | 106.71 |
| 25 | 8 | 602 | CLA | C4A-NA-C1A | 8.35 | 110.46 | 106.71 |
| 25 | A | 1124 | CLA | C4A-NA-C1A | 8.34 | 110.45 | 106.71 |
| 25 | 7 | 604 | CLA | C4A-NA-C1A | 8.34 | 110.45 | 106.71 |
| 25 | 4 | 602 | CLA | C4A-NA-C1A | 8.33 | 110.45 | 106.71 |
| 25 | 8 | 605 | CLA | C4A-NA-C1A | 8.33 | 110.45 | 106.71 |
| 25 | B | 1208 | CLA | C4A-NA-C1A | 8.33 | 110.45 | 106.71 |
| 25 | A | 1138 | CLA | C4A-NA-C1A | 8.32 | 110.45 | 106.71 |
| 25 | 5 | 605 | CLA | C4A-NA-C1A | 8.32 | 110.45 | 106.71 |
| 25 | 2 | 604 | CLA | C4A-NA-C1A | 8.32 | 110.44 | 106.71 |
| 25 | A | 1116 | CLA | C4A-NA-C1A | 8.31 | 110.44 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 7 | 606 | CLA | C4A-NA-C1A | 8.30 | 110.44 | 106.71 |
| 25 | B | 1229 | CLA | C4A-NA-C1A | 8.30 | 110.44 | 106.71 |
| 25 | 2 | 602 | CLA | C4A-NA-C1A | 8.30 | 110.44 | 106.71 |
| 25 | B | 1211 | CLA | C4A-NA-C1A | 8.29 | 110.44 | 106.71 |
| 29 | 8 | 503 | BCR | C20-C19-C18 | 8.29 | 149.72 | 126.42 |
| 25 | 9 | 605 | CLA | C4A-NA-C1A | 8.29 | 110.43 | 106.71 |
| 25 | H | 1703 | CLA | C4A-NA-C1A | 8.28 | 110.43 | 106.71 |
| 25 | A | 1121 | CLA | C4A-NA-C1A | 8.28 | 110.43 | 106.71 |
| 25 | B | 1240 | CLA | C4A-NA-C1A | 8.28 | 110.43 | 106.71 |
| 25 | 4 | 615 | CLA | C4A-NA-C1A | 8.27 | 110.43 | 106.71 |
| 25 | B | 1218 | CLA | C4A-NA-C1A | 8.27 | 110.42 | 106.71 |
| 25 | 4 | 603 | CLA | C4A-NA-C1A | 8.26 | 110.42 | 106.71 |
| 25 | A | 1113 | CLA | C4A-NA-C1A | 8.26 | 110.42 | 106.71 |
| 25 | B | 1207 | CLA | C4A-NA-C1A | 8.25 | 110.42 | 106.71 |
| 25 | 6 | 618 | CLA | C4A-NA-C1A | 8.25 | 110.42 | 106.71 |
| 25 | 5 | 603 | CLA | C4A-NA-C1A | 8.25 | 110.42 | 106.71 |
| 25 | 1 | 607 | CLA | C4A-NA-C1A | 8.25 | 110.41 | 106.71 |
| 25 | A | 1107 | CLA | C4A-NA-C1A | 8.23 | 110.41 | 106.71 |
| 25 | G | 1603 | CLA | C4A-NA-C1A | 8.23 | 110.41 | 106.71 |
| 25 | A | 1105 | CLA | C4A-NA-C1A | 8.23 | 110.41 | 106.71 |
| 25 | 1 | 601 | CLA | C4A-NA-C1A | 8.23 | 110.41 | 106.71 |
| 25 | A | 1135 | CLA | C4A-NA-C1A | 8.23 | 110.40 | 106.71 |
| 25 | 6 | 602 | CLA | C4A-NA-C1A | 8.23 | 110.40 | 106.71 |
| 25 | A | 1129 | CLA | C4A-NA-C1A | 8.22 | 110.40 | 106.71 |
| 25 | A | 1108 | CLA | C4A-NA-C1A | 8.20 | 110.39 | 106.71 |
| 25 | A | 1110 | CLA | C4A-NA-C1A | 8.19 | 110.39 | 106.71 |
| 25 | 4 | 605 | CLA | C4A-NA-C1A | 8.19 | 110.39 | 106.71 |
| 25 | 4 | 616 | CLA | C4A-NA-C1A | 8.18 | 110.39 | 106.71 |
| 25 | B | 1216 | CLA | C4A-NA-C1A | 8.17 | 110.38 | 106.71 |
| 25 | A | 1104 | CLA | C4A-NA-C1A | 8.17 | 110.38 | 106.71 |
| 29 | A | 4004 | BCR | C20-C19-C18 | 8.17 | 149.37 | 126.42 |
| 25 | 7 | 602 | CLA | C4A-NA-C1A | 8.17 | 110.38 | 106.71 |
| 25 | 6 | 601 | CLA | C4A-NA-C1A | 8.16 | 110.38 | 106.71 |
| 25 | 5 | 602 | CLA | C4A-NA-C1A | 8.15 | 110.37 | 106.71 |
| 29 | B | 4003 | BCR | C20-C19-C18 | 8.13 | 149.26 | 126.42 |
| 25 | B | 1203 | CLA | C4A-NA-C1A | 8.13 | 110.36 | 106.71 |
| 25 | 6 | 605 | CLA | C4A-NA-C1A | 8.11 | 110.35 | 106.71 |
| 25 | 9 | 606 | CLA | C4A-NA-C1A | 8.10 | 110.35 | 106.71 |
| 25 | L | 1504 | CLA | C4A-NA-C1A | 8.08 | 110.34 | 106.71 |
| 25 | A | 1130 | CLA | C4A-NA-C1A | 8.08 | 110.34 | 106.71 |
| 25 | B | 1225 | CLA | C4A-NA-C1A | 8.06 | 110.33 | 106.71 |
| 25 | A | 1119 | CLA | C4A-NA-C1A | 8.05 | 110.32 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 608 | CLA | C4A-NA-C1A | 8.03 | 110.31 | 106.71 |
| 25 | 2 | 605 | CLA | C4A-NA-C1A | 7.94 | 110.28 | 106.71 |
| 29 | B | 4007 | BCR | C20-C19-C18 | 7.92 | 148.66 | 126.42 |
| 25 | A | 1125 | CLA | C4A-NA-C1A | 7.90 | 110.26 | 106.71 |
| 29 | A | 4002 | BCR | C20-C19-C18 | 7.87 | 148.53 | 126.42 |
| 29 | L | 4001 | BCR | C20-C19-C18 | 7.86 | 148.49 | 126.42 |
| 25 | B | 1231 | CLA | C4A-NA-C1A | 7.80 | 110.21 | 106.71 |
| 25 | B | 1209 | CLA | C4A-NA-C1A | 7.75 | 110.19 | 106.71 |
| 29 | H | 4001 | BCR | C20-C19-C18 | 7.74 | 148.15 | 126.42 |
| 29 | J | 4001 | BCR | C20-C19-C18 | 7.64 | 147.89 | 126.42 |
| 29 | 6 | 504 | BCR | C20-C19-C18 | 7.63 | 147.85 | 126.42 |
| 25 | 6 | 604 | CLA | C4A-NA-C1A | 7.61 | 110.13 | 106.71 |
| 29 | B | 4006 | BCR | C20-C19-C18 | 7.58 | 147.70 | 126.42 |
| 25 | B | 1226 | CLA | C4A-NA-C1A | 7.58 | 110.11 | 106.71 |
| 25 | B | 1022 | CLA | C4A-NA-C1A | 7.55 | 110.10 | 106.71 |
| 29 | L | 4002 | BCR | C20-C19-C18 | 7.55 | 147.61 | 126.42 |
| 29 | G | 4001 | BCR | C20-C19-C18 | 7.48 | 147.42 | 126.42 |
| 29 | 3 | 505 | BCR | C20-C19-C18 | 7.43 | 147.28 | 126.42 |
| 43 | 7 | 501 | LUT | C21-C26-C27 | 7.41 | 122.07 | 112.70 |
| 39 | F | 4001 | NEX | C2-C1-C6 | 7.40 | 116.41 | 109.21 |
| 24 | A | 1011 | CL0 | CMD-C2D-C1D | 7.23 | 137.46 | 124.71 |
| 29 | B | 4001 | BCR | C20-C19-C18 | 7.19 | 146.62 | 126.42 |
| 29 | 3 | 504 | BCR | C20-C19-C18 | 7.13 | 146.45 | 126.42 |
| 29 | A | 4001 | BCR | C20-C19-C18 | 7.10 | 146.35 | 126.42 |
| 29 | K | 4001 | BCR | C20-C19-C18 | 7.02 | 146.14 | 126.42 |
| 29 | K | 4002 | BCR | C20-C19-C18 | 6.93 | 145.87 | 126.42 |
| 44 | 7 | 504 | AXT | C1-C6-C5 | -6.89 | 112.91 | 122.61 |
| 39 | F | 4001 | NEX | O24-C25-C38 | -6.84 | 106.86 | 115.06 |
| 24 | A | 1011 | CL0 | C4A-NA-C1A | 6.72 | 109.73 | 106.71 |
| 43 | 2 | 507 | LUT | C31-C30-C29 | -6.70 | 117.74 | 127.31 |
| 40 | 3 | 506 | RRX | C20-C21-C22 | -6.67 | 117.79 | 127.31 |
| 48 | 8 | 804 | DGA | CDB-CCB-CBB | -6.66 | 80.61 | 114.42 |
| 43 | 4 | 501 | LUT | C21-C26-C27 | 6.65 | 121.11 | 112.70 |
| 25 | 2 | 601 | CLA | O2A-C1-C2 | 6.60 | 125.99 | 108.64 |
| 29 | G | 4001 | BCR | C15-C14-C13 | -6.57 | 117.94 | 127.31 |
| 25 | A | 1117 | CLA | O2D-CGD-CBD | 6.51 | 122.84 | 111.27 |
| 43 | 2 | 507 | LUT | C21-C26-C27 | 6.49 | 120.91 | 112.70 |
| 25 | B | 1218 | CLA | O2D-CGD-CBD | 6.42 | 122.67 | 111.27 |
| 43 | 1 | 503 | LUT | C15-C35-C34 | -6.39 | 110.38 | 123.47 |
| 25 | 4 | 610 | CLA | O2A-C1-C2 | 6.36 | 125.34 | 108.64 |
| 29 | A | 4003 | BCR | C20-C19-C18 | 6.29 | 144.09 | 126.42 |
| 43 | a | 503 | LUT | C35-C34-C33 | -6.27 | 118.36 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 612 | CLA | O2D-CGD-CBD | 6.25 | 122.38 | 111.27 |
| 24 | A | 1011 | CL0 | C2C-C1C-NC | 6.23 | 115.81 | 109.97 |
| 50 | 9 | 507 | XAT | C15-C14-C13 | -6.21 | 118.44 | 127.31 |
| 25 | 1 | 605 | CLA | O2A-C1-C2 | 6.19 | 124.92 | 108.64 |
| 25 | 2 | 604 | CLA | O2A-C1-C2 | 6.19 | 124.90 | 108.64 |
| 25 | 1 | 606 | CLA | O2D-CGD-CBD | 6.16 | 122.21 | 111.27 |
| 25 | 8 | 618 | CLA | CMD-C2D-C1D | 6.12 | 135.51 | 124.71 |
| 25 | B | 1205 | CLA | O2D-CGD-CBD | 6.12 | 122.14 | 111.27 |
| 25 | B | 1201 | CLA | O2D-CGD-CBD | 6.09 | 122.09 | 111.27 |
| 25 | A | 1106 | CLA | O2D-CGD-CBD | 6.09 | 122.08 | 111.27 |
| 25 | A | 1121 | CLA | CMD-C2D-C1D | 6.06 | 135.39 | 124.71 |
| 25 | B | 1231 | CLA | CMD-C2D-C1D | 6.00 | 135.29 | 124.71 |
| 43 | a | 503 | LUT | C21-C26-C25 | 5.99 | 122.16 | 111.42 |
| 25 | A | 1128 | CLA | O2D-CGD-CBD | 5.98 | 121.89 | 111.27 |
| 25 | H | 1702 | CLA | O2D-CGD-CBD | 5.96 | 121.86 | 111.27 |
| 25 | A | 1132 | CLA | O2D-CGD-CBD | 5.94 | 121.83 | 111.27 |
| 43 | 2 | 507 | LUT | C11-C10-C9 | -5.93 | 118.84 | 127.31 |
| 25 | B | 1221 | CLA | O2D-CGD-CBD | 5.93 | 121.81 | 111.27 |
| 43 | 1 | 501 | LUT | C21-C26-C25 | 5.93 | 122.04 | 111.42 |
| 25 | A | 1112 | CLA | O2D-CGD-CBD | 5.93 | 121.80 | 111.27 |
| 29 | 7 | 503 | BCR | C23-C24-C25 | -5.93 | 110.56 | 127.20 |
| 43 | a | 502 | LUT | C21-C26-C25 | 5.92 | 122.02 | 111.42 |
| 25 | 2 | 604 | CLA | CMD-C2D-C1D | 5.91 | 135.14 | 124.71 |
| 25 | A | 1101 | CLA | O2D-CGD-CBD | 5.90 | 121.75 | 111.27 |
| 26 | 3 | 604 | CHL | C1-O2A-CGA | 5.87 | 131.86 | 116.44 |
| 43 | 8 | 501 | LUT | C21-C26-C25 | 5.87 | 121.94 | 111.42 |
| 25 | 6 | 608 | CLA | CMD-C2D-C1D | 5.86 | 135.03 | 124.71 |
| 43 | 6 | 502 | LUT | C21-C26-C25 | 5.85 | 121.89 | 111.42 |
| 25 | B | 1240 | CLA | O2D-CGD-CBD | 5.85 | 121.66 | 111.27 |
| 25 | 2 | 605 | CLA | CMD-C2D-C1D | 5.84 | 135.00 | 124.71 |
| 25 | 6 | 605 | CLA | CMD-C2D-C1D | 5.83 | 135.00 | 124.71 |
| 25 | 1 | 605 | CLA | O2D-CGD-CBD | 5.83 | 121.63 | 111.27 |
| 25 | B | 1238 | CLA | O2A-C1-C2 | 5.83 | 123.95 | 108.64 |
| 43 | 3 | 502 | LUT | C21-C26-C25 | 5.83 | 121.86 | 111.42 |
| 25 | B | 1230 | CLA | O2D-CGD-CBD | 5.82 | 121.61 | 111.27 |
| 25 | A | 1120 | CLA | O2D-CGD-CBD | 5.82 | 121.60 | 111.27 |
| 25 | 7 | 604 | CLA | CMD-C2D-C1D | 5.81 | 134.95 | 124.71 |
| 25 | B | 1214 | CLA | O2A-C1-C2 | 5.80 | 123.88 | 108.64 |
| 43 | 5 | 505 | LUT | C21-C26-C27 | 5.80 | 120.03 | 112.70 |
| 25 | A | 1137 | CLA | O2A-C1-C2 | 5.80 | 123.87 | 108.64 |
| 25 | A | 1129 | CLA | O2D-CGD-CBD | 5.79 | 121.56 | 111.27 |
| 25 | A | 1115 | CLA | O2D-CGD-CBD | 5.79 | 121.55 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 5 | 501 | LUT | C21-C26-C25 | 5.78 | 121.78 | 111.42 |
| 25 | B | 1226 | CLA | CMD-C2D-C1D | 5.78 | 134.89 | 124.71 |
| 25 | B | 1211 | CLA | O2D-CGD-CBD | 5.77 | 121.52 | 111.27 |
| 43 | a | 501 | LUT | C21-C26-C25 | 5.76 | 121.74 | 111.42 |
| 25 | 5 | 604 | CLA | CMD-C2D-C1D | 5.76 | 134.86 | 124.71 |
| 43 | 9 | 502 | LUT | C21-C26-C25 | 5.75 | 121.72 | 111.42 |
| 25 | 8 | 609 | CLA | O2D-CGD-CBD | 5.75 | 121.48 | 111.27 |
| 25 | B | 1212 | CLA | O2D-CGD-CBD | 5.75 | 121.48 | 111.27 |
| 24 | A | 1011 | CL0 | C2D-C1D-ND | 5.75 | 114.34 | 110.10 |
| 25 | A | 1109 | CLA | CMD-C2D-C1D | 5.74 | 134.83 | 124.71 |
| 43 | 5 | 502 | LUT | C21-C26-C25 | 5.72 | 121.67 | 111.42 |
| 43 | 3 | 501 | LUT | C21-C26-C25 | 5.72 | 121.66 | 111.42 |
| 25 | 5 | 603 | CLA | CMD-C2D-C1D | 5.72 | 134.79 | 124.71 |
| 25 | 7 | 601 | CLA | CMD-C2D-C1D | 5.71 | 134.78 | 124.71 |
| 25 | B | 1228 | CLA | O2A-C1-C2 | 5.71 | 123.65 | 108.64 |
| 43 | 4 | 502 | LUT | C21-C26-C25 | 5.71 | 121.65 | 111.42 |
| 25 | 2 | 615 | CLA | O2D-CGD-CBD | 5.71 | 121.41 | 111.27 |
| 25 | A | 1012 | CLA | O2A-C1-C2 | 5.71 | 123.63 | 108.64 |
| 25 | A | 1134 | CLA | O2D-CGD-CBD | 5.70 | 121.39 | 111.27 |
| 25 | 4 | 606 | CLA | O2D-CGD-CBD | 5.69 | 121.38 | 111.27 |
| 44 | 7 | 504 | AXT | C8-C9-C10 | 5.69 | 127.67 | 118.94 |
| 25 | L | 1502 | CLA | O2A-C1-C2 | 5.68 | 123.57 | 108.64 |
| 25 | A | 1102 | CLA | O2D-CGD-CBD | 5.67 | 121.35 | 111.27 |
| 25 | 3 | 601 | CLA | O2A-C1-C2 | 5.66 | 123.52 | 108.64 |
| 25 | 7 | 607 | CLA | O2A-C1-C2 | 5.65 | 122.19 | 108.97 |
| 43 | a | 503 | LUT | C21-C26-C27 | 5.65 | 119.85 | 112.70 |
| 25 | 1 | 605 | CLA | CMD-C2D-C1D | 5.64 | 134.66 | 124.71 |
| 25 | a | 605 | CLA | CMD-C2D-C1D | 5.64 | 134.66 | 124.71 |
| 25 | B | 1208 | CLA | O2D-CGD-CBD | 5.64 | 121.28 | 111.27 |
| 25 | B | 1227 | CLA | O2D-CGD-CBD | 5.63 | 121.28 | 111.27 |
| 25 | B | 1209 | CLA | O2A-C1-C2 | 5.63 | 123.43 | 108.64 |
| 25 | 9 | 605 | CLA | CMD-C2D-C1D | 5.63 | 134.63 | 124.71 |
| 25 | B | 1210 | CLA | O2D-CGD-CBD | 5.63 | 121.27 | 111.27 |
| 46 | a | 504 | QTB | C09-C02-C03 | 5.62 | 127.57 | 118.94 |
| 25 | 6 | 604 | CLA | CMD-C2D-C1D | 5.62 | 134.62 | 124.71 |
| 40 | 3 | 506 | RRX | C15-C16-C17 | -5.62 | 111.95 | 123.47 |
| 25 | 1 | 601 | CLA | CMD-C2D-C1D | 5.62 | 134.62 | 124.71 |
| 25 | A | 1113 | CLA | O2D-CGD-CBD | 5.62 | 121.25 | 111.27 |
| 25 | A | 1141 | CLA | CMD-C2D-C1D | 5.61 | 134.61 | 124.71 |
| 25 | A | 1111 | CLA | CMD-C2D-C1D | 5.61 | 134.61 | 124.71 |
| 25 | 4 | 606 | CLA | CMD-C2D-C1D | 5.61 | 134.60 | 124.71 |
| 25 | 6 | 606 | CLA | O2D-CGD-CBD | 5.61 | 121.23 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | J | 4002 | RRX | C15-C16-C17 | 5.60 | 134.95 | 123.47 |
| 25 | 7 | 606 | CLA | CMD-C2D-C1D | 5.60 | 134.59 | 124.71 |
| 25 | A | 1101 | CLA | CMD-C2D-C1D | 5.60 | 134.58 | 124.71 |
| 25 | A | 1120 | CLA | O2A-C1-C2 | 5.60 | 122.06 | 108.97 |
| 25 | O | 1802 | CLA | CMD-C2D-C1D | 5.60 | 134.57 | 124.71 |
| 43 | 2 | 507 | LUT | C21-C26-C25 | 5.59 | 121.43 | 111.42 |
| 25 | B | 1217 | CLA | CMD-C2D-C1D | 5.59 | 134.56 | 124.71 |
| 25 | 1 | 606 | CLA | CMD-C2D-C1D | 5.58 | 134.55 | 124.71 |
| 43 | 5 | 505 | LUT | C21-C26-C25 | 5.58 | 121.41 | 111.42 |
| 25 | 8 | 620 | CLA | CMD-C2D-C1D | 5.58 | 134.54 | 124.71 |
| 25 | B | 1209 | CLA | CMD-C2D-C1D | 5.57 | 134.54 | 124.71 |
| 25 | A | 1126 | CLA | CMD-C2D-C1D | 5.56 | 134.52 | 124.71 |
| 25 | 5 | 601 | CLA | CMD-C2D-C1D | 5.56 | 134.52 | 124.71 |
| 25 | 8 | 602 | CLA | CMD-C2D-C1D | 5.56 | 134.52 | 124.71 |
| 25 | A | 1113 | CLA | CMD-C2D-C1D | 5.56 | 134.52 | 124.71 |
| 25 | 4 | 617 | CLA | CMD-C2D-C1D | 5.56 | 134.51 | 124.71 |
| 43 | 9 | 501 | LUT | C21-C26-C25 | 5.56 | 121.38 | 111.42 |
| 25 | B | 1218 | CLA | CMD-C2D-C1D | 5.56 | 134.51 | 124.71 |
| 25 | A | 1103 | CLA | O2D-CGD-CBD | 5.55 | 121.14 | 111.27 |
| 25 | A | 1123 | CLA | O2D-CGD-CBD | 5.55 | 121.14 | 111.27 |
| 25 | B | 1211 | CLA | CMD-C2D-C1D | 5.55 | 134.50 | 124.71 |
| 25 | a | 601 | CLA | CMD-C2D-C1D | 5.55 | 134.50 | 124.71 |
| 25 | A | 1109 | CLA | O2A-C1-C2 | 5.55 | 123.22 | 108.64 |
| 25 | O | 1802 | CLA | O2D-CGD-CBD | 5.55 | 121.13 | 111.27 |
| 25 | B | 1228 | CLA | CMD-C2D-C1D | 5.55 | 134.49 | 124.71 |
| 25 | 3 | 602 | CLA | CMD-C2D-C1D | 5.55 | 134.49 | 124.71 |
| 25 | A | 1130 | CLA | O2A-C1-C2 | 5.54 | 123.21 | 108.64 |
| 25 | 5 | 605 | CLA | CMD-C2D-C1D | 5.54 | 134.48 | 124.71 |
| 43 | 8 | 502 | LUT | C21-C26-C25 | 5.54 | 121.34 | 111.42 |
| 25 | a | 605 | CLA | O2D-CGD-CBD | 5.54 | 121.11 | 111.27 |
| 43 | 2 | 502 | LUT | C21-C26-C25 | 5.54 | 121.34 | 111.42 |
| 25 | 4 | 604 | CLA | CMD-C2D-C1D | 5.53 | 134.46 | 124.71 |
| 25 | 4 | 605 | CLA | CMD-C2D-C1D | 5.53 | 134.46 | 124.71 |
| 25 | A | 1119 | CLA | O2A-C1-C2 | 5.53 | 123.17 | 108.64 |
| 25 | a | 603 | CLA | CMD-C2D-C1D | 5.53 | 134.46 | 124.71 |
| 25 | B | 1203 | CLA | CMD-C2D-C1D | 5.53 | 134.46 | 124.71 |
| 25 | 4 | 610 | CLA | CMD-C2D-C1D | 5.53 | 134.46 | 124.71 |
| 25 | B | 1216 | CLA | O2A-C1-C2 | 5.53 | 123.16 | 108.64 |
| 25 | 6 | 606 | CLA | CMD-C2D-C1D | 5.53 | 134.45 | 124.71 |
| 25 | O | 1801 | CLA | CMD-C2D-C1D | 5.52 | 134.45 | 124.71 |
| 25 | 6 | 601 | CLA | CMD-C2D-C1D | 5.52 | 134.44 | 124.71 |
| 25 | 9 | 604 | CLA | CMD-C2D-C1D | 5.52 | 134.44 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 2 | 607 | CLA | O2D-CGD-CBD | 5.52 | 121.07 | 111.27 |
| 25 | 2 | 621 | CLA | O2A-C1-C2 | 5.52 | 123.13 | 108.64 |
| 25 | A | 1132 | CLA | CMD-C2D-C1D | 5.52 | 134.43 | 124.71 |
| 25 | 8 | 607 | CLA | O2D-CGD-CBD | 5.51 | 121.07 | 111.27 |
| 25 | A | 1106 | CLA | CMD-C2D-C1D | 5.51 | 134.43 | 124.71 |
| 24 | A | 1011 | CL0 | C1C-C2C-C3C | -5.51 | 101.16 | 106.96 |
| 25 | 4 | 603 | CLA | CMD-C2D-C1D | 5.51 | 134.43 | 124.71 |
| 25 | A | 1136 | CLA | CMD-C2D-C1D | 5.51 | 134.43 | 124.71 |
| 25 | a | 603 | CLA | O2A-C1-C2 | 5.51 | 123.12 | 108.64 |
| 25 | 8 | 605 | CLA | CMD-C2D-C1D | 5.51 | 134.42 | 124.71 |
| 25 | A | 1125 | CLA | O2D-CGD-CBD | 5.51 | 121.05 | 111.27 |
| 25 | 4 | 608 | CLA | O2D-CGD-CBD | 5.51 | 121.05 | 111.27 |
| 25 | B | 1023 | CLA | O2A-C1-C2 | 5.51 | 123.10 | 108.64 |
| 25 | B | 1223 | CLA | O2D-CGD-CBD | 5.50 | 121.05 | 111.27 |
| 25 | 6 | 604 | CLA | O2D-CGD-CBD | 5.50 | 121.05 | 111.27 |
| 25 | B | 1229 | CLA | CMD-C2D-C1D | 5.50 | 134.41 | 124.71 |
| 25 | 3 | 605 | CLA | CMD-C2D-C1D | 5.50 | 134.41 | 124.71 |
| 25 | 2 | 606 | CLA | CMD-C2D-C1D | 5.50 | 134.41 | 124.71 |
| 25 | A | 1105 | CLA | CMD-C2D-C1D | 5.50 | 134.41 | 124.71 |
| 25 | G | 1602 | CLA | CMD-C2D-C1D | 5.50 | 134.41 | 124.71 |
| 25 | A | 1138 | CLA | CMD-C2D-C1D | 5.50 | 134.40 | 124.71 |
| 25 | A | 1121 | CLA | O2D-CGD-CBD | 5.50 | 121.03 | 111.27 |
| 25 | A | 1134 | CLA | CMD-C2D-C1D | 5.50 | 134.40 | 124.71 |
| 25 | O | 1803 | CLA | CMD-C2D-C1D | 5.50 | 134.40 | 124.71 |
| 25 | 5 | 606 | CLA | CMD-C2D-C1D | 5.49 | 134.40 | 124.71 |
| 25 | A | 1125 | CLA | CMD-C2D-C1D | 5.49 | 134.39 | 124.71 |
| 25 | K | 1402 | CLA | O2A-C1-C2 | 5.49 | 123.07 | 108.64 |
| 25 | A | 1102 | CLA | CMD-C2D-C1D | 5.49 | 134.39 | 124.71 |
| 25 | 4 | 611 | CLA | CMD-C2D-C1D | 5.49 | 134.39 | 124.71 |
| 25 | B | 1225 | CLA | O2A-C1-C2 | 5.49 | 123.06 | 108.64 |
| 25 | 7 | 603 | CLA | CMD-C2D-C1D | 5.49 | 134.38 | 124.71 |
| 25 | K | 1404 | CLA | CMD-C2D-C1D | 5.49 | 134.38 | 124.71 |
| 25 | G | 1603 | CLA | CMD-C2D-C1D | 5.49 | 134.38 | 124.71 |
| 25 | A | 1103 | CLA | CMD-C2D-C1D | 5.48 | 134.38 | 124.71 |
| 25 | B | 1238 | CLA | CMD-C2D-C1D | 5.48 | 134.37 | 124.71 |
| 25 | A | 1140 | CLA | CMD-C2D-C1D | 5.48 | 134.37 | 124.71 |
| 25 | 9 | 606 | CLA | CMD-C2D-C1D | 5.48 | 134.37 | 124.71 |
| 25 | 3 | 606 | CLA | CMD-C2D-C1D | 5.48 | 134.37 | 124.71 |
| 25 | 3 | 610 | CLA | CMD-C2D-C1D | 5.48 | 134.37 | 124.71 |
| 25 | H | 1703 | CLA | O2A-C1-C2 | 5.48 | 123.03 | 108.64 |
| 25 | 9 | 609 | CLA | CMD-C2D-C1D | 5.48 | 134.37 | 124.71 |
| 25 | B | 1221 | CLA | CMD-C2D-C1D | 5.47 | 134.36 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 7 | 605 | CLA | CMD-C2D-C1D | 5.47 | 134.36 | 124.71 |
| 25 | L | 1503 | CLA | CMD-C2D-C1D | 5.47 | 134.36 | 124.71 |
| 25 | L | 1503 | CLA | O2D-CGD-CBD | 5.47 | 120.99 | 111.27 |
| 25 | B | 1222 | CLA | CMD-C2D-C1D | 5.47 | 134.36 | 124.71 |
| 25 | 8 | 606 | CLA | CMD-C2D-C1D | 5.47 | 134.35 | 124.71 |
| 25 | A | 1130 | CLA | CMD-C2D-C1D | 5.47 | 134.35 | 124.71 |
| 25 | B | 1229 | CLA | O2D-CGD-CBD | 5.47 | 120.99 | 111.27 |
| 25 | 2 | 601 | CLA | CMD-C2D-C1D | 5.47 | 134.35 | 124.71 |
| 25 | 2 | 603 | CLA | CMD-C2D-C1D | 5.47 | 134.35 | 124.71 |
| 25 | A | 1122 | CLA | CMD-C2D-C1D | 5.47 | 134.35 | 124.71 |
| 25 | B | 1217 | CLA | O2D-CGD-CBD | 5.46 | 120.98 | 111.27 |
| 25 | L | 1504 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | B | 1202 | CLA | O2D-CGD-CBD | 5.46 | 120.97 | 111.27 |
| 25 | B | 1213 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | B | 1239 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | A | 1116 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | K | 1403 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | B | 1216 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | F | 1301 | CLA | CMD-C2D-C1D | 5.46 | 134.34 | 124.71 |
| 25 | 4 | 616 | CLA | CMD-C2D-C1D | 5.46 | 134.33 | 124.71 |
| 25 | a | 611 | CLA | CMD-C2D-C1D | 5.45 | 134.32 | 124.71 |
| 25 | B | 1208 | CLA | CMD-C2D-C1D | 5.45 | 134.32 | 124.71 |
| 50 | 2 | 501 | XAT | C38-C25-C24 | 5.45 | 120.41 | 114.28 |
| 25 | H | 1703 | CLA | CMD-C2D-C1D | 5.45 | 134.32 | 124.71 |
| 25 | B | 1223 | CLA | CMD-C2D-C1D | 5.45 | 134.31 | 124.71 |
| 25 | 8 | 611 | CLA | CMD-C2D-C1D | 5.45 | 134.31 | 124.71 |
| 25 | B | 1220 | CLA | CMD-C2D-C1D | 5.44 | 134.31 | 124.71 |
| 25 | 1 | 612 | CLA | CMD-C2D-C1D | 5.44 | 134.31 | 124.71 |
| 25 | B | 1210 | CLA | CMD-C2D-C1D | 5.44 | 134.30 | 124.71 |
| 25 | H | 1702 | CLA | CMD-C2D-C1D | 5.44 | 134.30 | 124.71 |
| 25 | B | 1224 | CLA | CMD-C2D-C1D | 5.44 | 134.30 | 124.71 |
| 25 | 1 | 607 | CLA | CMD-C2D-C1D | 5.44 | 134.30 | 124.71 |
| 25 | 8 | 615 | CLA | CMD-C2D-C1D | 5.44 | 134.30 | 124.71 |
| 25 | L | 1501 | CLA | CMD-C2D-C1D | 5.44 | 134.30 | 124.71 |
| 25 | B | 1214 | CLA | CMD-C2D-C1D | 5.44 | 134.29 | 124.71 |
| 25 | A | 1135 | CLA | CMD-C2D-C1D | 5.43 | 134.29 | 124.71 |
| 25 | A | 1137 | CLA | CMD-C2D-C1D | 5.43 | 134.29 | 124.71 |
| 25 | H | 1701 | CLA | CMD-C2D-C1D | 5.43 | 134.29 | 124.71 |
| 40 | J | 4002 | RRX | C24-C23-C22 | -5.43 | 118.02 | 126.23 |
| 25 | B | 1235 | CLA | CMD-C2D-C1D | 5.43 | 134.29 | 124.71 |
| 25 | 3 | 610 | CLA | O2D-CGD-CBD | 5.43 | 120.92 | 111.27 |
| 25 | A | 1117 | CLA | CMD-C2D-C1D | 5.43 | 134.28 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1129 | CLA | CMD-C2D-C1D | 5.43 | 134.28 | 124.71 |
| 25 | B | 1227 | CLA | O2A-C1-C2 | 5.43 | 122.91 | 108.64 |
| 25 | O | 1802 | CLA | O2A-C1-C2 | 5.42 | 122.89 | 108.64 |
| 25 | 3 | 613 | CLA | O2D-CGD-CBD | 5.42 | 120.91 | 111.27 |
| 25 | 3 | 612 | CLA | CMD-C2D-C1D | 5.42 | 134.27 | 124.71 |
| 25 | A | 1139 | CLA | CMD-C2D-C1D | 5.42 | 134.27 | 124.71 |
| 25 | 1 | 603 | CLA | CMD-C2D-C1D | 5.42 | 134.27 | 124.71 |
| 25 | 7 | 602 | CLA | CMD-C2D-C1D | 5.42 | 134.27 | 124.71 |
| 25 | B | 1232 | CLA | CMD-C2D-C1D | 5.42 | 134.27 | 124.71 |
| 25 | A | 1110 | CLA | CMD-C2D-C1D | 5.42 | 134.26 | 124.71 |
| 25 | B | 1207 | CLA | CMD-C2D-C1D | 5.42 | 134.26 | 124.71 |
| 25 | A | 1112 | CLA | O2A-C1-C2 | 5.42 | 122.87 | 108.64 |
| 25 | K | 1403 | CLA | O2A-C1-C2 | 5.41 | 121.63 | 108.97 |
| 25 | K | 1402 | CLA | CMD-C2D-C1D | 5.41 | 134.25 | 124.71 |
| 25 | 7 | 610 | CLA | CMD-C2D-C1D | 5.41 | 134.25 | 124.71 |
| 25 | A | 1108 | CLA | CMD-C2D-C1D | 5.41 | 134.25 | 124.71 |
| 46 | a | 504 | QTB | C04-C03-C02 | 5.41 | 135.03 | 127.31 |
| 25 | A | 1104 | CLA | CMD-C2D-C1D | 5.40 | 134.24 | 124.71 |
| 25 | a | 601 | CLA | O2A-C1-C2 | 5.40 | 122.82 | 108.64 |
| 25 | J | 1901 | CLA | CMD-C2D-C1D | 5.40 | 134.23 | 124.71 |
| 25 | 8 | 608 | CLA | CMD-C2D-C1D | 5.40 | 134.23 | 124.71 |
| 25 | A | 1115 | CLA | O2A-C1-C2 | 5.40 | 122.82 | 108.64 |
| 25 | 4 | 604 | CLA | O2D-CGD-CBD | 5.40 | 120.86 | 111.27 |
| 25 | 4 | 601 | CLA | CMD-C2D-C1D | 5.40 | 134.22 | 124.71 |
| 25 | B | 1208 | CLA | O2A-C1-C2 | 5.39 | 122.81 | 108.64 |
| 25 | B | 1235 | CLA | O2A-C1-C2 | 5.39 | 122.80 | 108.64 |
| 43 | 6 | 501 | LUT | C21-C26-C25 | 5.39 | 121.07 | 111.42 |
| 25 | B | 1240 | CLA | O2A-C1-C2 | 5.39 | 122.80 | 108.64 |
| 25 | B | 1212 | CLA | CMD-C2D-C1D | 5.39 | 134.21 | 124.71 |
| 25 | 4 | 602 | CLA | O2D-CGD-CBD | 5.39 | 120.84 | 111.27 |
| 25 | B | 1202 | CLA | CMD-C2D-C1D | 5.39 | 134.21 | 124.71 |
| 25 | 1 | 602 | CLA | CMD-C2D-C1D | 5.39 | 134.21 | 124.71 |
| 25 | 2 | 605 | CLA | O2A-C1-C2 | 5.39 | 122.79 | 108.64 |
| 25 | A | 1107 | CLA | CMD-C2D-C1D | 5.38 | 134.20 | 124.71 |
| 25 | 8 | 602 | CLA | O2D-CGD-CBD | 5.38 | 120.83 | 111.27 |
| 25 | A | 1119 | CLA | CMD-C2D-C1D | 5.38 | 134.20 | 124.71 |
| 25 | a | 608 | CLA | CMD-C2D-C1D | 5.38 | 134.19 | 124.71 |
| 25 | 9 | 604 | CLA | O2D-CGD-CBD | 5.38 | 120.82 | 111.27 |
| 25 | 6 | 603 | CLA | CMD-C2D-C1D | 5.38 | 134.19 | 124.71 |
| 25 | 8 | 609 | CLA | CMD-C2D-C1D | 5.38 | 134.19 | 124.71 |
| 25 | A | 1136 | CLA | O2A-C1-C2 | 5.37 | 122.76 | 108.64 |
| 25 | B | 1235 | CLA | O2D-CGD-CBD | 5.37 | 120.82 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1110 | CLA | O2D-CGD-CBD | 5.37 | 120.81 | 111.27 |
| 25 | 6 | 615 | CLA | O2D-CGD-CBD | 5.37 | 120.81 | 111.27 |
| 25 | B | 1209 | CLA | O2D-CGD-CBD | 5.36 | 120.80 | 111.27 |
| 25 | 5 | 603 | CLA | O2A-C1-C2 | 5.36 | 122.73 | 108.64 |
| 25 | A | 1013 | CLA | O2A-C1-C2 | 5.36 | 122.72 | 108.64 |
| 25 | 5 | 606 | CLA | O2A-C1-C2 | 5.36 | 122.72 | 108.64 |
| 25 | B | 1227 | CLA | CMD-C2D-C1D | 5.36 | 134.15 | 124.71 |
| 25 | B | 1236 | CLA | CMD-C2D-C1D | 5.36 | 134.15 | 124.71 |
| 25 | B | 1231 | CLA | O2D-CGD-CBD | 5.36 | 120.78 | 111.27 |
| 25 | A | 1128 | CLA | O2A-C1-C2 | 5.35 | 122.70 | 108.64 |
| 25 | 3 | 607 | CLA | CMD-C2D-C1D | 5.35 | 134.14 | 124.71 |
| 25 | 6 | 618 | CLA | CMD-C2D-C1D | 5.35 | 134.14 | 124.71 |
| 25 | 8 | 608 | CLA | O2D-CGD-CBD | 5.35 | 120.77 | 111.27 |
| 25 | 3 | 613 | CLA | CMD-C2D-C1D | 5.35 | 134.14 | 124.71 |
| 25 | a | 612 | CLA | CMD-C2D-C1D | 5.35 | 134.14 | 124.71 |
| 25 | 2 | 608 | CLA | CMD-C2D-C1D | 5.35 | 134.14 | 124.71 |
| 25 | A | 1125 | CLA | O2A-C1-C2 | 5.35 | 122.69 | 108.64 |
| 25 | A | 1112 | CLA | CMD-C2D-C1D | 5.35 | 134.13 | 124.71 |
| 25 | A | 1131 | CLA | CMD-C2D-C1D | 5.34 | 134.13 | 124.71 |
| 25 | 5 | 615 | CLA | CMD-C2D-C1D | 5.34 | 134.13 | 124.71 |
| 25 | 1 | 615 | CLA | CMD-C2D-C1D | 5.34 | 134.13 | 124.71 |
| 25 | B | 1021 | CLA | O2D-CGD-CBD | 5.34 | 120.76 | 111.27 |
| 25 | B | 1230 | CLA | CMD-C2D-C1D | 5.34 | 134.13 | 124.71 |
| 25 | 2 | 621 | CLA | CMD-C2D-C1D | 5.34 | 134.12 | 124.71 |
| 25 | 2 | 602 | CLA | O2A-C1-C2 | 5.34 | 122.66 | 108.64 |
| 25 | 7 | 604 | CLA | O2D-CGD-CBD | 5.33 | 120.75 | 111.27 |
| 25 | 9 | 607 | CLA | CMD-C2D-C1D | 5.33 | 134.11 | 124.71 |
| 25 | 3 | 618 | CLA | CMD-C2D-C1D | 5.33 | 134.11 | 124.71 |
| 25 | 3 | 605 | CLA | O2A-C1-C2 | 5.33 | 122.64 | 108.64 |
| 25 | 2 | 612 | CLA | CMD-C2D-C1D | 5.33 | 134.10 | 124.71 |
| 25 | 1 | 606 | CLA | O2A-C1-C2 | 5.33 | 122.63 | 108.64 |
| 25 | A | 1105 | CLA | O2D-CGD-CBD | 5.32 | 120.73 | 111.27 |
| 25 | B | 1204 | CLA | CMD-C2D-C1D | 5.32 | 134.09 | 124.71 |
| 25 | 2 | 607 | CLA | CMD-C2D-C1D | 5.32 | 134.09 | 124.71 |
| 25 | 8 | 618 | CLA | O2D-CGD-CBD | 5.32 | 120.72 | 111.27 |
| 25 | 4 | 602 | CLA | CMD-C2D-C1D | 5.32 | 134.08 | 124.71 |
| 25 | 6 | 602 | CLA | CMD-C2D-C1D | 5.31 | 134.07 | 124.71 |
| 25 | 7 | 610 | CLA | O2A-C1-C2 | 5.30 | 122.58 | 108.64 |
| 25 | 5 | 609 | CLA | CMD-C2D-C1D | 5.30 | 134.06 | 124.71 |
| 25 | B | 1022 | CLA | CMD-C2D-C1D | 5.30 | 134.06 | 124.71 |
| 25 | B | 1205 | CLA | CMD-C2D-C1D | 5.30 | 134.06 | 124.71 |
| 25 | 5 | 612 | CLA | CMD-C2D-C1D | 5.30 | 134.06 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | a | 607 | CLA | CMD-C2D-C1D | 5.29 | 134.04 | 124.71 |
| 25 | F | 1302 | CLA | O2A-C1-C2 | 5.29 | 122.54 | 108.64 |
| 25 | A | 1118 | CLA | CMD-C2D-C1D | 5.29 | 134.04 | 124.71 |
| 25 | B | 1201 | CLA | O2A-C1-C2 | 5.29 | 122.54 | 108.64 |
| 25 | 9 | 606 | CLA | O2D-CGD-CBD | 5.29 | 120.67 | 111.27 |
| 25 | 3 | 616 | CLA | CMD-C2D-C1D | 5.29 | 134.03 | 124.71 |
| 25 | A | 1135 | CLA | O2A-C1-C2 | 5.28 | 122.52 | 108.64 |
| 25 | L | 1502 | CLA | O2D-CGD-CBD | 5.28 | 120.65 | 111.27 |
| 25 | 2 | 621 | CLA | O2D-CGD-CBD | 5.28 | 120.65 | 111.27 |
| 25 | A | 1133 | CLA | O2A-C1-C2 | 5.28 | 122.51 | 108.64 |
| 25 | 4 | 607 | CLA | CMD-C2D-C1D | 5.28 | 134.01 | 124.71 |
| 25 | a | 602 | CLA | CMD-C2D-C1D | 5.28 | 134.01 | 124.71 |
| 25 | 3 | 606 | CLA | O2A-C1-C2 | 5.27 | 122.49 | 108.64 |
| 25 | 7 | 601 | CLA | O2A-C1-C2 | 5.27 | 122.49 | 108.64 |
| 25 | B | 1201 | CLA | CMD-C2D-C1D | 5.27 | 134.00 | 124.71 |
| 40 | J | 4002 | RRX | C7-C8-C9 | -5.27 | 118.27 | 126.23 |
| 25 | 9 | 609 | CLA | O2D-CGD-CBD | 5.27 | 120.63 | 111.27 |
| 25 | B | 1237 | CLA | CMD-C2D-C1D | 5.27 | 134.00 | 124.71 |
| 25 | 7 | 606 | CLA | O2A-C1-C2 | 5.27 | 122.48 | 108.64 |
| 25 | A | 1107 | CLA | O2D-CGD-CBD | 5.27 | 120.63 | 111.27 |
| 25 | 3 | 602 | CLA | O2D-CGD-CBD | 5.27 | 120.62 | 111.27 |
| 25 | 5 | 614 | CLA | CMD-C2D-C1D | 5.27 | 133.99 | 124.71 |
| 25 | 6 | 602 | CLA | O2D-CGD-CBD | 5.26 | 120.62 | 111.27 |
| 25 | a | 607 | CLA | O2D-CGD-CBD | 5.26 | 120.62 | 111.27 |
| 25 | B | 1212 | CLA | O2A-C1-C2 | 5.26 | 122.46 | 108.64 |
| 25 | A | 1139 | CLA | O2D-CGD-CBD | 5.26 | 120.61 | 111.27 |
| 25 | K | 1403 | CLA | O2D-CGD-CBD | 5.25 | 120.61 | 111.27 |
| 25 | B | 1215 | CLA | O2D-CGD-CBD | 5.25 | 120.60 | 111.27 |
| 24 | A | 1011 | CL0 | O2A-CGA-O1A | -5.25 | 110.34 | 123.59 |
| 25 | A | 1137 | CLA | O2D-CGD-CBD | 5.25 | 120.60 | 111.27 |
| 25 | 9 | 605 | CLA | O2D-CGD-CBD | 5.25 | 120.59 | 111.27 |
| 25 | 9 | 602 | CLA | CMD-C2D-C1D | 5.24 | 133.96 | 124.71 |
| 25 | K | 1402 | CLA | O2D-CGD-CBD | 5.24 | 120.59 | 111.27 |
| 25 | 9 | 612 | CLA | CMD-C2D-C1D | 5.24 | 133.95 | 124.71 |
| 44 | 7 | 504 | AXT | C40-C33-C34 | -5.24 | 115.58 | 122.92 |
| 25 | 3 | 601 | CLA | CMD-C2D-C1D | 5.24 | 133.95 | 124.71 |
| 25 | A | 1132 | CLA | O2A-C1-C2 | 5.24 | 122.40 | 108.64 |
| 25 | 4 | 615 | CLA | O2A-C1-C2 | 5.24 | 122.40 | 108.64 |
| 25 | 8 | 612 | CLA | CMD-C2D-C1D | 5.23 | 133.94 | 124.71 |
| 25 | B | 1234 | CLA | O2A-C1-C2 | 5.23 | 122.38 | 108.64 |
| 25 | 7 | 608 | CLA | CMD-C2D-C1D | 5.23 | 133.93 | 124.71 |
| 25 | 5 | 607 | CLA | CMD-C2D-C1D | 5.23 | 133.93 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 607 | CLA | O2D-CGD-CBD | 5.23 | 120.56 | 111.27 |
| 25 | B | 1219 | CLA | CMD-C2D-C1D | 5.23 | 133.93 | 124.71 |
| 25 | 6 | 605 | CLA | O2D-CGD-CBD | 5.22 | 120.55 | 111.27 |
| 25 | A | 1117 | CLA | O2A-C1-C2 | 5.22 | 122.36 | 108.64 |
| 46 | a | 504 | QTB | C13-C12-C11 | 5.22 | 122.90 | 112.60 |
| 43 | 5 | 505 | LUT | C15-C14-C13 | -5.22 | 119.86 | 127.31 |
| 25 | F | 1301 | CLA | O2A-C1-C2 | 5.22 | 122.35 | 108.64 |
| 25 | A | 1124 | CLA | CMD-C2D-C1D | 5.22 | 133.91 | 124.71 |
| 25 | 2 | 606 | CLA | O2D-CGD-CBD | 5.22 | 120.54 | 111.27 |
| 25 | B | 1211 | CLA | O2A-C1-C2 | 5.22 | 122.35 | 108.64 |
| 25 | B | 1218 | CLA | O2A-C1-C2 | 5.22 | 122.35 | 108.64 |
| 25 | F | 1302 | CLA | CMD-C2D-C1D | 5.22 | 133.91 | 124.71 |
| 44 | 1 | 502 | AXT | C1-C6-C5 | -5.22 | 115.27 | 122.61 |
| 25 | 6 | 615 | CLA | CMD-C2D-C1D | 5.21 | 133.90 | 124.71 |
| 25 | 2 | 601 | CLA | O2D-CGD-CBD | 5.21 | 120.53 | 111.27 |
| 25 | 4 | 601 | CLA | O2D-CGD-CBD | 5.21 | 120.53 | 111.27 |
| 25 | A | 1133 | CLA | CMD-C2D-C1D | 5.21 | 133.89 | 124.71 |
| 25 | B | 1240 | CLA | CMD-C2D-C1D | 5.21 | 133.89 | 124.71 |
| 25 | B | 1234 | CLA | O2D-CGD-CBD | 5.20 | 120.51 | 111.27 |
| 42 | M | 4001 | ECH | C20-C21-C22 | -5.20 | 119.89 | 127.31 |
| 25 | A | 1111 | CLA | O2D-CGD-CBD | 5.20 | 120.51 | 111.27 |
| 25 | 4 | 611 | CLA | O2A-C1-C2 | 5.19 | 122.29 | 108.64 |
| 25 | 4 | 601 | CLA | O2A-C1-C2 | 5.19 | 122.27 | 108.64 |
| 25 | 5 | 605 | CLA | O2D-CGD-CBD | 5.19 | 120.49 | 111.27 |
| 25 | 5 | 601 | CLA | O2D-CGD-CBD | 5.19 | 120.48 | 111.27 |
| 43 | 5 | 505 | LUT | C11-C10-C9 | -5.19 | 119.91 | 127.31 |
| 25 | B | 1226 | CLA | O2D-CGD-CBD | 5.19 | 120.48 | 111.27 |
| 25 | 7 | 608 | CLA | O2D-CGD-CBD | 5.18 | 120.48 | 111.27 |
| 25 | 6 | 608 | CLA | O2D-CGD-CBD | 5.18 | 120.48 | 111.27 |
| 25 | 6 | 607 | CLA | CMD-C2D-C1D | 5.18 | 133.85 | 124.71 |
| 25 | K | 1404 | CLA | O2D-CGD-CBD | 5.18 | 120.47 | 111.27 |
| 25 | B | 1215 | CLA | CMD-C2D-C1D | 5.18 | 133.84 | 124.71 |
| 25 | a | 611 | CLA | O2D-CGD-CBD | 5.18 | 120.46 | 111.27 |
| 25 | B | 1225 | CLA | CMD-C2D-C1D | 5.17 | 133.83 | 124.71 |
| 25 | 2 | 603 | CLA | O2A-C1-C2 | 5.17 | 122.21 | 108.64 |
| 25 | B | 1204 | CLA | O2D-CGD-CBD | 5.16 | 120.44 | 111.27 |
| 26 | a | 604 | CHL | C1-C2-C3 | -5.16 | 117.11 | 126.04 |
| 42 | M | 4001 | ECH | C11-C10-C9 | -5.16 | 119.94 | 127.31 |
| 25 | 4 | 607 | CLA | O2A-C1-C2 | 5.16 | 122.20 | 108.64 |
| 25 | 5 | 602 | CLA | O2A-C1-C2 | 5.16 | 122.20 | 108.64 |
| 25 | A | 1134 | CLA | O2A-C1-C2 | 5.16 | 122.19 | 108.64 |
| 25 | A | 1120 | CLA | CMD-C2D-C1D | 5.16 | 133.80 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | G | 1602 | CLA | O2A-C1-C2 | 5.16 | 122.19 | 108.64 |
| 25 | 1 | 612 | CLA | O2A-C1-C2 | 5.16 | 122.18 | 108.64 |
| 25 | A | 1121 | CLA | O2A-C1-C2 | 5.15 | 122.18 | 108.64 |
| 25 | B | 1224 | CLA | O2D-CGD-CBD | 5.15 | 120.43 | 111.27 |
| 25 | B | 1214 | CLA | O2D-CGD-CBD | 5.15 | 120.42 | 111.27 |
| 25 | 2 | 605 | CLA | O2D-CGD-CBD | 5.15 | 120.42 | 111.27 |
| 25 | 5 | 602 | CLA | CMD-C2D-C1D | 5.15 | 133.79 | 124.71 |
| 25 | B | 1206 | CLA | O2A-C1-C2 | 5.15 | 122.17 | 108.64 |
| 25 | A | 1131 | CLA | O2D-CGD-CBD | 5.15 | 120.41 | 111.27 |
| 25 | 6 | 601 | CLA | O2D-CGD-CBD | 5.15 | 120.41 | 111.27 |
| 25 | a | 608 | CLA | O2A-C1-C2 | 5.14 | 122.15 | 108.64 |
| 43 | 1 | 503 | LUT | C21-C26-C27 | 5.14 | 119.20 | 112.70 |
| 25 | 5 | 602 | CLA | O2D-CGD-CBD | 5.14 | 120.41 | 111.27 |
| 25 | 4 | 612 | CLA | CMD-C2D-C1D | 5.14 | 133.78 | 124.71 |
| 25 | A | 1104 | CLA | O2D-CGD-CBD | 5.14 | 120.40 | 111.27 |
| 43 | 2 | 507 | LUT | C35-C34-C33 | -5.14 | 119.97 | 127.31 |
| 25 | G | 1601 | CLA | CMD-C2D-C1D | 5.14 | 133.77 | 124.71 |
| 25 | 6 | 603 | CLA | O2D-CGD-CBD | 5.14 | 120.40 | 111.27 |
| 25 | 7 | 602 | CLA | O2D-CGD-CBD | 5.14 | 120.39 | 111.27 |
| 25 | A | 1135 | CLA | O2D-CGD-CBD | 5.14 | 120.39 | 111.27 |
| 25 | 1 | 608 | CLA | CMD-C2D-C1D | 5.14 | 133.76 | 124.71 |
| 25 | 8 | 609 | CLA | O2A-C1-C2 | 5.13 | 122.13 | 108.64 |
| 50 | 7 | 502 | XAT | C31-C30-C29 | -5.13 | 119.98 | 127.31 |
| 50 | 2 | 501 | XAT | C31-C30-C29 | -5.13 | 119.98 | 127.31 |
| 25 | 4 | 605 | CLA | O2D-CGD-CBD | 5.13 | 120.39 | 111.27 |
| 25 | 7 | 607 | CLA | CMD-C2D-C1D | 5.13 | 133.75 | 124.71 |
| 25 | A | 1113 | CLA | O2A-C1-C2 | 5.13 | 122.11 | 108.64 |
| 25 | G | 1603 | CLA | O2D-CGD-CBD | 5.13 | 120.38 | 111.27 |
| 25 | 4 | 615 | CLA | CMD-C2D-C1D | 5.13 | 133.75 | 124.71 |
| 25 | 3 | 616 | CLA | O2A-C1-C2 | 5.13 | 122.11 | 108.64 |
| 46 | a | 504 | QTB | C01-C02-C09 | -5.13 | 110.00 | 118.08 |
| 25 | 2 | 602 | CLA | CMD-C2D-C1D | 5.12 | 133.75 | 124.71 |
| 25 | A | 1123 | CLA | CMD-C2D-C1D | 5.12 | 133.74 | 124.71 |
| 25 | A | 1140 | CLA | O2A-C1-C2 | 5.12 | 122.09 | 108.64 |
| 25 | 3 | 616 | CLA | O2D-CGD-CBD | 5.12 | 120.36 | 111.27 |
| 25 | B | 1204 | CLA | O2A-C1-C2 | 5.11 | 122.07 | 108.64 |
| 25 | A | 1136 | CLA | O2D-CGD-CBD | 5.11 | 120.35 | 111.27 |
| 44 | 7 | 504 | AXT | C19-C9-C10 | -5.11 | 115.76 | 122.92 |
| 25 | B | 1207 | CLA | O2D-CGD-CBD | 5.11 | 120.35 | 111.27 |
| 25 | 5 | 607 | CLA | O2A-C1-C2 | 5.11 | 122.06 | 108.64 |
| 25 | A | 1116 | CLA | O2D-CGD-CBD | 5.11 | 120.34 | 111.27 |
| 25 | a | 607 | CLA | O2A-C1-C2 | 5.11 | 122.06 | 108.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 607 | CLA | O2D-CGD-CBD | 5.11 | 120.34 | 111.27 |
| 25 | 5 | 604 | CLA | O2D-CGD-CBD | 5.10 | 120.34 | 111.27 |
| 25 | A | 1140 | CLA | O2D-CGD-CBD | 5.10 | 120.33 | 111.27 |
| 25 | B | 1239 | CLA | O2D-CGD-CBD | 5.10 | 120.33 | 111.27 |
| 25 | 6 | 601 | CLA | O2A-C1-C2 | 5.09 | 122.02 | 108.64 |
| 25 | 4 | 607 | CLA | O2D-CGD-CBD | 5.09 | 120.31 | 111.27 |
| 25 | B | 1239 | CLA | O2A-C1-C2 | 5.09 | 122.01 | 108.64 |
| 25 | 7 | 603 | CLA | O2D-CGD-CBD | 5.09 | 120.31 | 111.27 |
| 25 | A | 1126 | CLA | O2D-CGD-CBD | 5.09 | 120.31 | 111.27 |
| 25 | 8 | 607 | CLA | CMD-C2D-C1D | 5.09 | 133.68 | 124.71 |
| 25 | A | 1127 | CLA | O2A-C1-C2 | 5.09 | 122.00 | 108.64 |
| 25 | H | 1703 | CLA | O2D-CGD-CBD | 5.09 | 120.30 | 111.27 |
| 25 | A | 1105 | CLA | O2A-C1-C2 | 5.08 | 121.99 | 108.64 |
| 25 | B | 1224 | CLA | O2A-C1-C2 | 5.08 | 121.98 | 108.64 |
| 25 | 3 | 612 | CLA | O2D-CGD-CBD | 5.08 | 120.29 | 111.27 |
| 50 | 7 | 502 | XAT | C38-C25-C24 | 5.07 | 119.99 | 114.28 |
| 25 | B | 1023 | CLA | CMD-C2D-C1D | 5.07 | 133.65 | 124.71 |
| 43 | 1 | 503 | LUT | C21-C26-C25 | 5.07 | 120.50 | 111.42 |
| 25 | A | 1122 | CLA | O2A-C1-C2 | 5.07 | 121.96 | 108.64 |
| 25 | B | 1238 | CLA | O2D-CGD-CBD | 5.07 | 120.27 | 111.27 |
| 25 | B | 1236 | CLA | O2D-CGD-CBD | 5.07 | 120.27 | 111.27 |
| 25 | 4 | 608 | CLA | CMD-C2D-C1D | 5.07 | 133.64 | 124.71 |
| 25 | 7 | 612 | CLA | CMD-C2D-C1D | 5.06 | 133.64 | 124.71 |
| 25 | 3 | 613 | CLA | O2A-C1-C2 | 5.06 | 121.94 | 108.64 |
| 25 | 2 | 602 | CLA | O2D-CGD-CBD | 5.06 | 120.26 | 111.27 |
| 25 | B | 1022 | CLA | O2A-C1-C2 | 5.06 | 121.94 | 108.64 |
| 50 | 9 | 504 | XAT | C31-C30-C29 | -5.06 | 120.09 | 127.31 |
| 25 | 3 | 618 | CLA | O2D-CGD-CBD | 5.06 | 120.26 | 111.27 |
| 40 | 3 | 506 | RRX | C24-C23-C22 | -5.06 | 118.60 | 126.23 |
| 25 | B | 1219 | CLA | O2D-CGD-CBD | 5.06 | 120.25 | 111.27 |
| 25 | B | 1213 | CLA | O2A-C1-C2 | 5.05 | 121.92 | 108.64 |
| 25 | 8 | 608 | CLA | O2A-C1-C2 | 5.05 | 121.92 | 108.64 |
| 25 | 5 | 614 | CLA | O2D-CGD-CBD | 5.05 | 120.25 | 111.27 |
| 50 | 9 | 507 | XAT | C38-C25-C24 | 5.05 | 119.96 | 114.28 |
| 25 | 1 | 602 | CLA | O2D-CGD-CBD | 5.05 | 120.24 | 111.27 |
| 25 | 9 | 602 | CLA | O2D-CGD-CBD | 5.05 | 120.24 | 111.27 |
| 40 | J | 4002 | RRX | C11-C10-C9 | -5.05 | 120.11 | 127.31 |
| 25 | B | 1213 | CLA | O2D-CGD-CBD | 5.05 | 120.24 | 111.27 |
| 25 | A | 1106 | CLA | O2A-C1-C2 | 5.04 | 121.89 | 108.64 |
| 25 | 8 | 606 | CLA | O2A-C1-C2 | 5.04 | 121.88 | 108.64 |
| 25 | 6 | 615 | CLA | O2A-C1-C2 | 5.04 | 121.88 | 108.64 |
| 25 | A | 1130 | CLA | O2D-CGD-CBD | 5.04 | 120.22 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1220 | CLA | O2A-C1-C2 | 5.04 | 121.87 | 108.64 |
| 25 | 5 | 601 | CLA | O2A-C1-C2 | 5.04 | 121.87 | 108.64 |
| 25 | B | 1228 | CLA | O2D-CGD-CBD | 5.03 | 120.22 | 111.27 |
| 25 | J | 1901 | CLA | O2D-CGD-CBD | 5.03 | 120.22 | 111.27 |
| 25 | B | 1219 | CLA | O2A-C1-C2 | 5.03 | 121.87 | 108.64 |
| 25 | L | 1501 | CLA | O2D-CGD-CBD | 5.03 | 120.21 | 111.27 |
| 25 | B | 1203 | CLA | O2A-C1-C2 | 5.03 | 121.85 | 108.64 |
| 25 | G | 1601 | CLA | O2A-C1-C2 | 5.03 | 121.85 | 108.64 |
| 25 | A | 1124 | CLA | O2D-CGD-CBD | 5.03 | 120.20 | 111.27 |
| 25 | B | 1234 | CLA | CHC-C1C-NC | -5.02 | 121.86 | 128.83 |
| 25 | 4 | 608 | CLA | O2A-C1-C2 | 5.02 | 121.84 | 108.64 |
| 25 | 6 | 612 | CLA | CMD-C2D-C1D | 5.02 | 133.56 | 124.71 |
| 25 | G | 1602 | CLA | O2D-CGD-CBD | 5.02 | 120.19 | 111.27 |
| 25 | A | 1111 | CLA | O2A-C1-C2 | 5.02 | 121.82 | 108.64 |
| 25 | 1 | 608 | CLA | O2A-C1-C2 | 5.02 | 121.82 | 108.64 |
| 25 | A | 1141 | CLA | O2D-CGD-CBD | 5.01 | 120.17 | 111.27 |
| 43 | 2 | 507 | LUT | C15-C14-C13 | -5.01 | 120.16 | 127.31 |
| 25 | 7 | 607 | CLA | O2D-CGD-CBD | 5.01 | 120.17 | 111.27 |
| 25 | a | 602 | CLA | O2D-CGD-CBD | 5.01 | 120.17 | 111.27 |
| 25 | 2 | 604 | CLA | O2D-CGD-CBD | 5.00 | 120.16 | 111.27 |
| 25 | 8 | 605 | CLA | O2D-CGD-CBD | 5.00 | 120.15 | 111.27 |
| 25 | 1 | 601 | CLA | O2A-C1-C2 | 5.00 | 121.77 | 108.64 |
| 25 | 9 | 612 | CLA | O2D-CGD-CBD | 5.00 | 120.15 | 111.27 |
| 43 | 3 | 502 | LUT | C21-C26-C27 | 4.99 | 119.01 | 112.70 |
| 25 | L | 1504 | CLA | O2A-C1-C2 | 4.99 | 121.76 | 108.64 |
| 25 | B | 1229 | CLA | O2A-C1-C2 | 4.99 | 121.76 | 108.64 |
| 25 | a | 612 | CLA | O2A-C1-C2 | 4.99 | 121.75 | 108.64 |
| 25 | a | 601 | CLA | O2D-CGD-CBD | 4.99 | 120.14 | 111.27 |
| 25 | L | 1501 | CLA | O2A-C1-C2 | 4.99 | 121.75 | 108.64 |
| 25 | 5 | 608 | CLA | O2D-CGD-CBD | 4.99 | 120.13 | 111.27 |
| 25 | A | 1104 | CLA | O2A-C1-C2 | 4.99 | 121.74 | 108.64 |
| 26 | 6 | 619 | CHL | C1-O2A-CGA | 4.98 | 129.52 | 116.44 |
| 25 | B | 1230 | CLA | O2A-C1-C2 | 4.98 | 121.73 | 108.64 |
| 25 | 4 | 604 | CLA | O2A-C1-C2 | 4.98 | 121.73 | 108.64 |
| 25 | B | 1022 | CLA | O2D-CGD-CBD | 4.98 | 120.12 | 111.27 |
| 25 | A | 1115 | CLA | CMD-C2D-C1D | 4.98 | 133.49 | 124.71 |
| 25 | B | 1205 | CLA | O2A-C1-C2 | 4.97 | 121.71 | 108.64 |
| 25 | 4 | 606 | CLA | O2A-C1-C2 | 4.97 | 121.70 | 108.64 |
| 25 | B | 1206 | CLA | CMD-C2D-C1D | 4.96 | 133.46 | 124.71 |
| 25 | 6 | 602 | CLA | O2A-C1-C2 | 4.96 | 121.67 | 108.64 |
| 25 | 7 | 612 | CLA | O2A-C1-C2 | 4.96 | 121.67 | 108.64 |
| 25 | 5 | 608 | CLA | CMD-C2D-C1D | 4.96 | 133.45 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 8 | 601 | CHL | C1-C2-C3 | -4.96 | 117.47 | 126.04 |
| 25 | 6 | 606 | CLA | O2A-C1-C2 | 4.96 | 121.66 | 108.64 |
| 25 | 6 | 612 | CLA | O2D-CGD-CBD | 4.96 | 120.07 | 111.27 |
| 40 | 3 | 506 | RRX | C7-C8-C9 | -4.95 | 118.75 | 126.23 |
| 25 | A | 1110 | CLA | O2A-C1-C2 | 4.95 | 121.65 | 108.64 |
| 25 | 5 | 606 | CLA | O2D-CGD-CBD | 4.95 | 120.07 | 111.27 |
| 25 | B | 1210 | CLA | O2A-C1-C2 | 4.95 | 121.64 | 108.64 |
| 25 | A | 1131 | CLA | O2A-C1-C2 | 4.95 | 121.64 | 108.64 |
| 25 | B | 1223 | CLA | O2A-C1-C2 | 4.95 | 121.63 | 108.64 |
| 25 | 4 | 611 | CLA | O2D-CGD-CBD | 4.95 | 120.06 | 111.27 |
| 25 | B | 1225 | CLA | O2D-CGD-CBD | 4.94 | 120.05 | 111.27 |
| 25 | L | 1502 | CLA | CMD-C2D-C1D | 4.94 | 133.43 | 124.71 |
| 25 | 4 | 616 | CLA | O2A-C1-C2 | 4.94 | 121.63 | 108.64 |
| 42 | M | 4001 | ECH | C15-C14-C13 | -4.94 | 120.26 | 127.31 |
| 25 | K | 1401 | CLA | O2D-CGD-CBD | 4.94 | 120.04 | 111.27 |
| 25 | 2 | 607 | CLA | O2A-C1-C2 | 4.94 | 121.61 | 108.64 |
| 25 | A | 1133 | CLA | O2D-CGD-CBD | 4.93 | 120.04 | 111.27 |
| 25 | a | 615 | CLA | O2D-CGD-CBD | 4.93 | 120.03 | 111.27 |
| 24 | A | 1011 | CL0 | O2D-CGD-CBD | 4.93 | 120.03 | 111.27 |
| 25 | 8 | 605 | CLA | O2A-C1-C2 | 4.93 | 121.59 | 108.64 |
| 25 | 8 | 615 | CLA | O2D-CGD-CBD | 4.93 | 120.02 | 111.27 |
| 25 | A | 1123 | CLA | O2A-C1-C2 | 4.93 | 121.58 | 108.64 |
| 25 | 3 | 606 | CLA | O2D-CGD-CBD | 4.93 | 120.02 | 111.27 |
| 25 | B | 1021 | CLA | O2A-C1-C2 | 4.93 | 121.58 | 108.64 |
| 25 | 1 | 601 | CLA | O2D-CGD-CBD | 4.92 | 120.01 | 111.27 |
| 25 | 5 | 609 | CLA | O2D-CGD-CBD | 4.91 | 120.00 | 111.27 |
| 25 | A | 1012 | CLA | O2D-CGD-CBD | 4.91 | 120.00 | 111.27 |
| 25 | B | 1206 | CLA | O2D-CGD-CBD | 4.91 | 119.99 | 111.27 |
| 30 | 2 | 802 | LHG | O7-C7-C8 | 4.91 | 122.08 | 111.50 |
| 25 | L | 1504 | CLA | O2D-CGD-CBD | 4.91 | 119.99 | 111.27 |
| 25 | 3 | 607 | CLA | O2D-CGD-CBD | 4.91 | 119.98 | 111.27 |
| 25 | B | 1023 | CLA | O2D-CGD-CBD | 4.90 | 119.98 | 111.27 |
| 25 | A | 1139 | CLA | O2A-C1-C2 | 4.90 | 121.52 | 108.64 |
| 25 | H | 1701 | CLA | O2A-C1-C2 | 4.90 | 121.52 | 108.64 |
| 25 | K | 1401 | CLA | CMD-C2D-C1D | 4.90 | 133.35 | 124.71 |
| 25 | B | 1222 | CLA | O2A-C1-C2 | 4.90 | 121.51 | 108.64 |
| 25 | 4 | 602 | CLA | O2A-C1-C2 | 4.90 | 121.50 | 108.64 |
| 25 | B | 1203 | CLA | O2D-CGD-CBD | 4.90 | 119.97 | 111.27 |
| 25 | H | 1701 | CLA | O2D-CGD-CBD | 4.89 | 119.96 | 111.27 |
| 25 | A | 1116 | CLA | O2A-C1-C2 | 4.89 | 121.49 | 108.64 |
| 25 | 1 | 615 | CLA | O2D-CGD-CBD | 4.89 | 119.96 | 111.27 |
| 25 | A | 1124 | CLA | O2A-C1-C2 | 4.89 | 121.48 | 108.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 612 | CLA | O2A-C1-C2 | 4.89 | 121.48 | 108.64 |
| 25 | 8 | 612 | CLA | O2A-C1-C2 | 4.87 | 121.44 | 108.64 |
| 25 | 2 | 612 | CLA | O2A-C1-C2 | 4.87 | 121.44 | 108.64 |
| 25 | 4 | 615 | CLA | O2D-CGD-CBD | 4.87 | 119.93 | 111.27 |
| 25 | B | 1237 | CLA | O2D-CGD-CBD | 4.87 | 119.92 | 111.27 |
| 25 | G | 1601 | CLA | O2D-CGD-CBD | 4.87 | 119.92 | 111.27 |
| 25 | B | 1216 | CLA | O2D-CGD-CBD | 4.87 | 119.92 | 111.27 |
| 25 | 6 | 607 | CLA | O2D-CGD-CBD | 4.87 | 119.92 | 111.27 |
| 25 | B | 1021 | CLA | CMD-C2D-C1D | 4.86 | 133.29 | 124.71 |
| 40 | J | 4002 | RRX | C16-C15-C14 | 4.86 | 133.44 | 123.47 |
| 25 | 3 | 610 | CLA | O2A-C1-C2 | 4.86 | 121.42 | 108.64 |
| 25 | A | 1107 | CLA | O2A-C1-C2 | 4.86 | 121.41 | 108.64 |
| 25 | 3 | 601 | CLA | O2D-CGD-CBD | 4.86 | 119.90 | 111.27 |
| 24 | A | 1011 | CL0 | O2A-C1-C2 | 4.86 | 121.41 | 108.64 |
| 25 | F | 1301 | CLA | O2D-CGD-CBD | 4.86 | 119.90 | 111.27 |
| 25 | 7 | 601 | CLA | O2D-CGD-CBD | 4.86 | 119.90 | 111.27 |
| 25 | B | 1234 | CLA | C4D-ND-C1D | -4.86 | 102.59 | 109.68 |
| 25 | A | 1103 | CLA | O2A-C1-C2 | 4.85 | 121.39 | 108.64 |
| 39 | F | 4001 | NEX | C17-C1-C2 | -4.85 | 87.28 | 109.05 |
| 25 | 4 | 610 | CLA | O2D-CGD-CBD | 4.85 | 119.88 | 111.27 |
| 25 | a | 605 | CLA | O2A-C1-C2 | 4.84 | 121.36 | 108.64 |
| 25 | B | 1226 | CLA | O2A-C1-C2 | 4.84 | 121.35 | 108.64 |
| 25 | 5 | 604 | CLA | O2A-C1-C2 | 4.83 | 121.34 | 108.64 |
| 25 | B | 1231 | CLA | O2A-C1-C2 | 4.83 | 121.34 | 108.64 |
| 25 | 5 | 603 | CLA | O2D-CGD-CBD | 4.83 | 119.86 | 111.27 |
| 25 | 1 | 603 | CLA | O2A-C1-C2 | 4.83 | 121.33 | 108.64 |
| 25 | 8 | 602 | CLA | O2A-C1-C2 | 4.83 | 121.33 | 108.64 |
| 25 | 5 | 612 | CLA | O2D-CGD-CBD | 4.83 | 119.84 | 111.27 |
| 25 | 8 | 618 | CLA | O2A-C1-C2 | 4.82 | 121.31 | 108.64 |
| 25 | 6 | 607 | CLA | O2A-C1-C2 | 4.81 | 121.28 | 108.64 |
| 25 | 6 | 618 | CLA | O2D-CGD-CBD | 4.81 | 119.82 | 111.27 |
| 43 | 5 | 505 | LUT | C7-C8-C9 | -4.81 | 118.96 | 126.23 |
| 25 | 9 | 605 | CLA | O2A-C1-C2 | 4.81 | 121.27 | 108.64 |
| 25 | 7 | 610 | CLA | O2D-CGD-CBD | 4.81 | 119.81 | 111.27 |
| 25 | 1 | 607 | CLA | O2A-C1-C2 | 4.80 | 121.26 | 108.64 |
| 25 | A | 1118 | CLA | O2A-C1-C2 | 4.80 | 121.26 | 108.64 |
| 25 | 2 | 608 | CLA | O2D-CGD-CBD | 4.80 | 119.80 | 111.27 |
| 25 | a | 615 | CLA | CMD-C2D-C1D | 4.80 | 133.17 | 124.71 |
| 25 | a | 602 | CLA | O2A-C1-C2 | 4.80 | 121.25 | 108.64 |
| 25 | 3 | 605 | CLA | O2D-CGD-CBD | 4.80 | 119.80 | 111.27 |
| 43 | 3 | 501 | LUT | C21-C26-C27 | 4.80 | 118.77 | 112.70 |
| 25 | 4 | 617 | CLA | O2D-CGD-CBD | 4.79 | 119.79 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 9 | 607 | CLA | O2D-CGD-CBD | 4.79 | 119.79 | 111.27 |
| 50 | 9 | 504 | XAT | C18-C5-C4 | 4.79 | 119.67 | 114.28 |
| 25 | B | 1221 | CLA | O2A-C1-C2 | 4.79 | 121.21 | 108.64 |
| 25 | 7 | 604 | CLA | O2A-C1-C2 | 4.79 | 121.21 | 108.64 |
| 25 | A | 1127 | CLA | O2D-CGD-CBD | 4.78 | 119.75 | 111.27 |
| 25 | a | 611 | CLA | O2A-C1-C2 | 4.77 | 121.16 | 108.64 |
| 25 | B | 1237 | CLA | O2A-C1-C2 | 4.76 | 121.16 | 108.64 |
| 25 | 2 | 615 | CLA | CMD-C2D-C1D | 4.76 | 133.11 | 124.71 |
| 43 | 7 | 501 | LUT | C21-C26-C25 | 4.76 | 119.95 | 111.42 |
| 25 | A | 1119 | CLA | O2D-CGD-CBD | 4.76 | 119.73 | 111.27 |
| 25 | B | 1217 | CLA | O2A-C1-C2 | 4.76 | 121.14 | 108.64 |
| 25 | 8 | 620 | CLA | O2D-CGD-CBD | 4.76 | 119.72 | 111.27 |
| 26 | 8 | 604 | CHL | C1-C2-C3 | -4.76 | 117.82 | 126.04 |
| 25 | F | 1302 | CLA | O2D-CGD-CBD | 4.76 | 119.72 | 111.27 |
| 25 | 6 | 612 | CLA | O2A-C1-C2 | 4.75 | 121.12 | 108.64 |
| 25 | A | 1101 | CLA | O2A-C1-C2 | 4.75 | 121.12 | 108.64 |
| 25 | 7 | 612 | CLA | O2D-CGD-CBD | 4.75 | 119.70 | 111.27 |
| 50 | 9 | 504 | XAT | O24-C25-C24 | 4.75 | 116.95 | 113.38 |
| 25 | 7 | 603 | CLA | O2A-C1-C2 | 4.75 | 121.11 | 108.64 |
| 25 | 8 | 612 | CLA | O2D-CGD-CBD | 4.74 | 119.70 | 111.27 |
| 25 | A | 1108 | CLA | O2A-C1-C2 | 4.74 | 121.10 | 108.64 |
| 25 | a | 608 | CLA | O2D-CGD-CBD | 4.74 | 119.69 | 111.27 |
| 25 | 2 | 612 | CLA | O2D-CGD-CBD | 4.74 | 119.69 | 111.27 |
| 29 | I | 4001 | BCR | C23-C24-C25 | -4.73 | 113.91 | 127.20 |
| 25 | 2 | 615 | CLA | O2A-C1-C2 | 4.73 | 121.07 | 108.64 |
| 25 | 8 | 611 | CLA | O2D-CGD-CBD | 4.73 | 119.67 | 111.27 |
| 25 | 9 | 604 | CLA | O2A-C1-C2 | 4.72 | 121.05 | 108.64 |
| 25 | B | 1236 | CLA | O2A-C1-C2 | 4.72 | 121.04 | 108.64 |
| 25 | 6 | 608 | CLA | O2A-C1-C2 | 4.72 | 121.04 | 108.64 |
| 25 | A | 1013 | CLA | CMD-C2D-C1D | 4.72 | 133.03 | 124.71 |
| 25 | 4 | 616 | CLA | O2D-CGD-CBD | 4.72 | 119.65 | 111.27 |
| 25 | 6 | 604 | CLA | O2A-C1-C2 | 4.72 | 121.03 | 108.64 |
| 25 | O | 1803 | CLA | O2D-CGD-CBD | 4.71 | 119.65 | 111.27 |
| 25 | 1 | 603 | CLA | O2D-CGD-CBD | 4.71 | 119.64 | 111.27 |
| 24 | A | 1011 | CL0 | CHD-C1D-ND | -4.71 | 120.13 | 124.45 |
| 25 | 4 | 603 | CLA | O2D-CGD-CBD | 4.70 | 119.62 | 111.27 |
| 25 | a | 603 | CLA | O2D-CGD-CBD | 4.70 | 119.62 | 111.27 |
| 25 | 7 | 608 | CLA | O2A-C1-C2 | 4.70 | 120.99 | 108.64 |
| 29 | 7 | 503 | BCR | C23-C22-C21 | -4.69 | 111.74 | 118.94 |
| 25 | 5 | 609 | CLA | O2A-C1-C2 | 4.69 | 120.96 | 108.64 |
| 25 | B | 1232 | CLA | O2D-CGD-CBD | 4.69 | 119.60 | 111.27 |
| 25 | 1 | 612 | CLA | O2D-CGD-CBD | 4.69 | 119.60 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1202 | CLA | O2A-C1-C2 | 4.68 | 120.93 | 108.64 |
| 40 | 3 | 506 | RRX | C33-C5-C6 | -4.67 | 119.28 | 124.53 |
| 43 | a | 501 | LUT | C15-C14-C13 | -4.67 | 120.65 | 127.31 |
| 25 | A | 1012 | CLA | CMD-C2D-C1D | 4.67 | 132.94 | 124.71 |
| 25 | a | 612 | CLA | O2D-CGD-CBD | 4.66 | 119.56 | 111.27 |
| 43 | 4 | 501 | LUT | C35-C34-C33 | -4.65 | 120.67 | 127.31 |
| 25 | A | 1138 | CLA | O2A-C1-C2 | 4.65 | 120.85 | 108.64 |
| 24 | A | 1011 | CL0 | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 25 | A | 1127 | CLA | CMD-C2D-C1D | 4.64 | 132.89 | 124.71 |
| 25 | A | 1128 | CLA | CMD-C2D-C1D | 4.64 | 132.89 | 124.71 |
| 25 | 5 | 612 | CLA | O2A-C1-C2 | 4.63 | 120.81 | 108.64 |
| 30 | 6 | 802 | LHG | O7-C7-C8 | 4.61 | 121.43 | 111.50 |
| 25 | 8 | 611 | CLA | O2A-C1-C2 | 4.60 | 120.73 | 108.64 |
| 25 | A | 1129 | CLA | O2A-C1-C2 | 4.60 | 120.72 | 108.64 |
| 25 | A | 1118 | CLA | O2D-CGD-CBD | 4.60 | 119.44 | 111.27 |
| 25 | 1 | 608 | CLA | O2D-CGD-CBD | 4.60 | 119.44 | 111.27 |
| 26 | 1 | 604 | CHL | CHD-C1D-ND | -4.60 | 120.23 | 124.45 |
| 26 | 8 | 601 | CHL | CHD-C1D-ND | -4.59 | 120.24 | 124.45 |
| 25 | A | 1109 | CLA | O2D-CGD-CBD | 4.58 | 119.41 | 111.27 |
| 25 | A | 1013 | CLA | O2D-CGD-CBD | 4.58 | 119.41 | 111.27 |
| 25 | 7 | 606 | CLA | O2D-CGD-CBD | 4.58 | 119.40 | 111.27 |
| 25 | 8 | 606 | CLA | O2D-CGD-CBD | 4.58 | 119.40 | 111.27 |
| 25 | 9 | 606 | CLA | O2A-C1-C2 | 4.58 | 120.66 | 108.64 |
| 50 | 7 | 502 | XAT | C18-C5-C4 | 4.57 | 119.43 | 114.28 |
| 43 | a | 503 | LUT | C31-C30-C29 | -4.57 | 120.78 | 127.31 |
| 36 | 8 | 803 | DGD | O2G-C1B-C2B | 4.56 | 121.33 | 111.50 |
| 25 | 2 | 603 | CLA | O2D-CGD-CBD | 4.56 | 119.37 | 111.27 |
| 25 | A | 1102 | CLA | O2A-C1-C2 | 4.56 | 120.62 | 108.64 |
| 25 | B | 1207 | CLA | O2A-C1-C2 | 4.55 | 120.59 | 108.64 |
| 40 | 3 | 506 | RRX | C11-C12-C13 | -4.53 | 113.69 | 126.42 |
| 26 | a | 604 | CHL | CHD-C1D-ND | -4.53 | 120.29 | 124.45 |
| 40 | 3 | 506 | RRX | C20-C19-C18 | -4.51 | 113.73 | 126.42 |
| 25 | 2 | 603 | CLA | CAA-C2A-C3A | -4.51 | 100.42 | 112.78 |
| 50 | 2 | 501 | XAT | C18-C5-C4 | 4.51 | 119.36 | 114.28 |
| 43 | 6 | 502 | LUT | C7-C8-C9 | -4.51 | 119.42 | 126.23 |
| 25 | B | 1222 | CLA | O2D-CGD-CBD | 4.51 | 119.27 | 111.27 |
| 25 | 9 | 612 | CLA | O2A-C1-C2 | 4.48 | 120.42 | 108.64 |
| 25 | 5 | 606 | CLA | C1-C2-C3 | -4.48 | 119.51 | 126.75 |
| 43 | 9 | 501 | LUT | C21-C26-C27 | 4.46 | 118.34 | 112.70 |
| 25 | B | 1021 | CLA | C1-C2-C3 | -4.46 | 118.34 | 126.04 |
| 43 | a | 502 | LUT | C21-C26-C27 | 4.44 | 118.32 | 112.70 |
| 43 | a | 501 | LUT | C11-C10-C9 | -4.44 | 120.97 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | 5 | 802 | PTY | O7-C8-C11 | 4.44 | 121.07 | 111.50 |
| 30 | F | 5002 | LHG | O7-C7-C8 | 4.44 | 121.06 | 111.50 |
| 40 | 3 | 506 | RRX | C19-C18-C17 | 4.43 | 125.74 | 118.94 |
| 30 | A | 5001 | LHG | O7-C7-C8 | 4.43 | 121.05 | 111.50 |
| 30 | 9 | 802 | LHG | O7-C7-C8 | 4.43 | 121.05 | 111.50 |
| 25 | 6 | 603 | CLA | O2A-C1-C2 | 4.43 | 120.27 | 108.64 |
| 25 | A | 1108 | CLA | O2D-CGD-CBD | 4.43 | 119.13 | 111.27 |
| 43 | a | 501 | LUT | C18-C5-C6 | -4.42 | 119.56 | 124.53 |
| 50 | 9 | 504 | XAT | C15-C14-C13 | -4.42 | 121.01 | 127.31 |
| 43 | 5 | 502 | LUT | C21-C26-C27 | 4.40 | 118.27 | 112.70 |
| 26 | 3 | 611 | CHL | CHD-C1D-ND | -4.40 | 120.41 | 124.45 |
| 30 | 5 | 801 | LHG | O7-C7-C8 | 4.38 | 120.94 | 111.50 |
| 25 | 4 | 603 | CLA | O2A-C1-C2 | 4.38 | 120.15 | 108.64 |
| 43 | 6 | 502 | LUT | C21-C26-C27 | 4.37 | 118.23 | 112.70 |
| 26 | 3 | 604 | CHL | CHD-C1D-ND | -4.37 | 120.43 | 124.45 |
| 43 | 5 | 505 | LUT | C35-C34-C33 | -4.37 | 121.07 | 127.31 |
| 44 | 7 | 504 | AXT | C10-C11-C12 | 4.37 | 136.85 | 123.22 |
| 43 | 8 | 502 | LUT | C21-C26-C27 | 4.37 | 118.22 | 112.70 |
| 40 | J | 4002 | RRX | C20-C19-C18 | -4.37 | 114.15 | 126.42 |
| 25 | A | 1121 | CLA | C1-C2-C3 | -4.37 | 118.49 | 126.04 |
| 43 | 8 | 502 | LUT | C7-C8-C9 | -4.36 | 119.65 | 126.23 |
| 43 | 6 | 501 | LUT | C21-C26-C27 | 4.35 | 118.20 | 112.70 |
| 43 | 2 | 507 | LUT | C18-C5-C6 | -4.35 | 119.64 | 124.53 |
| 25 | B | 1234 | CLA | C4D-CHA-C1A | -4.35 | 120.00 | 127.26 |
| 25 | A | 1122 | CLA | O2D-CGD-CBD | 4.35 | 118.99 | 111.27 |
| 43 | a | 503 | LUT | C15-C14-C13 | -4.34 | 121.11 | 127.31 |
| 43 | 4 | 501 | LUT | C21-C26-C25 | 4.34 | 119.19 | 111.42 |
| 25 | B | 1215 | CLA | O2A-C1-C2 | 4.33 | 120.01 | 108.64 |
| 25 | A | 1126 | CLA | O2A-C1-C2 | 4.33 | 120.00 | 108.64 |
| 30 | 2 | 801 | LHG | O7-C7-C8 | 4.32 | 120.82 | 111.50 |
| 25 | B | 1234 | CLA | C2D-C1D-ND | 4.32 | 113.31 | 106.99 |
| 25 | 5 | 615 | CLA | O2D-CGD-CBD | 4.31 | 118.92 | 111.27 |
| 43 | 4 | 502 | LUT | C35-C34-C33 | -4.31 | 121.16 | 127.31 |
| 44 | 7 | 504 | AXT | C39-C29-C30 | -4.28 | 116.93 | 122.92 |
| 26 | 1 | 604 | CHL | C1-C2-C3 | -4.28 | 118.64 | 126.04 |
| 44 | 1 | 502 | AXT | C39-C29-C30 | -4.27 | 116.94 | 122.92 |
| 30 | B | 5002 | LHG | O7-C7-C8 | 4.27 | 120.71 | 111.50 |
| 25 | A | 1012 | CLA | C1-C2-C3 | -4.27 | 118.67 | 126.04 |
| 30 | F | 5001 | LHG | O7-C7-C8 | 4.26 | 120.69 | 111.50 |
| 43 | 5 | 505 | LUT | C22-C23-C24 | -4.26 | 106.89 | 111.74 |
| 26 | A | 1114 | CHL | CHD-C1D-ND | -4.26 | 120.54 | 124.45 |
| 26 | 9 | 601 | CHL | CHD-C1D-ND | -4.25 | 120.55 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | 7 | 804 | PTY | O7-C8-C11 | 4.25 | 120.65 | 111.50 |
| 39 | F | 4001 | NEX | C26-C27-C28 | -4.23 | 117.05 | 125.99 |
| 29 | L | 4002 | BCR | C33-C5-C6 | -4.23 | 119.78 | 124.53 |
| 43 | a | 501 | LUT | C35-C34-C33 | -4.22 | 121.28 | 127.31 |
| 25 | 3 | 607 | CLA | O2A-C1-C2 | 4.22 | 119.72 | 108.64 |
| 24 | A | 1011 | CL0 | O2A-CGA-CBA | 4.21 | 125.12 | 111.91 |
| 42 | M | 4001 | ECH | C16-C17-C18 | -4.21 | 121.30 | 127.31 |
| 29 | 3 | 503 | BCR | C33-C5-C6 | -4.21 | 119.80 | 124.53 |
| 26 | 8 | 604 | CHL | CHD-C1D-ND | -4.21 | 120.59 | 124.45 |
| 44 | 1 | 502 | AXT | C40-C33-C34 | -4.20 | 117.04 | 122.92 |
| 46 | a | 504 | QTB | C19-C17-C11 | -4.19 | 104.56 | 110.60 |
| 25 | 4 | 612 | CLA | O2A-C1-C2 | 4.18 | 119.63 | 108.64 |
| 42 | M | 4001 | ECH | C24-C23-C22 | -4.17 | 119.93 | 126.23 |
| 29 | G | 4001 | BCR | C33-C5-C6 | -4.17 | 119.85 | 124.53 |
| 37 | B | 5004 | PCW | O2-C31-C32 | 4.17 | 120.49 | 111.50 |
| 25 | B | 1220 | CLA | O2D-CGD-CBD | 4.17 | 118.67 | 111.27 |
| 43 | a | 502 | LUT | C7-C8-C9 | -4.17 | 119.94 | 126.23 |
| 40 | 3 | 506 | RRX | C38-C26-C25 | -4.16 | 119.85 | 124.53 |
| 30 | 6 | 801 | LHG | O7-C7-C8 | 4.15 | 120.45 | 111.50 |
| 25 | A | 1126 | CLA | C1-C2-C3 | -4.15 | 118.87 | 126.04 |
| 43 | 1 | 501 | LUT | C35-C34-C33 | -4.14 | 121.39 | 127.31 |
| 44 | 1 | 502 | AXT | C19-C9-C10 | -4.14 | 117.12 | 122.92 |
| 29 | 8 | 503 | BCR | C33-C5-C6 | -4.13 | 119.89 | 124.53 |
| 37 | 6 | 803 | PCW | O2-C31-C32 | 4.12 | 120.38 | 111.50 |
| 40 | 3 | 506 | RRX | C1-C6-C5 | -4.12 | 116.81 | 122.61 |
| 33 | 9 | 803 | PTY | O7-C8-C11 | 4.12 | 120.37 | 111.50 |
| 48 | 3 | 803 | DGA | OG2-CB1-CB2 | 4.11 | 120.35 | 111.50 |
| 43 | 9 | 501 | LUT | C18-C5-C6 | -4.11 | 119.92 | 124.53 |
| 29 | L | 4003 | BCR | C33-C5-C6 | -4.10 | 119.93 | 124.53 |
| 30 | 9 | 801 | LHG | O7-C7-C8 | 4.10 | 120.33 | 111.50 |
| 29 | 7 | 503 | BCR | C33-C5-C6 | -4.09 | 119.93 | 124.53 |
| 43 | 2 | 502 | LUT | C21-C26-C27 | 4.09 | 117.87 | 112.70 |
| 44 | 1 | 502 | AXT | C20-C13-C14 | -4.09 | 117.20 | 122.92 |
| 25 | 2 | 621 | CLA | C1-C2-C3 | -4.08 | 118.98 | 126.04 |
| 52 | 8 | 805 | P5S | O37-C38-C39 | 4.08 | 120.29 | 111.50 |
| 51 | 7 | 807 | 4RF | O21-C22-C24 | 4.08 | 120.29 | 111.50 |
| 34 | A | 5007 | 3PH | O21-C21-C22 | 4.07 | 120.28 | 111.50 |
| 25 | A | 1127 | CLA | C1-C2-C3 | -4.07 | 119.00 | 126.04 |
| 50 | 7 | 502 | XAT | C15-C14-C13 | -4.07 | 121.51 | 127.31 |
| 26 | 6 | 613 | CHL | CHD-C1D-ND | -4.06 | 120.72 | 124.45 |
| 30 | 7 | 803 | LHG | O7-C7-C8 | 4.05 | 120.23 | 111.50 |
| 26 | 2 | 609 | CHL | CHD-C1D-ND | -4.05 | 120.73 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 8 | 801 | LHG | O7-C7-C8 | 4.05 | 120.23 | 111.50 |
| 25 | 3 | 605 | CLA | C1-C2-C3 | -4.05 | 119.05 | 126.04 |
| 53 | 8 | 810 | LAP | O7-P9-O5 | 4.04 | 132.22 | 112.24 |
| 25 | 7 | 603 | CLA | C1-C2-C3 | -4.04 | 119.05 | 126.04 |
| 43 | 1 | 503 | LUT | C22-C23-C24 | -4.04 | 107.14 | 111.74 |
| 44 | 7 | 504 | AXT | C8-C7-C6 | 4.04 | 138.55 | 127.20 |
| 30 | 1 | 801 | LHG | O7-C7-C8 | 4.03 | 120.19 | 111.50 |
| 25 | 4 | 601 | CLA | C1-C2-C3 | -4.03 | 119.07 | 126.04 |
| 25 | 3 | 612 | CLA | C1-C2-C3 | -4.03 | 120.23 | 126.75 |
| 29 | B | 4002 | BCR | C33-C5-C6 | -4.03 | 120.00 | 124.53 |
| 43 | 4 | 501 | LUT | C7-C8-C9 | -4.02 | 120.16 | 126.23 |
| 26 | A | 1114 | CHL | C1-O2A-CGA | 4.02 | 126.99 | 116.44 |
| 33 | J | 5001 | PTY | O7-C8-C11 | 4.02 | 120.16 | 111.50 |
| 26 | 9 | 608 | CHL | CHD-C1D-ND | -4.02 | 120.76 | 124.45 |
| 43 | 2 | 502 | LUT | C15-C14-C13 | -4.01 | 121.59 | 127.31 |
| 26 | 4 | 609 | CHL | CHD-C1D-ND | -4.01 | 120.77 | 124.45 |
| 25 | 8 | 606 | CLA | C1-C2-C3 | -4.01 | 119.12 | 126.04 |
| 29 | A | 4003 | BCR | C28-C27-C26 | -4.00 | 106.93 | 114.08 |
| 43 | 4 | 502 | LUT | C7-C8-C9 | -4.00 | 120.19 | 126.23 |
| 25 | B | 1231 | CLA | CHD-C1D-ND | -4.00 | 120.78 | 124.45 |
| 26 | 3 | 608 | CHL | CHD-C1D-ND | -4.00 | 120.78 | 124.45 |
| 33 | B | 5005 | PTY | O7-C8-C11 | 4.00 | 120.11 | 111.50 |
| 50 | 2 | 501 | XAT | C15-C14-C13 | -3.99 | 121.62 | 127.31 |
| 25 | A | 1130 | CLA | C1-C2-C3 | -3.99 | 119.14 | 126.04 |
| 37 | K | 5001 | PCW | O2-C31-C32 | 3.99 | 120.10 | 111.50 |
| 31 | A | 5004 | LMG | O7-C10-C11 | 3.98 | 120.08 | 111.50 |
| 25 | L | 1504 | CLA | C1-C2-C3 | -3.98 | 120.31 | 126.75 |
| 36 | 8 | 802 | DGD | O2G-C1B-C2B | 3.98 | 120.07 | 111.50 |
| 43 | 1 | 501 | LUT | C21-C26-C27 | 3.97 | 117.72 | 112.70 |
| 43 | 3 | 501 | LUT | C22-C23-C24 | -3.97 | 107.23 | 111.74 |
| 25 | F | 1301 | CLA | C1-C2-C3 | -3.97 | 120.33 | 126.75 |
| 43 | 5 | 501 | LUT | C21-C26-C27 | 3.96 | 117.71 | 112.70 |
| 25 | H | 1703 | CLA | C1-C2-C3 | -3.96 | 119.19 | 126.04 |
| 29 | 6 | 504 | BCR | C33-C5-C6 | -3.96 | 120.08 | 124.53 |
| 30 | 4 | 802 | LHG | O7-C7-C8 | 3.96 | 120.04 | 111.50 |
| 25 | 2 | 612 | CLA | C1-C2-C3 | -3.96 | 120.35 | 126.75 |
| 48 | 5 | 803 | DGA | OG2-CB1-CB2 | 3.95 | 120.02 | 111.50 |
| 33 | G | 5002 | PTY | O7-C8-C11 | 3.95 | 120.02 | 111.50 |
| 25 | A | 1128 | CLA | C1-C2-C3 | -3.95 | 119.22 | 126.04 |
| 26 | 5 | 617 | CHL | CHD-C1D-ND | -3.94 | 120.83 | 124.45 |
| 36 | B | 5003 | DGD | O2G-C1B-C2B | 3.94 | 119.98 | 111.50 |
| 43 | 8 | 502 | LUT | C35-C34-C33 | -3.93 | 121.70 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | A | 5002 | LHG | O7-C7-C8 | 3.93 | 119.97 | 111.50 |
| 40 | J | 4002 | RRX | C38-C26-C25 | -3.92 | 120.12 | 124.53 |
| 42 | M | 4001 | ECH | C33-C5-C6 | -3.92 | 120.12 | 124.53 |
| 25 | A | 1136 | CLA | C1-C2-C3 | -3.92 | 119.26 | 126.04 |
| 40 | 3 | 506 | RRX | C36-C18-C17 | -3.92 | 117.44 | 122.92 |
| 50 | 2 | 501 | XAT | O4-C5-C4 | -3.92 | 110.44 | 113.38 |
| 25 | 8 | 611 | CLA | C1-C2-C3 | -3.91 | 120.42 | 126.75 |
| 25 | G | 1601 | CLA | C1-C2-C3 | -3.91 | 120.42 | 126.75 |
| 30 | 1 | 802 | LHG | O7-C7-C8 | 3.91 | 119.92 | 111.50 |
| 25 | 8 | 605 | CLA | C1-C2-C3 | -3.90 | 119.29 | 126.04 |
| 48 | 2 | 803 | DGA | OG2-CB1-CB2 | 3.90 | 119.91 | 111.50 |
| 30 | 3 | 801 | LHG | O7-C7-C8 | 3.90 | 119.90 | 111.50 |
| 25 | B | 1229 | CLA | C1-C2-C3 | -3.90 | 119.30 | 126.04 |
| 25 | A | 1138 | CLA | O2D-CGD-CBD | 3.90 | 118.19 | 111.27 |
| 25 | 4 | 616 | CLA | C1-C2-C3 | -3.89 | 120.45 | 126.75 |
| 29 | 5 | 503 | BCR | C33-C5-C6 | -3.89 | 120.16 | 124.53 |
| 48 | 8 | 804 | DGA | OG2-CB1-CB2 | 3.89 | 119.88 | 111.50 |
| 26 | 6 | 619 | CHL | CHD-C1D-ND | -3.89 | 120.88 | 124.45 |
| 33 | G | 5003 | PTY | O7-C8-C11 | 3.88 | 119.87 | 111.50 |
| 24 | A | 1011 | CL0 | C1-C2-C3 | -3.88 | 119.33 | 126.04 |
| 26 | 6 | 611 | CHL | CHD-C1D-ND | -3.88 | 120.89 | 124.45 |
| 26 | 6 | 609 | CHL | CHD-C1D-ND | -3.87 | 120.89 | 124.45 |
| 40 | J | 4002 | RRX | C4-C5-C6 | -3.87 | 117.11 | 122.73 |
| 29 | 6 | 504 | BCR | C15-C14-C13 | -3.87 | 121.78 | 127.31 |
| 26 | 4 | 613 | CHL | CHD-C1D-ND | -3.86 | 120.90 | 124.45 |
| 25 | a | 601 | CLA | C1-C2-C3 | -3.86 | 119.36 | 126.04 |
| 25 | B | 1204 | CLA | C1-C2-C3 | -3.86 | 119.37 | 126.04 |
| 25 | 6 | 615 | CLA | C1-C2-C3 | -3.86 | 119.37 | 126.04 |
| 43 | 1 | 501 | LUT | C22-C23-C24 | -3.86 | 107.35 | 111.74 |
| 43 | 2 | 502 | LUT | C7-C8-C9 | -3.86 | 120.40 | 126.23 |
| 26 | 1 | 613 | CHL | CHD-C1D-ND | -3.86 | 120.91 | 124.45 |
| 44 | 1 | 502 | AXT | C8-C9-C10 | 3.86 | 124.86 | 118.94 |
| 30 | a | 801 | LHG | O7-C7-C8 | 3.85 | 119.81 | 111.50 |
| 25 | B | 1206 | CLA | C2C-C1C-NC | 3.85 | 113.58 | 109.97 |
| 26 | 5 | 618 | CHL | CHD-C1D-ND | -3.85 | 120.92 | 124.45 |
| 43 | 2 | 502 | LUT | C22-C23-C24 | -3.85 | 107.36 | 111.74 |
| 43 | 6 | 502 | LUT | C35-C34-C33 | -3.85 | 121.82 | 127.31 |
| 25 | 7 | 604 | CLA | C1-C2-C3 | -3.85 | 119.39 | 126.04 |
| 29 | B | 4007 | BCR | C33-C5-C6 | -3.85 | 120.21 | 124.53 |
| 25 | A | 1112 | CLA | C1-C2-C3 | -3.84 | 119.39 | 126.04 |
| 30 | A | 5003 | LHG | O7-C7-C8 | 3.84 | 119.78 | 111.50 |
| 30 | 7 | 801 | LHG | O7-C7-C8 | 3.84 | 119.78 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 5 | 611 | CHL | CHD-C1D-ND | -3.84 | 120.93 | 124.45 |
| 33 | a | 802 | PTY | O7-C8-C11 | 3.83 | 119.76 | 111.50 |
| 50 | 9 | 507 | XAT | O4-C5-C4 | -3.83 | 110.50 | 113.38 |
| 25 | B | 1224 | CLA | C1-C2-C3 | -3.83 | 119.42 | 126.04 |
| 43 | 6 | 501 | LUT | C18-C5-C6 | -3.83 | 120.23 | 124.53 |
| 43 | a | 501 | LUT | C21-C26-C27 | 3.83 | 117.54 | 112.70 |
| 26 | 8 | 610 | CHL | CHD-C1D-ND | -3.82 | 120.94 | 124.45 |
| 43 | 3 | 502 | LUT | C15-C14-C13 | -3.82 | 121.86 | 127.31 |
| 40 | J | 4002 | RRX | C33-C5-C6 | -3.82 | 120.24 | 124.53 |
| 43 | 1 | 503 | LUT | C10-C11-C12 | -3.82 | 111.31 | 123.22 |
| 25 | 7 | 606 | CLA | C1-C2-C3 | -3.82 | 119.44 | 126.04 |
| 43 | 5 | 501 | LUT | C18-C5-C6 | -3.81 | 120.25 | 124.53 |
| 33 | A | 5006 | PTY | O7-C8-C11 | 3.81 | 119.71 | 111.50 |
| 26 | 1 | 611 | CHL | CHD-C1D-ND | -3.81 | 120.95 | 124.45 |
| 43 | a | 503 | LUT | C18-C5-C6 | -3.81 | 120.25 | 124.53 |
| 26 | 1 | 610 | CHL | CHD-C1D-ND | -3.81 | 120.96 | 124.45 |
| 25 | B | 1234 | CLA | C3D-C4D-ND | 3.81 | 113.14 | 107.38 |
| 43 | 7 | 501 | LUT | C35-C34-C33 | -3.80 | 121.88 | 127.31 |
| 26 | 6 | 610 | CHL | CHD-C1D-ND | -3.80 | 120.96 | 124.45 |
| 43 | 4 | 501 | LUT | C18-C5-C6 | -3.80 | 120.26 | 124.53 |
| 33 | 3 | 802 | PTY | O7-C8-C11 | 3.80 | 119.68 | 111.50 |
| 43 | 4 | 502 | LUT | C18-C5-C6 | -3.79 | 120.27 | 124.53 |
| 26 | a | 606 | CHL | CHD-C1D-ND | -3.79 | 120.97 | 124.45 |
| 25 | 3 | 606 | CLA | C1-C2-C3 | -3.79 | 119.49 | 126.04 |
| 26 | 9 | 613 | CHL | CHD-C1D-ND | -3.78 | 120.98 | 124.45 |
| 43 | a | 502 | LUT | C35-C34-C33 | -3.78 | 121.91 | 127.31 |
| 50 | 9 | 507 | XAT | C18-C5-C4 | 3.78 | 118.53 | 114.28 |
| 25 | 2 | 604 | CLA | CHD-C1D-ND | -3.77 | 120.99 | 124.45 |
| 25 | 4 | 606 | CLA | C1-C2-C3 | -3.77 | 120.65 | 126.75 |
| 30 | 4 | 801 | LHG | O7-C7-C8 | 3.77 | 119.62 | 111.50 |
| 25 | A | 1109 | CLA | C1-C2-C3 | -3.77 | 119.53 | 126.04 |
| 43 | 2 | 507 | LUT | C22-C23-C24 | -3.76 | 107.46 | 111.74 |
| 33 | a | 803 | PTY | O7-C8-C11 | 3.76 | 119.61 | 111.50 |
| 25 | 5 | 601 | CLA | C1-C2-C3 | -3.76 | 119.55 | 126.04 |
| 25 | L | 1501 | CLA | C1-C2-C3 | -3.75 | 120.68 | 126.75 |
| 25 | B | 1201 | CLA | C1-C2-C3 | -3.75 | 119.56 | 126.04 |
| 39 | F | 4001 | NEX | O24-C25-C24 | 3.74 | 116.19 | 113.38 |
| 25 | A | 1131 | CLA | C1-C2-C3 | -3.74 | 119.57 | 126.04 |
| 25 | 1 | 606 | CLA | C1-C2-C3 | -3.74 | 119.58 | 126.04 |
| 43 | 8 | 501 | LUT | C18-C5-C6 | -3.73 | 120.34 | 124.53 |
| 26 | 7 | 609 | CHL | CHD-C1D-ND | -3.73 | 121.03 | 124.45 |
| 43 | a | 501 | LUT | C22-C23-C24 | -3.73 | 107.50 | 111.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | 7 | 504 | AXT | C32-C33-C34 | 3.73 | 124.66 | 118.94 |
| 26 | 7 | 611 | CHL | CHD-C1D-ND | -3.73 | 121.03 | 124.45 |
| 26 | 8 | 603 | CHL | CHD-C1D-ND | -3.73 | 121.03 | 124.45 |
| 29 | A | 4003 | BCR | C33-C5-C6 | -3.73 | 120.34 | 124.53 |
| 40 | 3 | 506 | RRX | C30-C25-C26 | -3.72 | 117.37 | 122.61 |
| 43 | 3 | 502 | LUT | C22-C23-C24 | -3.72 | 107.50 | 111.74 |
| 44 | 7 | 504 | AXT | C11-C10-C9 | -3.72 | 122.00 | 127.31 |
| 25 | 5 | 601 | CLA | CHD-C1D-ND | -3.72 | 121.03 | 124.45 |
| 43 | 4 | 502 | LUT | C21-C26-C27 | 3.72 | 117.41 | 112.70 |
| 43 | 6 | 501 | LUT | C35-C34-C33 | -3.72 | 122.00 | 127.31 |
| 25 | 2 | 601 | CLA | C1-O2A-CGA | 3.72 | 126.20 | 116.44 |
| 43 | 1 | 501 | LUT | C15-C14-C13 | -3.71 | 122.01 | 127.31 |
| 25 | A | 1108 | CLA | C1-C2-C3 | -3.71 | 119.63 | 126.04 |
| 43 | 8 | 501 | LUT | C21-C26-C27 | 3.71 | 117.39 | 112.70 |
| 29 | A | 4005 | BCR | C23-C24-C25 | -3.71 | 116.79 | 127.20 |
| 26 | 7 | 613 | CHL | CHD-C1D-ND | -3.71 | 121.05 | 124.45 |
| 37 | K | 5002 | PCW | O2-C31-C32 | 3.70 | 119.48 | 111.50 |
| 26 | 2 | 610 | CHL | CHD-C1D-ND | -3.70 | 121.05 | 124.45 |
| 43 | 5 | 501 | LUT | C35-C34-C33 | -3.70 | 122.03 | 127.31 |
| 43 | a | 503 | LUT | C22-C23-C24 | -3.70 | 107.53 | 111.74 |
| 25 | A | 1140 | CLA | C1-C2-C3 | -3.69 | 119.65 | 126.04 |
| 25 | 6 | 612 | CLA | C1-C2-C3 | -3.69 | 120.79 | 126.75 |
| 25 | A | 1129 | CLA | C1-C2-C3 | -3.68 | 120.79 | 126.75 |
| 25 | B | 1022 | CLA | CHD-C1D-ND | -3.68 | 121.07 | 124.45 |
| 48 | 2 | 803 | DGA | CDB-CCB-CBB | -3.68 | 81.15 | 115.30 |
| 25 | A | 1121 | CLA | CHD-C1D-ND | -3.68 | 121.07 | 124.45 |
| 25 | 2 | 601 | CLA | C1-C2-C3 | -3.68 | 119.69 | 126.04 |
| 25 | 3 | 612 | CLA | CHD-C1D-ND | -3.67 | 121.08 | 124.45 |
| 25 | 8 | 608 | CLA | C1-C2-C3 | -3.67 | 119.70 | 126.04 |
| 43 | 7 | 501 | LUT | C18-C5-C6 | -3.66 | 120.42 | 124.53 |
| 25 | B | 1203 | CLA | C1-C2-C3 | -3.66 | 119.71 | 126.04 |
| 50 | 7 | 502 | XAT | C7-C8-C9 | -3.66 | 119.85 | 125.53 |
| 50 | 7 | 502 | XAT | O4-C5-C18 | -3.66 | 110.67 | 115.06 |
| 29 | A | 4004 | BCR | C23-C24-C25 | -3.66 | 116.93 | 127.20 |
| 29 | I | 4001 | BCR | C27-C26-C25 | -3.66 | 117.42 | 122.73 |
| 25 | 8 | 612 | CLA | CHD-C1D-ND | -3.66 | 121.09 | 124.45 |
| 25 | 6 | 604 | CLA | CHD-C1D-ND | -3.66 | 121.09 | 124.45 |
| 29 | A | 4004 | BCR | C33-C5-C6 | -3.65 | 120.43 | 124.53 |
| 43 | 1 | 501 | LUT | C18-C5-C6 | -3.65 | 120.43 | 124.53 |
| 32 | I | 5001 | SQD | O7-S-C6 | -3.65 | 102.60 | 106.94 |
| 26 | a | 610 | CHL | CHD-C1D-ND | -3.65 | 121.10 | 124.45 |
| 50 | 9 | 504 | XAT | C7-C8-C9 | -3.65 | 119.87 | 125.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 4 | 618 | CHL | CHD-C1D-ND | -3.65 | 121.10 | 124.45 |
| 25 | 8 | 618 | CLA | CHD-C1D-ND | -3.65 | 121.10 | 124.45 |
| 43 | 9 | 501 | LUT | C35-C34-C33 | -3.65 | 122.11 | 127.31 |
| 25 | B | 1218 | CLA | C1-C2-C3 | -3.65 | 119.74 | 126.04 |
| 29 | O | 4001 | BCR | C33-C5-C6 | -3.65 | 120.43 | 124.53 |
| 25 | B | 1222 | CLA | CHD-C1D-ND | -3.64 | 121.11 | 124.45 |
| 43 | 7 | 501 | LUT | C22-C23-C24 | -3.64 | 107.60 | 111.74 |
| 43 | 8 | 501 | LUT | C22-C23-C24 | -3.64 | 107.60 | 111.74 |
| 25 | B | 1222 | CLA | C1-C2-C3 | -3.64 | 119.75 | 126.04 |
| 25 | 9 | 607 | CLA | O2A-C1-C2 | 3.64 | 121.79 | 108.42 |
| 25 | K | 1402 | CLA | C1-C2-C3 | -3.64 | 119.75 | 126.04 |
| 29 | 6 | 503 | BCR | C33-C5-C6 | -3.64 | 120.44 | 124.53 |
| 29 | B | 4001 | BCR | C33-C5-C6 | -3.64 | 120.44 | 124.53 |
| 30 | B | 5001 | LHG | O7-C7-C8 | 3.63 | 119.33 | 111.50 |
| 43 | 5 | 502 | LUT | C7-C8-C9 | -3.63 | 120.75 | 126.23 |
| 43 | 6 | 502 | LUT | C18-C5-C6 | -3.63 | 120.45 | 124.53 |
| 25 | 6 | 606 | CLA | C1-C2-C3 | -3.63 | 119.77 | 126.04 |
| 25 | A | 1134 | CLA | C1-C2-C3 | -3.63 | 119.77 | 126.04 |
| 25 | 8 | 615 | CLA | CHD-C1D-ND | -3.62 | 121.12 | 124.45 |
| 25 | A | 1116 | CLA | C1-C2-C3 | -3.62 | 119.78 | 126.04 |
| 29 | G | 4001 | BCR | C12-C13-C14 | 3.62 | 124.49 | 118.94 |
| 26 | 6 | 617 | CHL | CHD-C1D-ND | -3.61 | 121.14 | 124.45 |
| 29 | B | 4005 | BCR | C33-C5-C6 | -3.61 | 120.48 | 124.53 |
| 30 | 7 | 802 | LHG | O7-C7-C8 | 3.61 | 119.27 | 111.50 |
| 50 | 9 | 507 | XAT | C26-C27-C28 | -3.60 | 118.37 | 125.99 |
| 43 | 3 | 501 | LUT | C35-C34-C33 | -3.60 | 122.17 | 127.31 |
| 25 | B | 1218 | CLA | CHD-C1D-ND | -3.60 | 121.14 | 124.45 |
| 26 | 7 | 617 | CHL | CHD-C1D-ND | -3.60 | 121.15 | 124.45 |
| 25 | A | 1119 | CLA | CHD-C1D-ND | -3.60 | 121.15 | 124.45 |
| 25 | 3 | 616 | CLA | C1-C2-C3 | -3.60 | 119.82 | 126.04 |
| 25 | 6 | 601 | CLA | CHD-C1D-ND | -3.60 | 121.15 | 124.45 |
| 26 | 9 | 610 | CHL | CHD-C1D-ND | -3.60 | 121.15 | 124.45 |
| 26 | 9 | 603 | CHL | CHD-C1D-ND | -3.60 | 121.15 | 124.45 |
| 43 | 5 | 502 | LUT | C35-C34-C33 | -3.59 | 122.19 | 127.31 |
| 32 | G | 5001 | SQD | O7-S-C6 | -3.59 | 102.68 | 106.94 |
| 25 | A | 1135 | CLA | C1-C2-C3 | -3.59 | 119.84 | 126.04 |
| 25 | A | 1111 | CLA | C1-C2-C3 | -3.58 | 119.85 | 126.04 |
| 43 | 9 | 502 | LUT | C21-C26-C27 | 3.58 | 117.23 | 112.70 |
| 25 | B | 1209 | CLA | C1-C2-C3 | -3.58 | 119.85 | 126.04 |
| 25 | F | 1302 | CLA | C1-C2-C3 | -3.58 | 119.85 | 126.04 |
| 25 | A | 1119 | CLA | C1-C2-C3 | -3.58 | 119.86 | 126.04 |
| 29 | I | 4001 | BCR | C33-C5-C6 | -3.57 | 120.52 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | 7 | 504 | AXT | C28-C29-C30 | 3.57 | 124.42 | 118.94 |
| 25 | A | 1104 | CLA | C1-C2-C3 | -3.57 | 119.87 | 126.04 |
| 40 | 3 | 506 | RRX | C12-C13-C14 | 3.57 | 124.42 | 118.94 |
| 25 | a | 603 | CLA | C1-C2-C3 | -3.57 | 119.87 | 126.04 |
| 25 | 7 | 604 | CLA | CHD-C1D-ND | -3.57 | 121.18 | 124.45 |
| 29 | H | 4001 | BCR | C33-C5-C4 | 3.56 | 120.45 | 113.62 |
| 25 | 7 | 601 | CLA | C1-C2-C3 | -3.56 | 119.89 | 126.04 |
| 43 | 9 | 502 | LUT | C18-C5-C6 | -3.56 | 120.53 | 124.53 |
| 25 | A | 1138 | CLA | CHD-C1D-ND | -3.55 | 121.19 | 124.45 |
| 26 | 5 | 617 | CHL | C2C-C3C-C4C | 3.55 | 109.02 | 106.49 |
| 32 | H | 5001 | SQD | O7-S-C6 | -3.55 | 102.72 | 106.94 |
| 26 | 1 | 604 | CHL | C3C-C4C-NC | -3.55 | 106.59 | 110.57 |
| 25 | 1 | 608 | CLA | CHD-C1D-ND | -3.54 | 121.20 | 124.45 |
| 25 | 5 | 604 | CLA | CHD-C1D-ND | -3.54 | 121.20 | 124.45 |
| 29 | A | 4003 | BCR | C36-C18-C17 | -3.54 | 117.97 | 122.92 |
| 25 | A | 1133 | CLA | CHD-C1D-ND | -3.54 | 121.20 | 124.45 |
| 43 | 3 | 501 | LUT | C18-C5-C6 | -3.53 | 120.56 | 124.53 |
| 43 | 9 | 501 | LUT | C7-C8-C9 | -3.53 | 120.90 | 126.23 |
| 43 | 1 | 503 | LUT | C35-C15-C14 | 3.53 | 130.70 | 123.47 |
| 25 | B | 1204 | CLA | CHD-C1D-ND | -3.53 | 121.21 | 124.45 |
| 25 | 8 | 602 | CLA | C1-C2-C3 | -3.53 | 119.94 | 126.04 |
| 25 | B | 1240 | CLA | C1-C2-C3 | -3.52 | 119.95 | 126.04 |
| 29 | 6 | 504 | BCR | C33-C5-C4 | 3.51 | 120.36 | 113.62 |
| 25 | L | 1502 | CLA | C2D-C1D-ND | 3.51 | 112.69 | 110.10 |
| 43 | 5 | 502 | LUT | C18-C5-C6 | -3.51 | 120.58 | 124.53 |
| 26 | 5 | 613 | CHL | CHD-C1D-ND | -3.51 | 121.23 | 124.45 |
| 40 | J | 4002 | RRX | C11-C12-C13 | -3.51 | 116.56 | 126.42 |
| 26 | 8 | 601 | CHL | C3C-C4C-NC | -3.51 | 106.64 | 110.57 |
| 29 | B | 4003 | BCR | C33-C5-C6 | -3.51 | 120.59 | 124.53 |
| 25 | B | 1220 | CLA | C1-C2-C3 | -3.50 | 119.98 | 126.04 |
| 43 | 8 | 502 | LUT | C18-C5-C6 | -3.50 | 120.59 | 124.53 |
| 29 | G | 4001 | BCR | C35-C13-C14 | -3.50 | 118.02 | 122.92 |
| 25 | B | 1229 | CLA | CHD-C1D-ND | -3.50 | 121.23 | 124.45 |
| 29 | 7 | 503 | BCR | C37-C22-C23 | 3.50 | 123.59 | 118.08 |
| 29 | L | 4001 | BCR | C33-C5-C6 | -3.50 | 120.60 | 124.53 |
| 25 | H | 1703 | CLA | CHD-C1D-ND | -3.50 | 121.24 | 124.45 |
| 25 | B | 1220 | CLA | CHD-C1D-ND | -3.50 | 121.24 | 124.45 |
| 26 | 3 | 611 | CHL | C3C-C4C-NC | -3.50 | 106.65 | 110.57 |
| 25 | a | 602 | CLA | C1-C2-C3 | -3.49 | 121.10 | 126.75 |
| 25 | 8 | 608 | CLA | CHD-C1D-ND | -3.49 | 121.25 | 124.45 |
| 25 | A | 1113 | CLA | CHD-C1D-ND | -3.49 | 121.25 | 124.45 |
| 29 | 5 | 504 | BCR | C33-C5-C4 | 3.49 | 120.32 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1109 | CLA | CHD-C1D-ND | -3.48 | 121.25 | 124.45 |
| 25 | a | 601 | CLA | CHD-C1D-ND | -3.48 | 121.25 | 124.45 |
| 43 | 7 | 501 | LUT | C15-C14-C13 | -3.48 | 122.34 | 127.31 |
| 50 | 2 | 501 | XAT | C6-C7-C8 | -3.48 | 118.63 | 125.99 |
| 25 | 7 | 601 | CLA | CHD-C1D-ND | -3.48 | 121.25 | 124.45 |
| 43 | 6 | 502 | LUT | C15-C14-C13 | -3.48 | 122.34 | 127.31 |
| 32 | A | 5005 | SQD | O7-S-C6 | -3.48 | 102.80 | 106.94 |
| 25 | A | 1108 | CLA | CHD-C1D-ND | -3.48 | 121.26 | 124.45 |
| 44 | 1 | 502 | AXT | C28-C29-C30 | 3.48 | 124.28 | 118.94 |
| 26 | 8 | 613 | CHL | CHD-C1D-ND | -3.48 | 121.26 | 124.45 |
| 43 | 9 | 502 | LUT | C35-C34-C33 | -3.48 | 122.35 | 127.31 |
| 25 | B | 1211 | CLA | C1-C2-C3 | -3.48 | 120.03 | 126.04 |
| 40 | 3 | 506 | RRX | C35-C13-C14 | -3.48 | 118.06 | 122.92 |
| 36 | 7 | 806 | DGD | O2G-C1B-C2B | 3.47 | 118.99 | 111.50 |
| 25 | A | 1117 | CLA | C1-C2-C3 | -3.47 | 120.03 | 126.04 |
| 25 | A | 1123 | CLA | C2C-C1C-NC | 3.47 | 113.22 | 109.97 |
| 25 | B | 1226 | CLA | CHD-C1D-ND | -3.47 | 121.26 | 124.45 |
| 25 | A | 1137 | CLA | CHD-C1D-ND | -3.47 | 121.27 | 124.45 |
| 26 | 3 | 603 | CHL | CHD-C1D-ND | -3.47 | 121.27 | 124.45 |
| 29 | 5 | 503 | BCR | C23-C24-C25 | -3.47 | 117.46 | 127.20 |
| 29 | 4 | 503 | BCR | C15-C14-C13 | -3.46 | 122.37 | 127.31 |
| 29 | B | 4007 | BCR | C23-C24-C25 | -3.46 | 117.48 | 127.20 |
| 39 | F | 4001 | NEX | C28-C29-C30 | 3.46 | 124.25 | 118.94 |
| 25 | B | 1213 | CLA | CHD-C1D-ND | -3.46 | 121.28 | 124.45 |
| 25 | L | 1502 | CLA | C1-C2-C3 | -3.46 | 120.06 | 126.04 |
| 25 | B | 1225 | CLA | C1-C2-C3 | -3.46 | 120.07 | 126.04 |
| 29 | 3 | 504 | BCR | C36-C18-C17 | -3.45 | 118.09 | 122.92 |
| 24 | A | 1011 | CL0 | C1D-ND-C4D | -3.45 | 103.89 | 106.33 |
| 25 | B | 1208 | CLA | CHD-C1D-ND | -3.45 | 121.29 | 124.45 |
| 26 | 5 | 617 | CHL | C3C-C4C-NC | -3.45 | 106.71 | 110.57 |
| 43 | 9 | 501 | LUT | C15-C14-C13 | -3.45 | 122.39 | 127.31 |
| 26 | a | 609 | CHL | CHD-C1D-ND | -3.44 | 121.29 | 124.45 |
| 25 | A | 1126 | CLA | CHD-C1D-ND | -3.44 | 121.29 | 124.45 |
| 25 | 4 | 601 | CLA | CHD-C1D-ND | -3.44 | 121.29 | 124.45 |
| 43 | a | 502 | LUT | C18-C5-C6 | -3.44 | 120.67 | 124.53 |
| 25 | A | 1122 | CLA | CHD-C1D-ND | -3.44 | 121.30 | 124.45 |
| 25 | A | 1105 | CLA | CHD-C1D-ND | -3.43 | 121.30 | 124.45 |
| 25 | B | 1215 | CLA | CHD-C1D-ND | -3.43 | 121.30 | 124.45 |
| 26 | 7 | 613 | CHL | C3C-C4C-NC | -3.43 | 106.72 | 110.57 |
| 44 | 1 | 502 | AXT | C32-C33-C34 | 3.43 | 124.21 | 118.94 |
| 25 | 6 | 601 | CLA | C1-C2-C3 | -3.43 | 120.11 | 126.04 |
| 26 | 9 | 601 | CHL | C3C-C4C-NC | -3.43 | 106.73 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | a | 603 | CLA | CHD-C1D-ND | -3.42 | 121.31 | 124.45 |
| 25 | 6 | 608 | CLA | CHD-C1D-ND | -3.42 | 121.31 | 124.45 |
| 25 | 3 | 610 | CLA | CHD-C1D-ND | -3.42 | 121.31 | 124.45 |
| 43 | 9 | 502 | LUT | C15-C14-C13 | -3.42 | 122.43 | 127.31 |
| 25 | 4 | 607 | CLA | C1-C2-C3 | -3.42 | 120.13 | 126.04 |
| 25 | 4 | 604 | CLA | C1-C2-C3 | -3.42 | 120.13 | 126.04 |
| 25 | 6 | 603 | CLA | C1-C2-C3 | -3.42 | 120.14 | 126.04 |
| 25 | 8 | 615 | CLA | C2D-C1D-ND | 3.42 | 112.62 | 110.10 |
| 43 | a | 502 | LUT | C22-C23-C24 | -3.42 | 107.85 | 111.74 |
| 26 | 7 | 615 | CHL | C1-C2-C3 | -3.41 | 121.23 | 126.75 |
| 25 | 1 | 601 | CLA | CHD-C1D-ND | -3.41 | 121.32 | 124.45 |
| 26 | 1 | 611 | CHL | C3C-C4C-NC | -3.41 | 106.75 | 110.57 |
| 25 | A | 1123 | CLA | C1-C2-C3 | -3.41 | 120.15 | 126.04 |
| 26 | 7 | 609 | CHL | C3C-C4C-NC | -3.41 | 106.75 | 110.57 |
| 25 | B | 1216 | CLA | CHD-C1D-ND | -3.41 | 121.32 | 124.45 |
| 25 | 8 | 606 | CLA | CHD-C1D-ND | -3.41 | 121.32 | 124.45 |
| 25 | A | 1106 | CLA | C1-C2-C3 | -3.40 | 120.16 | 126.04 |
| 25 | 2 | 612 | CLA | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 26 | 7 | 615 | CHL | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 25 | B | 1222 | CLA | CMA-C3A-C4A | 3.40 | 120.92 | 111.77 |
| 25 | 6 | 618 | CLA | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 29 | A | 4002 | BCR | C23-C24-C25 | -3.40 | 117.65 | 127.20 |
| 26 | 4 | 609 | CHL | C3C-C4C-NC | -3.40 | 106.76 | 110.57 |
| 32 | 7 | 805 | SQD | O7-S-C6 | -3.40 | 102.90 | 106.94 |
| 25 | L | 1503 | CLA | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 25 | 5 | 612 | CLA | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 50 | 9 | 504 | XAT | C38-C25-C24 | 3.40 | 118.10 | 114.28 |
| 25 | B | 1236 | CLA | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 25 | 4 | 603 | CLA | CHD-C1D-ND | -3.40 | 121.33 | 124.45 |
| 25 | 6 | 604 | CLA | C1-C2-C3 | -3.40 | 120.17 | 126.04 |
| 25 | B | 1227 | CLA | C1-C2-C3 | -3.40 | 121.26 | 126.75 |
| 29 | 5 | 504 | BCR | C28-C27-C26 | -3.39 | 108.02 | 114.08 |
| 29 | 3 | 505 | BCR | C33-C5-C6 | -3.39 | 120.72 | 124.53 |
| 25 | L | 1502 | CLA | CHD-C1D-ND | -3.39 | 121.34 | 124.45 |
| 25 | 3 | 613 | CLA | C1-C2-C3 | -3.39 | 120.17 | 126.04 |
| 29 | H | 4001 | BCR | C4-C5-C6 | -3.39 | 117.82 | 122.73 |
| 25 | B | 1228 | CLA | CHD-C1D-ND | -3.38 | 121.34 | 124.45 |
| 43 | 5 | 501 | LUT | C22-C23-C24 | -3.38 | 107.89 | 111.74 |
| 25 | B | 1239 | CLA | CHD-C1D-ND | -3.38 | 121.35 | 124.45 |
| 25 | 5 | 603 | CLA | CHD-C1D-ND | -3.38 | 121.35 | 124.45 |
| 25 | 8 | 618 | CLA | C1-C2-C3 | -3.38 | 120.20 | 126.04 |
| 25 | a | 605 | CLA | C1-C2-C3 | -3.37 | 120.21 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | a | 613 | CHL | CHD-C1D-ND | -3.37 | 121.36 | 124.45 |
| 25 | 2 | 603 | CLA | C1-C2-C3 | -3.37 | 120.22 | 126.04 |
| 26 | 1 | 611 | CHL | C2C-C3C-C4C | 3.37 | 108.89 | 106.49 |
| 25 | B | 1219 | CLA | CHD-C1D-ND | -3.37 | 121.36 | 124.45 |
| 29 | 4 | 503 | BCR | C33-C5-C6 | -3.37 | 120.75 | 124.53 |
| 26 | A | 1114 | CHL | C2C-C3C-C4C | 3.36 | 108.89 | 106.49 |
| 25 | A | 1136 | CLA | CHD-C1D-ND | -3.36 | 121.36 | 124.45 |
| 25 | 1 | 601 | CLA | C1-C2-C3 | -3.36 | 120.23 | 126.04 |
| 43 | 3 | 502 | LUT | C7-C8-C9 | -3.36 | 121.16 | 126.23 |
| 25 | B | 1212 | CLA | C1-C2-C3 | -3.36 | 120.23 | 126.04 |
| 25 | 5 | 604 | CLA | C1-C2-C3 | -3.36 | 120.23 | 126.04 |
| 26 | 3 | 604 | CHL | C3C-C4C-NC | -3.36 | 106.80 | 110.57 |
| 26 | 5 | 610 | CHL | CHD-C1D-ND | -3.36 | 121.37 | 124.45 |
| 26 | 8 | 603 | CHL | C3C-C4C-NC | -3.36 | 106.81 | 110.57 |
| 25 | B | 1209 | CLA | CHD-C1D-ND | -3.35 | 121.37 | 124.45 |
| 25 | B | 1223 | CLA | C1-C2-C3 | -3.35 | 120.24 | 126.04 |
| 29 | H | 4001 | BCR | C1-C6-C5 | -3.35 | 117.89 | 122.61 |
| 43 | 3 | 502 | LUT | C18-C5-C6 | -3.35 | 120.77 | 124.53 |
| 25 | 3 | 616 | CLA | C2C-C1C-NC | 3.35 | 113.11 | 109.97 |
| 25 | A | 1110 | CLA | CHD-C1D-ND | -3.35 | 121.38 | 124.45 |
| 25 | 2 | 601 | CLA | CHD-C1D-ND | -3.35 | 121.38 | 124.45 |
| 25 | B | 1023 | CLA | CHD-C1D-ND | -3.35 | 121.38 | 124.45 |
| 29 | G | 4001 | BCR | C8-C9-C10 | 3.35 | 124.08 | 118.94 |
| 25 | A | 1112 | CLA | C2C-C1C-NC | 3.35 | 113.11 | 109.97 |
| 25 | a | 607 | CLA | C1-C2-C3 | -3.35 | 120.25 | 126.04 |
| 25 | O | 1802 | CLA | C1-C2-C3 | -3.35 | 120.26 | 126.04 |
| 43 | 5 | 502 | LUT | C15-C14-C13 | -3.34 | 122.54 | 127.31 |
| 25 | 6 | 603 | CLA | CHD-C1D-ND | -3.34 | 121.38 | 124.45 |
| 43 | a | 503 | LUT | C11-C10-C9 | -3.34 | 122.54 | 127.31 |
| 25 | O | 1802 | CLA | CHD-C1D-ND | -3.34 | 121.39 | 124.45 |
| 29 | K | 4002 | BCR | C33-C5-C6 | -3.34 | 120.78 | 124.53 |
| 25 | G | 1603 | CLA | CHD-C1D-ND | -3.34 | 121.39 | 124.45 |
| 25 | 1 | 607 | CLA | CHD-C1D-ND | -3.34 | 121.39 | 124.45 |
| 26 | 3 | 611 | CHL | C2C-C3C-C4C | 3.33 | 108.87 | 106.49 |
| 26 | 5 | 610 | CHL | C1-C2-C3 | -3.33 | 120.28 | 126.04 |
| 29 | B | 4001 | BCR | C23-C24-C25 | -3.33 | 117.84 | 127.20 |
| 25 | A | 1125 | CLA | C2D-C1D-ND | 3.33 | 112.56 | 110.10 |
| 25 | 5 | 609 | CLA | CHD-C1D-ND | -3.33 | 121.40 | 124.45 |
| 25 | B | 1224 | CLA | CHD-C1D-ND | -3.33 | 121.40 | 124.45 |
| 25 | 2 | 604 | CLA | C1-C2-C3 | -3.33 | 120.29 | 126.04 |
| 25 | 1 | 605 | CLA | CHD-C1D-ND | -3.33 | 121.40 | 124.45 |
| 25 | 3 | 606 | CLA | CHD-C1D-ND | -3.32 | 121.40 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | A | 4005 | BCR | C33-C5-C6 | -3.32 | 120.80 | 124.53 |
| 25 | B | 1234 | CLA | C1-C2-C3 | -3.32 | 120.29 | 126.04 |
| 25 | B | 1203 | CLA | CHD-C1D-ND | -3.32 | 121.40 | 124.45 |
| 25 | B | 1208 | CLA | C1-C2-C3 | -3.32 | 120.30 | 126.04 |
| 26 | 5 | 611 | CHL | C3C-C4C-NC | -3.32 | 106.84 | 110.57 |
| 25 | 8 | 620 | CLA | CHD-C1D-ND | -3.32 | 121.40 | 124.45 |
| 25 | A | 1102 | CLA | C1-C2-C3 | -3.32 | 120.30 | 126.04 |
| 44 | 1 | 502 | AXT | C12-C13-C14 | 3.32 | 124.04 | 118.94 |
| 26 | 6 | 609 | CHL | C3C-C4C-NC | -3.32 | 106.85 | 110.57 |
| 25 | 9 | 604 | CLA | C1-C2-C3 | -3.32 | 120.30 | 126.04 |
| 25 | A | 1131 | CLA | C2C-C1C-NC | 3.32 | 113.08 | 109.97 |
| 25 | 3 | 601 | CLA | CHD-C1D-ND | -3.32 | 121.41 | 124.45 |
| 25 | 2 | 606 | CLA | CHD-C1D-ND | -3.32 | 121.41 | 124.45 |
| 25 | 2 | 621 | CLA | C2C-C1C-NC | 3.32 | 113.08 | 109.97 |
| 29 | A | 4004 | BCR | C27-C26-C25 | -3.32 | 117.92 | 122.73 |
| 26 | a | 609 | CHL | C3C-C4C-NC | -3.32 | 106.85 | 110.57 |
| 25 | 4 | 611 | CLA | CHD-C1D-ND | -3.32 | 121.41 | 124.45 |
| 25 | J | 1901 | CLA | C2C-C1C-NC | 3.32 | 113.08 | 109.97 |
| 26 | a | 604 | CHL | C3C-C4C-NC | -3.31 | 106.86 | 110.57 |
| 25 | B | 1230 | CLA | CHD-C1D-ND | -3.31 | 121.41 | 124.45 |
| 25 | A | 1111 | CLA | CHD-C1D-ND | -3.31 | 121.41 | 124.45 |
| 25 | B | 1223 | CLA | C2D-C1D-ND | 3.31 | 112.55 | 110.10 |
| 26 | A | 1114 | CHL | C3C-C4C-NC | -3.31 | 106.86 | 110.57 |
| 25 | 7 | 602 | CLA | CHD-C1D-ND | -3.31 | 121.41 | 124.45 |
| 26 | 8 | 613 | CHL | C3C-C4C-NC | -3.31 | 106.86 | 110.57 |
| 25 | A | 1132 | CLA | CHD-C1D-ND | -3.31 | 121.41 | 124.45 |
| 25 | 7 | 612 | CLA | CHD-C1D-ND | -3.31 | 121.41 | 124.45 |
| 25 | A | 1125 | CLA | C1-C2-C3 | -3.31 | 120.32 | 126.04 |
| 25 | B | 1217 | CLA | CHD-C1D-ND | -3.31 | 121.42 | 124.45 |
| 25 | L | 1504 | CLA | C2C-C1C-NC | 3.30 | 113.07 | 109.97 |
| 25 | H | 1701 | CLA | C1-C2-C3 | -3.30 | 120.33 | 126.04 |
| 25 | 1 | 612 | CLA | CHD-C1D-ND | -3.30 | 121.42 | 124.45 |
| 25 | A | 1130 | CLA | CHD-C1D-ND | -3.30 | 121.42 | 124.45 |
| 29 | A | 4001 | BCR | C33-C5-C6 | -3.30 | 120.82 | 124.53 |
| 25 | 7 | 610 | CLA | C1-C2-C3 | -3.30 | 120.34 | 126.04 |
| 25 | 8 | 612 | CLA | C1-C2-C3 | -3.30 | 121.42 | 126.75 |
| 25 | A | 1117 | CLA | CHD-C1D-ND | -3.30 | 121.42 | 124.45 |
| 25 | A | 1138 | CLA | C1-C2-C3 | -3.30 | 120.34 | 126.04 |
| 25 | B | 1238 | CLA | CHD-C1D-ND | -3.30 | 121.42 | 124.45 |
| 29 | B | 4003 | BCR | C37-C22-C21 | -3.30 | 118.31 | 122.92 |
| 29 | 6 | 503 | BCR | C36-C18-C17 | -3.30 | 118.31 | 122.92 |
| 25 | 3 | 601 | CLA | C1-C2-C3 | -3.29 | 120.34 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1213 | CLA | C1-C2-C3 | -3.29 | 120.35 | 126.04 |
| 25 | A | 1139 | CLA | CHD-C1D-ND | -3.29 | 121.43 | 124.45 |
| 25 | G | 1602 | CLA | CHD-C1D-ND | -3.29 | 121.43 | 124.45 |
| 25 | 4 | 610 | CLA | C1-O2A-CGA | 3.29 | 125.08 | 116.44 |
| 25 | 9 | 612 | CLA | C2C-C1C-NC | 3.29 | 113.06 | 109.97 |
| 26 | 2 | 610 | CHL | CMA-C3A-C4A | 3.29 | 120.62 | 111.77 |
| 25 | A | 1102 | CLA | CHD-C1D-ND | -3.29 | 121.43 | 124.45 |
| 26 | 7 | 611 | CHL | C3C-C4C-NC | -3.29 | 106.88 | 110.57 |
| 25 | A | 1132 | CLA | C1-C2-C3 | -3.29 | 120.36 | 126.04 |
| 25 | B | 1206 | CLA | C1C-C2C-C3C | -3.29 | 103.50 | 106.96 |
| 25 | A | 1122 | CLA | C1-C2-C3 | -3.29 | 120.36 | 126.04 |
| 25 | a | 608 | CLA | CHD-C1D-ND | -3.29 | 121.44 | 124.45 |
| 25 | 8 | 609 | CLA | C2D-C1D-ND | 3.28 | 112.52 | 110.10 |
| 25 | 7 | 608 | CLA | C1-C2-C3 | -3.28 | 120.36 | 126.04 |
| 25 | B | 1202 | CLA | CHD-C1D-ND | -3.28 | 121.44 | 124.45 |
| 25 | 4 | 605 | CLA | C2C-C1C-NC | 3.28 | 113.05 | 109.97 |
| 29 | 3 | 504 | BCR | C19-C18-C17 | 3.28 | 123.97 | 118.94 |
| 25 | A | 1128 | CLA | C2C-C1C-NC | 3.28 | 113.04 | 109.97 |
| 25 | B | 1226 | CLA | C2C-C1C-NC | 3.28 | 113.04 | 109.97 |
| 25 | 7 | 606 | CLA | CHD-C1D-ND | -3.28 | 121.44 | 124.45 |
| 26 | 8 | 610 | CHL | CMA-C3A-C4A | 3.28 | 120.58 | 111.77 |
| 25 | H | 1701 | CLA | C2C-C1C-NC | 3.27 | 113.04 | 109.97 |
| 25 | a | 603 | CLA | CMA-C3A-C4A | 3.27 | 120.58 | 111.77 |
| 43 | 9 | 502 | LUT | C22-C23-C24 | -3.27 | 108.02 | 111.74 |
| 25 | 6 | 615 | CLA | O2D-CGD-O1D | -3.27 | 117.44 | 123.84 |
| 25 | 4 | 604 | CLA | CHD-C1D-ND | -3.27 | 121.45 | 124.45 |
| 25 | B | 1206 | CLA | C1-C2-C3 | -3.27 | 120.39 | 126.04 |
| 25 | L | 1501 | CLA | CHD-C1D-ND | -3.27 | 121.45 | 124.45 |
| 26 | 8 | 603 | CHL | C2C-C3C-C4C | 3.27 | 108.82 | 106.49 |
| 43 | 8 | 501 | LUT | C7-C8-C9 | -3.27 | 121.30 | 126.23 |
| 26 | 6 | 619 | CHL | C3C-C4C-NC | -3.27 | 106.91 | 110.57 |
| 25 | 4 | 617 | CLA | C2C-C1C-NC | 3.27 | 113.03 | 109.97 |
| 25 | 7 | 603 | CLA | CHD-C1D-ND | -3.27 | 121.45 | 124.45 |
| 25 | B | 1211 | CLA | CHD-C1D-ND | -3.26 | 121.45 | 124.45 |
| 25 | A | 1106 | CLA | CHD-C1D-ND | -3.26 | 121.45 | 124.45 |
| 25 | B | 1227 | CLA | CHD-C1D-ND | -3.26 | 121.46 | 124.45 |
| 25 | A | 1124 | CLA | CHD-C1D-ND | -3.26 | 121.46 | 124.45 |
| 25 | 6 | 606 | CLA | CHD-C1D-ND | -3.26 | 121.46 | 124.45 |
| 25 | 4 | 608 | CLA | C1-C2-C3 | -3.26 | 120.41 | 126.04 |
| 26 | 8 | 604 | CHL | C3C-C4C-NC | -3.26 | 106.92 | 110.57 |
| 25 | 4 | 611 | CLA | C1-C2-C3 | -3.26 | 120.41 | 126.04 |
| 26 | 6 | 619 | CHL | CMA-C3A-C4A | 3.26 | 120.53 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 6 | 612 | CLA | CHD-C1D-ND | -3.26 | 121.46 | 124.45 |
| 26 | 5 | 611 | CHL | C2C-C3C-C4C | 3.25 | 108.81 | 106.49 |
| 25 | A | 1134 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 25 | B | 1235 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 25 | 4 | 606 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 25 | 1 | 612 | CLA | C2C-C1C-NC | 3.25 | 113.02 | 109.97 |
| 25 | A | 1104 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 43 | 2 | 502 | LUT | C18-C5-C6 | -3.25 | 120.88 | 124.53 |
| 25 | B | 1207 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 29 | 3 | 505 | BCR | C36-C18-C17 | -3.25 | 118.37 | 122.92 |
| 25 | 2 | 607 | CLA | C2C-C1C-NC | 3.25 | 113.02 | 109.97 |
| 25 | 9 | 606 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 25 | B | 1207 | CLA | C1-C2-C3 | -3.25 | 120.43 | 126.04 |
| 26 | 7 | 611 | CHL | C2C-C3C-C4C | 3.25 | 108.80 | 106.49 |
| 25 | 5 | 607 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |
| 25 | a | 612 | CLA | CHD-C1D-ND | -3.24 | 121.47 | 124.45 |
| 29 | B | 4004 | BCR | C23-C24-C25 | -3.24 | 118.11 | 127.20 |
| 25 | B | 1219 | CLA | C1-C2-C3 | -3.24 | 120.44 | 126.04 |
| 25 | 5 | 602 | CLA | C1-C2-C3 | -3.24 | 120.44 | 126.04 |
| 25 | 4 | 610 | CLA | CHD-C1D-ND | -3.24 | 121.48 | 124.45 |
| 25 | 7 | 610 | CLA | CHD-C1D-ND | -3.24 | 121.48 | 124.45 |
| 26 | 6 | 613 | CHL | C3C-C4C-NC | -3.24 | 106.94 | 110.57 |
| 25 | A | 1131 | CLA | CHD-C1D-ND | -3.24 | 121.48 | 124.45 |
| 26 | 3 | 608 | CHL | C3C-C4C-NC | -3.23 | 106.94 | 110.57 |
| 25 | 7 | 608 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 25 | 9 | 604 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 25 | K | 1404 | CLA | C2C-C1C-NC | 3.23 | 113.00 | 109.97 |
| 25 | A | 1112 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 25 | 4 | 608 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 25 | 1 | 602 | CLA | C2C-C1C-NC | 3.23 | 113.00 | 109.97 |
| 25 | A | 1103 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 25 | 3 | 602 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 25 | 8 | 611 | CLA | CHD-C1D-ND | -3.23 | 121.48 | 124.45 |
| 26 | a | 606 | CHL | C3C-C4C-NC | -3.23 | 106.95 | 110.57 |
| 26 | 2 | 609 | CHL | C3C-C4C-NC | -3.23 | 106.95 | 110.57 |
| 25 | 7 | 608 | CLA | C2C-C1C-NC | 3.23 | 113.00 | 109.97 |
| 29 | B | 4003 | BCR | C33-C5-C4 | 3.23 | 119.81 | 113.62 |
| 26 | a | 604 | CHL | CMA-C3A-C4A | 3.23 | 120.44 | 111.77 |
| 25 | A | 1116 | CLA | CHD-C1D-ND | -3.23 | 121.49 | 124.45 |
| 29 | J | 4001 | BCR | C36-C18-C17 | -3.23 | 118.41 | 122.92 |
| 25 | B | 1226 | CLA | CMB-C2B-C1B | -3.23 | 123.51 | 128.46 |
| 25 | a | 608 | CLA | C2C-C1C-NC | 3.22 | 112.99 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 6 | 611 | CHL | C3C-C4C-NC | -3.22 | 106.96 | 110.57 |
| 25 | A | 1013 | CLA | CHD-C1D-ND | -3.22 | 121.49 | 124.45 |
| 25 | 5 | 607 | CLA | C1-C2-C3 | -3.22 | 120.47 | 126.04 |
| 25 | 1 | 603 | CLA | CHD-C1D-ND | -3.22 | 121.50 | 124.45 |
| 42 | M | 4001 | ECH | C28-C27-C26 | -3.22 | 115.68 | 118.65 |
| 25 | A | 1139 | CLA | C1-C2-C3 | -3.22 | 120.48 | 126.04 |
| 25 | B | 1201 | CLA | CHD-C1D-ND | -3.22 | 121.50 | 124.45 |
| 26 | 6 | 611 | CHL | C2C-C3C-C4C | 3.22 | 108.78 | 106.49 |
| 25 | 9 | 609 | CLA | CHD-C1D-ND | -3.22 | 121.50 | 124.45 |
| 26 | A | 1114 | CHL | CMA-C3A-C4A | 3.22 | 120.42 | 111.77 |
| 26 | 4 | 618 | CHL | C3C-C4C-NC | -3.22 | 106.96 | 110.57 |
| 25 | A | 1117 | CLA | C2C-C1C-NC | 3.22 | 112.98 | 109.97 |
| 25 | H | 1702 | CLA | C2C-C1C-NC | 3.22 | 112.98 | 109.97 |
| 25 | 5 | 602 | CLA | C2C-C1C-NC | 3.22 | 112.98 | 109.97 |
| 25 | A | 1120 | CLA | CHD-C1D-ND | -3.21 | 121.50 | 124.45 |
| 25 | 4 | 616 | CLA | C2C-C1C-NC | 3.21 | 112.98 | 109.97 |
| 25 | A | 1115 | CLA | C1-C2-C3 | -3.21 | 120.49 | 126.04 |
| 43 | a | 501 | LUT | C7-C8-C9 | -3.21 | 121.38 | 126.23 |
| 25 | B | 1237 | CLA | CHD-C1D-ND | -3.21 | 121.50 | 124.45 |
| 25 | F | 1301 | CLA | CHD-C1D-ND | -3.21 | 121.50 | 124.45 |
| 26 | 3 | 604 | CHL | C2C-C3C-C4C | 3.21 | 108.78 | 106.49 |
| 26 | 4 | 609 | CHL | C2C-C3C-C4C | 3.21 | 108.78 | 106.49 |
| 25 | 6 | 615 | CLA | CHD-C1D-ND | -3.21 | 121.51 | 124.45 |
| 35 | 2 | 804 | LMT | C1'-O5'-C5' | -3.21 | 107.39 | 113.69 |
| 50 | 9 | 507 | XAT | C31-C30-C29 | -3.21 | 122.73 | 127.31 |
| 25 | B | 1204 | CLA | C2D-C1D-ND | 3.20 | 112.47 | 110.10 |
| 25 | B | 1210 | CLA | C1-C2-C3 | -3.20 | 120.50 | 126.04 |
| 25 | O | 1801 | CLA | CHD-C1D-ND | -3.20 | 121.51 | 124.45 |
| 26 | 2 | 610 | CHL | C3C-C4C-NC | -3.20 | 106.98 | 110.57 |
| 50 | 7 | 502 | XAT | C26-C27-C28 | -3.20 | 119.22 | 125.99 |
| 25 | B | 1237 | CLA | CMA-C3A-C4A | 3.20 | 120.38 | 111.77 |
| 25 | B | 1205 | CLA | CHD-C1D-ND | -3.20 | 121.51 | 124.45 |
| 25 | a | 605 | CLA | CHD-C1D-ND | -3.20 | 121.51 | 124.45 |
| 25 | 6 | 602 | CLA | C1-C2-C3 | -3.20 | 120.51 | 126.04 |
| 25 | A | 1129 | CLA | CHD-C1D-ND | -3.20 | 121.52 | 124.45 |
| 26 | 6 | 617 | CHL | C2C-C3C-C4C | 3.20 | 108.77 | 106.49 |
| 26 | 5 | 611 | CHL | C1-C2-C3 | -3.20 | 121.58 | 126.75 |
| 25 | K | 1403 | CLA | C2C-C1C-NC | 3.19 | 112.97 | 109.97 |
| 44 | 7 | 504 | AXT | C15-C14-C13 | 3.19 | 131.87 | 127.31 |
| 39 | F | 4001 | NEX | C39-C29-C30 | -3.19 | 118.45 | 122.92 |
| 25 | B | 1214 | CLA | C1-C2-C3 | -3.19 | 120.53 | 126.04 |
| 26 | 9 | 608 | CHL | C3C-C4C-NC | -3.19 | 107.00 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | L | 4002 | BCR | C36-C18-C17 | -3.19 | 118.46 | 122.92 |
| 25 | A | 1135 | CLA | CHD-C1D-ND | -3.19 | 121.53 | 124.45 |
| 25 | 5 | 606 | CLA | CHD-C1D-ND | -3.19 | 121.53 | 124.45 |
| 25 | 1 | 606 | CLA | CHD-C1D-ND | -3.19 | 121.53 | 124.45 |
| 25 | 2 | 608 | CLA | CHD-C1D-ND | -3.19 | 121.53 | 124.45 |
| 25 | a | 615 | CLA | C2D-C1D-ND | 3.18 | 112.45 | 110.10 |
| 26 | 4 | 609 | CHL | C1-C2-C3 | -3.18 | 120.54 | 126.04 |
| 25 | 3 | 616 | CLA | CHD-C1D-ND | -3.18 | 121.53 | 124.45 |
| 26 | 6 | 609 | CHL | CMA-C3A-C4A | 3.18 | 120.32 | 111.77 |
| 43 | 1 | 503 | LUT | C18-C5-C6 | -3.18 | 120.96 | 124.53 |
| 25 | 9 | 605 | CLA | C2C-C1C-NC | 3.18 | 112.95 | 109.97 |
| 25 | A | 1118 | CLA | CHD-C1D-ND | -3.18 | 121.53 | 124.45 |
| 25 | a | 607 | CLA | CHD-C1D-ND | -3.18 | 121.53 | 124.45 |
| 29 | 3 | 503 | BCR | C23-C24-C25 | -3.18 | 118.28 | 127.20 |
| 25 | a | 611 | CLA | C1-C2-C3 | -3.18 | 121.61 | 126.75 |
| 25 | B | 1212 | CLA | CHD-C1D-ND | -3.18 | 121.53 | 124.45 |
| 25 | 1 | 615 | CLA | C2C-C1C-NC | 3.18 | 112.95 | 109.97 |
| 25 | B | 1210 | CLA | CHD-C1D-ND | -3.17 | 121.54 | 124.45 |
| 43 | 2 | 507 | LUT | C20-C13-C14 | -3.17 | 118.48 | 122.92 |
| 25 | a | 611 | CLA | C2C-C1C-NC | 3.17 | 112.94 | 109.97 |
| 27 | A | 2001 | PQN | C14-C13-C15 | 3.17 | 120.60 | 115.27 |
| 25 | 7 | 606 | CLA | C1C-C2C-C3C | -3.17 | 104.16 | 107.07 |
| 25 | 7 | 612 | CLA | C2C-C1C-NC | 3.17 | 112.94 | 109.97 |
| 25 | A | 1118 | CLA | C2C-C1C-NC | 3.17 | 112.94 | 109.97 |
| 25 | B | 1217 | CLA | C2C-C1C-NC | 3.17 | 112.94 | 109.97 |
| 25 | a | 612 | CLA | C2C-C1C-NC | 3.17 | 112.94 | 109.97 |
| 43 | 4 | 502 | LUT | C15-C14-C13 | -3.17 | 122.79 | 127.31 |
| 25 | 5 | 614 | CLA | CHD-C1D-ND | -3.17 | 121.55 | 124.45 |
| 26 | 8 | 601 | CHL | C2C-C3C-C4C | 3.16 | 108.75 | 106.49 |
| 26 | 6 | 617 | CHL | C3C-C4C-NC | -3.16 | 107.02 | 110.57 |
| 25 | 2 | 615 | CLA | C2D-C1D-ND | 3.16 | 112.44 | 110.10 |
| 25 | 4 | 612 | CLA | C2C-C1C-NC | 3.16 | 112.94 | 109.97 |
| 25 | B | 1230 | CLA | C1-C2-C3 | -3.16 | 120.57 | 126.04 |
| 25 | B | 1221 | CLA | CHD-C1D-ND | -3.16 | 121.55 | 124.45 |
| 25 | 3 | 605 | CLA | CHD-C1D-ND | -3.16 | 121.55 | 124.45 |
| 25 | 2 | 603 | CLA | C2C-C1C-NC | 3.16 | 112.94 | 109.97 |
| 29 | 3 | 504 | BCR | C27-C26-C25 | -3.16 | 118.14 | 122.73 |
| 26 | 3 | 608 | CHL | C2C-C3C-C4C | 3.16 | 108.74 | 106.49 |
| 25 | B | 1221 | CLA | C2C-C1C-NC | 3.16 | 112.93 | 109.97 |
| 25 | O | 1803 | CLA | C2C-C1C-NC | 3.16 | 112.93 | 109.97 |
| 25 | 6 | 602 | CLA | C2C-C1C-NC | 3.16 | 112.93 | 109.97 |
| 29 | 3 | 504 | BCR | C33-C5-C6 | -3.16 | 120.98 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | F | 4001 | NEX | C38-C25-C24 | 3.16 | 117.83 | 114.28 |
| 25 | A | 1135 | CLA | C2C-C1C-NC | 3.16 | 112.93 | 109.97 |
| 25 | 6 | 606 | CLA | C2C-C1C-NC | 3.16 | 112.93 | 109.97 |
| 43 | 5 | 501 | LUT | C15-C14-C13 | -3.16 | 122.81 | 127.31 |
| 25 | F | 1302 | CLA | CHD-C1D-ND | -3.16 | 121.55 | 124.45 |
| 25 | 3 | 607 | CLA | C2C-C1C-NC | 3.16 | 112.93 | 109.97 |
| 26 | 8 | 610 | CHL | C4D-CHA-C1A | 3.15 | 125.09 | 121.25 |
| 25 | 3 | 613 | CLA | CHD-C1D-ND | -3.15 | 121.56 | 124.45 |
| 25 | 7 | 603 | CLA | C2C-C1C-NC | 3.15 | 112.93 | 109.97 |
| 27 | B | 2002 | PQN | C11-C12-C13 | -3.15 | 121.54 | 126.79 |
| 25 | A | 1124 | CLA | C1-C2-C3 | -3.15 | 120.59 | 126.04 |
| 25 | 8 | 607 | CLA | CHD-C1D-ND | -3.15 | 121.56 | 124.45 |
| 26 | 7 | 609 | CHL | C2C-C3C-C4C | 3.15 | 108.73 | 106.49 |
| 29 | B | 4001 | BCR | C12-C13-C14 | -3.15 | 114.11 | 118.94 |
| 25 | 6 | 605 | CLA | CHD-C1D-ND | -3.15 | 121.56 | 124.45 |
| 25 | 4 | 616 | CLA | CHD-C1D-ND | -3.15 | 121.56 | 124.45 |
| 25 | A | 1141 | CLA | C2C-C1C-NC | 3.15 | 112.92 | 109.97 |
| 25 | B | 1204 | CLA | C2C-C1C-NC | 3.14 | 112.92 | 109.97 |
| 25 | 4 | 607 | CLA | C2C-C1C-NC | 3.14 | 112.92 | 109.97 |
| 25 | 5 | 608 | CLA | C2C-C1C-NC | 3.14 | 112.92 | 109.97 |
| 25 | 2 | 621 | CLA | CHD-C1D-ND | -3.14 | 121.56 | 124.45 |
| 25 | B | 1239 | CLA | C1-C2-C3 | -3.14 | 120.61 | 126.04 |
| 25 | 4 | 602 | CLA | C2C-C1C-NC | 3.14 | 112.92 | 109.97 |
| 25 | O | 1801 | CLA | C2C-C1C-NC | 3.14 | 112.92 | 109.97 |
| 26 | 3 | 604 | CHL | CMA-C3A-C4A | 3.14 | 120.22 | 111.77 |
| 26 | 1 | 604 | CHL | C2C-C3C-C4C | 3.14 | 108.73 | 106.49 |
| 25 | B | 1237 | CLA | C1-C2-C3 | -3.14 | 120.61 | 126.04 |
| 25 | 7 | 607 | CLA | C2C-C1C-NC | 3.14 | 112.92 | 109.97 |
| 25 | 3 | 618 | CLA | CHD-C1D-ND | -3.14 | 121.57 | 124.45 |
| 29 | B | 4002 | BCR | C23-C24-C25 | -3.14 | 118.38 | 127.20 |
| 25 | a | 608 | CLA | CMA-C3A-C4A | 3.14 | 120.21 | 111.77 |
| 25 | A | 1103 | CLA | C1-C2-C3 | -3.14 | 120.61 | 126.04 |
| 26 | 5 | 618 | CHL | C1-C2-C3 | -3.14 | 121.67 | 126.75 |
| 25 | 4 | 611 | CLA | C2C-C1C-NC | 3.14 | 112.91 | 109.97 |
| 25 | 4 | 615 | CLA | C2C-C1C-NC | 3.14 | 112.91 | 109.97 |
| 25 | 9 | 612 | CLA | CHD-C1D-ND | -3.14 | 121.57 | 124.45 |
| 25 | 1 | 603 | CLA | CMA-C3A-C4A | 3.14 | 120.21 | 111.77 |
| 25 | B | 1218 | CLA | O2D-CGD-O1D | -3.14 | 117.70 | 123.84 |
| 26 | a | 613 | CHL | CMA-C3A-C4A | 3.14 | 120.20 | 111.77 |
| 25 | 3 | 607 | CLA | CHD-C1D-ND | -3.14 | 121.57 | 124.45 |
| 25 | 8 | 602 | CLA | CHD-C1D-ND | -3.14 | 121.57 | 124.45 |
| 25 | B | 1215 | CLA | C2C-C1C-NC | 3.14 | 112.91 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1140 | CLA | CHD-C1D-ND | -3.13 | 121.57 | 124.45 |
| 25 | 9 | 607 | CLA | CHD-C1D-ND | -3.13 | 121.57 | 124.45 |
| 25 | B | 1219 | CLA | C2C-C1C-NC | 3.13 | 112.91 | 109.97 |
| 25 | a | 611 | CLA | CHD-C1D-ND | -3.13 | 121.58 | 124.45 |
| 25 | B | 1236 | CLA | C2D-C1D-ND | 3.13 | 112.41 | 110.10 |
| 25 | 4 | 617 | CLA | CMA-C3A-C4A | 3.13 | 120.19 | 111.77 |
| 26 | 2 | 613 | CHL | C3C-C4C-NC | -3.13 | 107.06 | 110.57 |
| 25 | 4 | 610 | CLA | C2C-C1C-NC | 3.13 | 112.90 | 109.97 |
| 25 | O | 1803 | CLA | CHD-C1D-ND | -3.13 | 121.58 | 124.45 |
| 25 | 5 | 615 | CLA | C2C-C1C-NC | 3.13 | 112.90 | 109.97 |
| 25 | 2 | 602 | CLA | C2C-C1C-NC | 3.13 | 112.90 | 109.97 |
| 25 | A | 1132 | CLA | C2C-C1C-NC | 3.13 | 112.90 | 109.97 |
| 25 | B | 1214 | CLA | C2C-C1C-NC | 3.13 | 112.90 | 109.97 |
| 25 | a | 607 | CLA | C2C-C1C-NC | 3.13 | 112.90 | 109.97 |
| 26 | 9 | 613 | CHL | C3C-C4C-NC | -3.13 | 107.07 | 110.57 |
| 26 | 7 | 617 | CHL | C3C-C4C-NC | -3.12 | 107.07 | 110.57 |
| 25 | B | 1240 | CLA | C2C-C1C-NC | 3.12 | 112.90 | 109.97 |
| 25 | 5 | 607 | CLA | C2C-C1C-NC | 3.12 | 112.90 | 109.97 |
| 25 | 8 | 609 | CLA | CHD-C1D-ND | -3.12 | 121.58 | 124.45 |
| 25 | 3 | 610 | CLA | C1-C2-C3 | -3.12 | 120.64 | 126.04 |
| 26 | 4 | 613 | CHL | CMA-C3A-C4A | 3.12 | 120.17 | 111.77 |
| 25 | 4 | 612 | CLA | O2D-CGD-O1D | -3.12 | 117.73 | 123.84 |
| 26 | 6 | 609 | CHL | C2C-C3C-C4C | 3.12 | 108.72 | 106.49 |
| 25 | B | 1225 | CLA | CHD-C1D-ND | -3.12 | 121.58 | 124.45 |
| 25 | 6 | 618 | CLA | C2C-C1C-NC | 3.12 | 112.90 | 109.97 |
| 26 | 9 | 610 | CHL | C1-C2-C3 | -3.12 | 121.70 | 126.75 |
| 25 | O | 1802 | CLA | C2C-C1C-NC | 3.12 | 112.89 | 109.97 |
| 25 | A | 1117 | CLA | O2D-CGD-O1D | -3.12 | 117.74 | 123.84 |
| 26 | 5 | 611 | CHL | CMA-C3A-C4A | 3.12 | 120.15 | 111.77 |
| 43 | 8 | 502 | LUT | C22-C23-C24 | -3.12 | 108.19 | 111.74 |
| 25 | O | 1801 | CLA | C1C-C2C-C3C | -3.12 | 104.21 | 107.07 |
| 26 | 3 | 608 | CHL | C4D-CHA-C1A | 3.12 | 125.04 | 121.25 |
| 43 | 1 | 503 | LUT | C12-C13-C14 | -3.12 | 114.16 | 118.94 |
| 26 | 1 | 610 | CHL | C4D-CHA-C1A | 3.11 | 125.04 | 121.25 |
| 25 | 2 | 603 | CLA | CHD-C1D-ND | -3.11 | 121.59 | 124.45 |
| 26 | 6 | 611 | CHL | CMA-C3A-C4A | 3.11 | 120.14 | 111.77 |
| 25 | B | 1229 | CLA | C2D-C1D-ND | 3.11 | 112.40 | 110.10 |
| 42 | M | 4001 | ECH | C23-C24-C25 | -3.11 | 118.46 | 127.20 |
| 25 | K | 1401 | CLA | C2C-C1C-NC | 3.11 | 112.89 | 109.97 |
| 29 | A | 4002 | BCR | C33-C5-C6 | -3.11 | 121.03 | 124.53 |
| 43 | 3 | 501 | LUT | C15-C14-C13 | -3.11 | 122.87 | 127.31 |
| 25 | G | 1601 | CLA | C2C-C1C-NC | 3.11 | 112.89 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 8 | 603 | CHL | CMA-C3A-C4A | 3.11 | 120.13 | 111.77 |
| 25 | 3 | 618 | CLA | C2C-C1C-NC | 3.11 | 112.88 | 109.97 |
| 25 | 6 | 607 | CLA | C2C-C1C-NC | 3.11 | 112.88 | 109.97 |
| 25 | B | 1232 | CLA | CHD-C1D-ND | -3.11 | 121.60 | 124.45 |
| 25 | 1 | 615 | CLA | CHD-C1D-ND | -3.11 | 121.60 | 124.45 |
| 26 | 5 | 613 | CHL | C3C-C4C-NC | -3.11 | 107.09 | 110.57 |
| 25 | L | 1504 | CLA | CMA-C3A-C4A | 3.11 | 120.12 | 111.77 |
| 25 | A | 1101 | CLA | CHD-C1D-ND | -3.11 | 121.60 | 124.45 |
| 25 | 7 | 602 | CLA | C2C-C1C-NC | 3.11 | 112.88 | 109.97 |
| 25 | B | 1239 | CLA | C2C-C1C-NC | 3.10 | 112.88 | 109.97 |
| 29 | A | 4003 | BCR | C27-C26-C25 | -3.10 | 118.22 | 122.73 |
| 25 | A | 1125 | CLA | CHD-C1D-ND | -3.10 | 121.60 | 124.45 |
| 26 | 2 | 613 | CHL | C1-C2-C3 | -3.10 | 121.73 | 126.75 |
| 26 | 7 | 617 | CHL | C2C-C3C-C4C | 3.10 | 108.70 | 106.49 |
| 26 | 1 | 604 | CHL | CMA-C3A-C4A | 3.10 | 120.11 | 111.77 |
| 26 | 1 | 610 | CHL | C3C-C4C-NC | -3.10 | 107.09 | 110.57 |
| 25 | 1 | 603 | CLA | C2C-C1C-NC | 3.10 | 112.88 | 109.97 |
| 29 | K | 4001 | BCR | C36-C18-C17 | -3.10 | 118.58 | 122.92 |
| 25 | 7 | 603 | CLA | CMA-C3A-C4A | 3.10 | 120.11 | 111.77 |
| 25 | 6 | 607 | CLA | C1-C2-C3 | -3.10 | 120.68 | 126.04 |
| 25 | A | 1141 | CLA | CMA-C3A-C4A | 3.10 | 120.11 | 111.77 |
| 25 | 6 | 604 | CLA | CMA-C3A-C4A | 3.10 | 120.11 | 111.77 |
| 43 | 7 | 501 | LUT | C35-C15-C14 | -3.10 | 117.12 | 123.47 |
| 25 | B | 1205 | CLA | C1-C2-C3 | -3.10 | 120.68 | 126.04 |
| 25 | B | 1206 | CLA | CHD-C1D-ND | -3.10 | 121.61 | 124.45 |
| 25 | L | 1503 | CLA | C2C-C1C-NC | 3.10 | 112.87 | 109.97 |
| 25 | 2 | 607 | CLA | CHD-C1D-ND | -3.10 | 121.61 | 124.45 |
| 29 | A | 4002 | BCR | C36-C18-C17 | -3.10 | 118.59 | 122.92 |
| 26 | 1 | 613 | CHL | C3C-C4C-NC | -3.09 | 107.10 | 110.57 |
| 25 | 9 | 602 | CLA | CHD-C1D-ND | -3.09 | 121.61 | 124.45 |
| 29 | 5 | 504 | BCR | C4-C5-C6 | -3.09 | 118.24 | 122.73 |
| 43 | 2 | 507 | LUT | C20-C13-C12 | 3.09 | 122.95 | 118.08 |
| 25 | 4 | 607 | CLA | CHD-C1D-ND | -3.09 | 121.61 | 124.45 |
| 43 | a | 502 | LUT | C15-C14-C13 | -3.09 | 122.90 | 127.31 |
| 29 | K | 4002 | BCR | C36-C18-C17 | -3.09 | 118.60 | 122.92 |
| 25 | 2 | 608 | CLA | C2C-C1C-NC | 3.09 | 112.86 | 109.97 |
| 25 | 5 | 609 | CLA | C2C-C1C-NC | 3.09 | 112.86 | 109.97 |
| 43 | 8 | 501 | LUT | C35-C34-C33 | -3.09 | 122.91 | 127.31 |
| 25 | 6 | 607 | CLA | CHD-C1D-ND | -3.08 | 121.62 | 124.45 |
| 26 | 2 | 613 | CHL | CHD-C1D-ND | -3.08 | 121.62 | 124.45 |
| 29 | A | 4003 | BCR | C19-C18-C17 | 3.08 | 123.67 | 118.94 |
| 25 | 6 | 608 | CLA | C1-C2-C3 | -3.08 | 120.71 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 606 | CLA | C2C-C1C-NC | 3.08 | 112.86 | 109.97 |
| 26 | 6 | 610 | CHL | C3C-C4C-NC | -3.08 | 107.12 | 110.57 |
| 26 | 1 | 609 | CHL | CHD-C1D-ND | -3.08 | 121.62 | 124.45 |
| 29 | B | 4003 | BCR | C34-C9-C10 | -3.08 | 118.61 | 122.92 |
| 25 | 9 | 607 | CLA | C2C-C1C-NC | 3.08 | 112.86 | 109.97 |
| 25 | H | 1701 | CLA | CHD-C1D-ND | -3.08 | 121.62 | 124.45 |
| 29 | B | 4005 | BCR | C23-C24-C25 | -3.08 | 118.56 | 127.20 |
| 25 | 6 | 603 | CLA | CMA-C3A-C4A | 3.08 | 120.04 | 111.77 |
| 25 | 6 | 608 | CLA | C2C-C1C-NC | 3.08 | 112.85 | 109.97 |
| 25 | A | 1110 | CLA | C1-O2A-CGA | 3.08 | 124.51 | 116.44 |
| 25 | G | 1603 | CLA | C2C-C1C-NC | 3.08 | 112.85 | 109.97 |
| 29 | K | 4001 | BCR | C33-C5-C6 | -3.07 | 121.08 | 124.53 |
| 26 | 1 | 611 | CHL | CMA-C3A-C4A | 3.07 | 120.04 | 111.77 |
| 25 | a | 603 | CLA | C2C-C1C-NC | 3.07 | 112.85 | 109.97 |
| 25 | 9 | 609 | CLA | C2C-C1C-NC | 3.07 | 112.85 | 109.97 |
| 27 | A | 2001 | PQN | C11-C12-C13 | -3.07 | 121.67 | 126.79 |
| 26 | a | 610 | CHL | C3C-C4C-NC | -3.07 | 107.12 | 110.57 |
| 26 | 4 | 613 | CHL | C3C-C4C-NC | -3.07 | 107.12 | 110.57 |
| 25 | K | 1402 | CLA | C2C-C1C-NC | 3.07 | 112.85 | 109.97 |
| 25 | L | 1501 | CLA | CMA-C3A-C4A | 3.07 | 120.03 | 111.77 |
| 26 | 6 | 610 | CHL | CMA-C3A-C4A | 3.07 | 120.02 | 111.77 |
| 25 | J | 1901 | CLA | CHD-C1D-ND | -3.07 | 121.63 | 124.45 |
| 25 | K | 1403 | CLA | CHD-C1D-ND | -3.07 | 121.63 | 124.45 |
| 25 | A | 1106 | CLA | C2D-C1D-ND | 3.07 | 112.36 | 110.10 |
| 43 | 2 | 502 | LUT | C11-C10-C9 | -3.07 | 122.93 | 127.31 |
| 25 | 1 | 607 | CLA | C1-C2-C3 | -3.07 | 120.74 | 126.04 |
| 26 | 6 | 613 | CHL | C1-C2-C3 | -3.07 | 121.79 | 126.75 |
| 25 | 6 | 615 | CLA | C2D-C1D-ND | 3.07 | 112.36 | 110.10 |
| 29 | A | 4004 | BCR | C38-C26-C27 | 3.07 | 119.50 | 113.62 |
| 25 | 2 | 612 | CLA | C2C-C1C-NC | 3.06 | 112.84 | 109.97 |
| 26 | a | 604 | CHL | C2C-C3C-C4C | 3.06 | 108.67 | 106.49 |
| 25 | B | 1224 | CLA | C2C-C1C-NC | 3.06 | 112.84 | 109.97 |
| 25 | 2 | 605 | CLA | C1-C2-C3 | -3.06 | 120.75 | 126.04 |
| 25 | 6 | 615 | CLA | C2C-C1C-NC | 3.06 | 112.84 | 109.97 |
| 25 | 1 | 606 | CLA | O2D-CGD-O1D | -3.06 | 117.85 | 123.84 |
| 25 | K | 1402 | CLA | CHD-C1D-ND | -3.06 | 121.64 | 124.45 |
| 26 | 5 | 618 | CHL | CMA-C3A-C4A | 3.06 | 120.00 | 111.77 |
| 25 | 9 | 602 | CLA | C2C-C1C-NC | 3.06 | 112.84 | 109.97 |
| 25 | B | 1225 | CLA | C2C-C1C-NC | 3.06 | 112.84 | 109.97 |
| 26 | 6 | 617 | CHL | CMA-C3A-C4A | 3.06 | 120.00 | 111.77 |
| 26 | 9 | 601 | CHL | C1-C2-C3 | -3.06 | 120.75 | 126.04 |
| 25 | 4 | 602 | CLA | CHD-C1D-ND | -3.06 | 121.64 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 1 | 609 | CHL | CMA-C3A-C4A | 3.06 | 119.99 | 111.77 |
| 29 | B | 4006 | BCR | C33-C5-C6 | -3.06 | 121.09 | 124.53 |
| 26 | 8 | 613 | CHL | C2C-C3C-C4C | 3.06 | 108.67 | 106.49 |
| 43 | 5 | 501 | LUT | C7-C8-C9 | -3.06 | 121.62 | 126.23 |
| 25 | 7 | 607 | CLA | CHD-C1D-ND | -3.06 | 121.65 | 124.45 |
| 25 | 8 | 609 | CLA | C2C-C1C-NC | 3.06 | 112.83 | 109.97 |
| 25 | 2 | 602 | CLA | CHD-C1D-ND | -3.05 | 121.65 | 124.45 |
| 25 | K | 1404 | CLA | O2D-CGD-O1D | -3.05 | 117.87 | 123.84 |
| 25 | 4 | 617 | CLA | CHD-C1D-ND | -3.05 | 121.65 | 124.45 |
| 25 | 2 | 605 | CLA | CHD-C1D-ND | -3.05 | 121.65 | 124.45 |
| 26 | 1 | 613 | CHL | CMA-C3A-C4A | 3.05 | 119.98 | 111.77 |
| 25 | B | 1227 | CLA | C2C-C1C-NC | 3.05 | 112.83 | 109.97 |
| 43 | 3 | 502 | LUT | C35-C34-C33 | -3.05 | 122.96 | 127.31 |
| 26 | 3 | 603 | CHL | CMA-C3A-C4A | 3.05 | 119.97 | 111.77 |
| 25 | 6 | 612 | CLA | C2C-C1C-NC | 3.05 | 112.83 | 109.97 |
| 26 | 5 | 610 | CHL | C3C-C4C-NC | -3.05 | 107.16 | 110.57 |
| 25 | A | 1107 | CLA | CHD-C1D-ND | -3.04 | 121.66 | 124.45 |
| 43 | 6 | 501 | LUT | C15-C14-C13 | -3.04 | 122.97 | 127.31 |
| 25 | B | 1203 | CLA | C2C-C1C-NC | 3.04 | 112.82 | 109.97 |
| 43 | 3 | 501 | LUT | C7-C8-C9 | -3.04 | 121.64 | 126.23 |
| 25 | L | 1504 | CLA | CHD-C1D-ND | -3.04 | 121.66 | 124.45 |
| 25 | a | 602 | CLA | C2C-C1C-NC | 3.04 | 112.82 | 109.97 |
| 25 | 4 | 615 | CLA | C1-C2-C3 | -3.04 | 120.78 | 126.04 |
| 26 | 8 | 610 | CHL | C3C-C4C-NC | -3.04 | 107.16 | 110.57 |
| 44 | 1 | 502 | AXT | C15-C35-C34 | 3.04 | 129.71 | 123.47 |
| 25 | A | 1128 | CLA | CMB-C2B-C1B | -3.04 | 123.79 | 128.46 |
| 26 | 9 | 601 | CHL | C2C-C3C-C4C | 3.04 | 108.66 | 106.49 |
| 25 | 8 | 608 | CLA | C2C-C1C-NC | 3.04 | 112.82 | 109.97 |
| 25 | A | 1136 | CLA | CMA-C3A-C4A | 3.04 | 119.94 | 111.77 |
| 26 | 9 | 601 | CHL | CMA-C3A-C4A | 3.04 | 119.94 | 111.77 |
| 29 | A | 4001 | BCR | C23-C24-C25 | -3.04 | 118.67 | 127.20 |
| 29 | 6 | 504 | BCR | C36-C18-C17 | -3.04 | 118.67 | 122.92 |
| 25 | 5 | 615 | CLA | CHD-C1D-ND | -3.04 | 121.66 | 124.45 |
| 25 | 7 | 610 | CLA | C2C-C1C-NC | 3.04 | 112.82 | 109.97 |
| 26 | 2 | 610 | CHL | C2C-C3C-C4C | 3.04 | 108.65 | 106.49 |
| 25 | H | 1702 | CLA | CHD-C1D-ND | -3.04 | 121.66 | 124.45 |
| 29 | B | 4004 | BCR | C33-C5-C4 | 3.04 | 119.45 | 113.62 |
| 25 | B | 1207 | CLA | C2C-C1C-NC | 3.04 | 112.82 | 109.97 |
| 25 | a | 602 | CLA | CHD-C1D-ND | -3.04 | 121.66 | 124.45 |
| 25 | A | 1012 | CLA | C2C-C1C-NC | 3.04 | 112.82 | 109.97 |
| 25 | B | 1214 | CLA | CHD-C1D-ND | -3.03 | 121.67 | 124.45 |
| 25 | B | 1022 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 2 | 613 | CHL | C2C-C3C-C4C | 3.03 | 108.65 | 106.49 |
| 25 | B | 1230 | CLA | C2D-C1D-ND | 3.03 | 112.34 | 110.10 |
| 25 | 1 | 607 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |
| 25 | 7 | 602 | CLA | C1C-C2C-C3C | -3.03 | 104.29 | 107.07 |
| 25 | 8 | 620 | CLA | C2D-C1D-ND | 3.03 | 112.34 | 110.10 |
| 25 | B | 1228 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |
| 25 | B | 1217 | CLA | C1-C2-C3 | -3.03 | 120.80 | 126.04 |
| 25 | A | 1129 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |
| 25 | L | 1501 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |
| 25 | 7 | 605 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |
| 43 | 9 | 502 | LUT | C7-C8-C9 | -3.03 | 121.66 | 126.23 |
| 26 | 8 | 604 | CHL | C2C-C3C-C4C | 3.03 | 108.65 | 106.49 |
| 25 | B | 1205 | CLA | C2C-C1C-NC | 3.03 | 112.81 | 109.97 |
| 25 | A | 1113 | CLA | C1-C2-C3 | -3.03 | 120.81 | 126.04 |
| 25 | B | 1022 | CLA | C1-C2-C3 | -3.02 | 120.81 | 126.04 |
| 25 | H | 1702 | CLA | CMA-C3A-C4A | 3.02 | 119.90 | 111.77 |
| 29 | B | 4003 | BCR | C23-C22-C21 | 3.02 | 123.58 | 118.94 |
| 25 | O | 1803 | CLA | CMA-C3A-C4A | 3.02 | 119.90 | 111.77 |
| 25 | 3 | 602 | CLA | C2C-C1C-NC | 3.02 | 112.80 | 109.97 |
| 29 | G | 4001 | BCR | C34-C9-C10 | -3.02 | 118.69 | 122.92 |
| 26 | 1 | 609 | CHL | C1-C2-C3 | -3.02 | 120.82 | 126.04 |
| 25 | 8 | 605 | CLA | C2C-C1C-NC | 3.02 | 112.80 | 109.97 |
| 25 | 4 | 611 | CLA | CMA-C3A-C4A | 3.02 | 119.89 | 111.77 |
| 26 | 5 | 618 | CHL | C3C-C4C-NC | -3.02 | 107.18 | 110.57 |
| 25 | A | 1141 | CLA | O2D-CGD-O1D | -3.02 | 117.93 | 123.84 |
| 25 | a | 615 | CLA | CMA-C3A-C4A | 3.02 | 119.89 | 111.77 |
| 25 | G | 1603 | CLA | CMA-C3A-C4A | 3.02 | 119.89 | 111.77 |
| 26 | 9 | 613 | CHL | CMA-C3A-C4A | 3.02 | 119.89 | 111.77 |
| 25 | A | 1115 | CLA | CHD-C1D-ND | -3.02 | 121.68 | 124.45 |
| 25 | 6 | 618 | CLA | CMA-C3A-C4A | 3.02 | 119.88 | 111.77 |
| 25 | 4 | 603 | CLA | CMA-C3A-C4A | 3.02 | 119.88 | 111.77 |
| 26 | 3 | 603 | CHL | C3C-C4C-NC | -3.02 | 107.19 | 110.57 |
| 29 | B | 4003 | BCR | C36-C18-C17 | -3.02 | 118.70 | 122.92 |
| 25 | A | 1111 | CLA | C2C-C1C-NC | 3.02 | 112.80 | 109.97 |
| 25 | A | 1134 | CLA | C2C-C1C-NC | 3.02 | 112.80 | 109.97 |
| 25 | 7 | 606 | CLA | C2C-C1C-NC | 3.02 | 112.80 | 109.97 |
| 25 | B | 1218 | CLA | C2C-C1C-NC | 3.01 | 112.80 | 109.97 |
| 25 | 6 | 603 | CLA | C2C-C1C-NC | 3.01 | 112.80 | 109.97 |
| 25 | 9 | 604 | CLA | C2C-C1C-NC | 3.01 | 112.80 | 109.97 |
| 40 | J | 4002 | RRX | C1-C6-C5 | -3.01 | 118.37 | 122.61 |
| 40 | J | 4002 | RRX | C33-C5-C4 | 3.01 | 119.41 | 113.62 |
| 25 | A | 1109 | CLA | CMA-C3A-C4A | 3.01 | 119.87 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1118 | CLA | C1-C2-C3 | -3.01 | 120.83 | 126.04 |
| 25 | A | 1133 | CLA | C2C-C1C-NC | 3.01 | 112.79 | 109.97 |
| 25 | 4 | 612 | CLA | CHD-C1D-ND | -3.01 | 121.69 | 124.45 |
| 25 | A | 1137 | CLA | C1-C2-C3 | -3.01 | 120.84 | 126.04 |
| 25 | B | 1235 | CLA | C1-C2-C3 | -3.01 | 120.84 | 126.04 |
| 25 | A | 1104 | CLA | C2C-C1C-NC | 3.01 | 112.79 | 109.97 |
| 29 | B | 4001 | BCR | C35-C13-C12 | 3.01 | 122.82 | 118.08 |
| 25 | 9 | 604 | CLA | CMA-C3A-C4A | 3.01 | 119.86 | 111.77 |
| 25 | A | 1107 | CLA | C2C-C1C-NC | 3.01 | 112.79 | 109.97 |
| 43 | 8 | 501 | LUT | C15-C14-C13 | -3.01 | 123.02 | 127.31 |
| 25 | 6 | 602 | CLA | CHD-C1D-ND | -3.01 | 121.69 | 124.45 |
| 26 | 2 | 613 | CHL | CHB-C4A-NA | 3.00 | 128.67 | 124.51 |
| 26 | 9 | 608 | CHL | C2C-C3C-C4C | 3.00 | 108.63 | 106.49 |
| 25 | B | 1220 | CLA | C2C-C1C-NC | 3.00 | 112.78 | 109.97 |
| 26 | a | 610 | CHL | CMA-C3A-C4A | 3.00 | 119.84 | 111.77 |
| 25 | A | 1141 | CLA | CHD-C1D-ND | -3.00 | 121.69 | 124.45 |
| 25 | B | 1218 | CLA | CMA-C3A-C4A | 3.00 | 119.84 | 111.77 |
| 25 | A | 1136 | CLA | C2C-C1C-NC | 3.00 | 112.78 | 109.97 |
| 25 | B | 1236 | CLA | C1-C2-C3 | -3.00 | 120.86 | 126.04 |
| 25 | B | 1240 | CLA | CHD-C1D-ND | -3.00 | 121.70 | 124.45 |
| 25 | G | 1601 | CLA | CMA-C3A-C4A | 3.00 | 119.83 | 111.77 |
| 25 | 1 | 606 | CLA | C2C-C1C-NC | 3.00 | 112.78 | 109.97 |
| 25 | 1 | 608 | CLA | C1-C2-C3 | -3.00 | 120.86 | 126.04 |
| 25 | a | 607 | CLA | CMA-C3A-C4A | 3.00 | 119.83 | 111.77 |
| 25 | F | 1302 | CLA | C2C-C1C-NC | 3.00 | 112.78 | 109.97 |
| 43 | 6 | 501 | LUT | C35-C15-C14 | -3.00 | 117.34 | 123.47 |
| 25 | 2 | 606 | CLA | C2C-C1C-NC | 3.00 | 112.78 | 109.97 |
| 50 | 2 | 501 | XAT | C7-C8-C9 | -2.99 | 120.88 | 125.53 |
| 50 | 2 | 501 | XAT | C26-C27-C28 | -2.99 | 119.67 | 125.99 |
| 25 | A | 1101 | CLA | C2D-C1D-ND | 2.99 | 112.31 | 110.10 |
| 25 | 8 | 620 | CLA | C2C-C1C-NC | 2.99 | 112.77 | 109.97 |
| 26 | 1 | 613 | CHL | C2C-C3C-C4C | 2.99 | 108.62 | 106.49 |
| 25 | 5 | 609 | CLA | C1-C2-C3 | -2.99 | 120.88 | 126.04 |
| 25 | K | 1401 | CLA | C2D-C1D-ND | 2.99 | 112.31 | 110.10 |
| 25 | 8 | 607 | CLA | C2C-C1C-NC | 2.99 | 112.77 | 109.97 |
| 25 | 4 | 603 | CLA | C1-C2-C3 | -2.98 | 120.88 | 126.04 |
| 29 | B | 4004 | BCR | C33-C5-C6 | -2.98 | 121.18 | 124.53 |
| 25 | F | 1301 | CLA | C2C-C1C-NC | 2.98 | 112.77 | 109.97 |
| 25 | A | 1012 | CLA | CHD-C1D-ND | -2.98 | 121.71 | 124.45 |
| 25 | 3 | 610 | CLA | C2C-C1C-NC | 2.98 | 112.77 | 109.97 |
| 25 | B | 1216 | CLA | C2C-C1C-NC | 2.98 | 112.76 | 109.97 |
| 25 | 5 | 614 | CLA | C2C-C1C-NC | 2.98 | 112.76 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 5 | 617 | CHL | CMA-C3A-C4A | 2.98 | 119.78 | 111.77 |
| 26 | 1 | 610 | CHL | CMA-C3A-C4A | 2.98 | 119.78 | 111.77 |
| 25 | A | 1127 | CLA | C2D-C1D-ND | 2.98 | 112.30 | 110.10 |
| 27 | B | 2002 | PQN | C14-C13-C15 | 2.98 | 120.28 | 115.27 |
| 25 | 2 | 601 | CLA | CAA-C2A-C3A | -2.98 | 104.62 | 112.78 |
| 25 | A | 1107 | CLA | CMB-C2B-C3B | 2.98 | 130.25 | 124.68 |
| 43 | 8 | 501 | LUT | C35-C15-C14 | -2.98 | 117.38 | 123.47 |
| 25 | A | 1128 | CLA | O2D-CGD-O1D | -2.98 | 118.02 | 123.84 |
| 26 | a | 606 | CHL | C2C-C3C-C4C | 2.98 | 108.61 | 106.49 |
| 25 | 4 | 608 | CLA | C2C-C1C-NC | 2.98 | 112.76 | 109.97 |
| 25 | 8 | 608 | CLA | C6-C5-C3 | -2.98 | 109.75 | 114.62 |
| 25 | K | 1402 | CLA | CMA-C3A-C4A | 2.98 | 119.77 | 111.77 |
| 26 | 2 | 609 | CHL | C2C-C3C-C4C | 2.97 | 108.61 | 106.49 |
| 25 | 6 | 604 | CLA | C2D-C1D-ND | 2.97 | 112.30 | 110.10 |
| 25 | 1 | 602 | CLA | CHD-C1D-ND | -2.97 | 121.72 | 124.45 |
| 25 | 8 | 606 | CLA | C2C-C1C-NC | 2.97 | 112.76 | 109.97 |
| 29 | A | 4001 | BCR | C12-C13-C14 | -2.97 | 114.38 | 118.94 |
| 25 | a | 602 | CLA | CMA-C3A-C4A | 2.97 | 119.76 | 111.77 |
| 25 | 8 | 602 | CLA | C2C-C1C-NC | 2.97 | 112.75 | 109.97 |
| 26 | a | 606 | CHL | C1-O2A-CGA | 2.97 | 124.24 | 116.44 |
| 25 | A | 1126 | CLA | C2C-C1C-NC | 2.97 | 112.75 | 109.97 |
| 25 | K | 1404 | CLA | CHD-C1D-ND | -2.97 | 121.72 | 124.45 |
| 25 | 9 | 607 | CLA | CMA-C3A-C4A | 2.97 | 119.75 | 111.77 |
| 25 | B | 1239 | CLA | C1C-C2C-C3C | -2.97 | 103.84 | 106.96 |
| 25 | a | 608 | CLA | C1-C2-C3 | -2.97 | 120.91 | 126.04 |
| 25 | 5 | 612 | CLA | C1-C2-C3 | -2.97 | 120.91 | 126.04 |
| 25 | B | 1236 | CLA | C2C-C1C-NC | 2.97 | 112.75 | 109.97 |
| 25 | B | 1226 | CLA | CMA-C3A-C4A | 2.97 | 119.74 | 111.77 |
| 25 | A | 1135 | CLA | CMA-C3A-C4A | 2.96 | 119.74 | 111.77 |
| 25 | 5 | 604 | CLA | CMA-C3A-C4A | 2.96 | 119.74 | 111.77 |
| 25 | 1 | 603 | CLA | C1-C2-C3 | -2.96 | 120.92 | 126.04 |
| 25 | B | 1210 | CLA | C2C-C1C-NC | 2.96 | 112.75 | 109.97 |
| 25 | B | 1238 | CLA | CMA-C3A-C4A | 2.96 | 119.74 | 111.77 |
| 25 | A | 1137 | CLA | C2D-C1D-ND | 2.96 | 112.29 | 110.10 |
| 29 | 5 | 503 | BCR | C36-C18-C17 | -2.96 | 118.77 | 122.92 |
| 25 | 8 | 618 | CLA | C2C-C1C-NC | 2.96 | 112.75 | 109.97 |
| 26 | 5 | 613 | CHL | C1-O2A-CGA | 2.96 | 124.22 | 116.44 |
| 26 | 4 | 618 | CHL | C2C-C3C-C4C | 2.96 | 108.60 | 106.49 |
| 25 | a | 605 | CLA | C2C-C1C-NC | 2.96 | 112.75 | 109.97 |
| 25 | 9 | 609 | CLA | CMA-C3A-C4A | 2.96 | 119.73 | 111.77 |
| 25 | 4 | 601 | CLA | C2C-C1C-NC | 2.96 | 112.74 | 109.97 |
| 25 | 5 | 606 | CLA | C2C-C1C-NC | 2.96 | 112.74 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 6 | 605 | CLA | C2C-C1C-NC | 2.96 | 112.74 | 109.97 |
| 25 | 5 | 603 | CLA | CMA-C3A-C4A | 2.96 | 119.72 | 111.77 |
| 25 | 4 | 604 | CLA | C2C-C1C-NC | 2.96 | 112.74 | 109.97 |
| 25 | A | 1103 | CLA | O2D-CGD-O1D | -2.96 | 118.06 | 123.84 |
| 25 | K | 1403 | CLA | CMA-C3A-C4A | 2.96 | 119.72 | 111.77 |
| 25 | A | 1013 | CLA | C2D-C1D-ND | 2.96 | 112.28 | 110.10 |
| 25 | 5 | 602 | CLA | C2D-C1D-ND | 2.96 | 112.28 | 110.10 |
| 25 | 2 | 615 | CLA | O2D-CGD-O1D | -2.95 | 118.06 | 123.84 |
| 25 | A | 1120 | CLA | C2D-C1D-ND | 2.95 | 112.28 | 110.10 |
| 25 | B | 1202 | CLA | C2D-C1D-ND | 2.95 | 112.28 | 110.10 |
| 25 | 8 | 615 | CLA | C2C-C1C-NC | 2.95 | 112.74 | 109.97 |
| 25 | A | 1117 | CLA | CMB-C2B-C3B | 2.95 | 130.20 | 124.68 |
| 25 | a | 615 | CLA | C2C-C1C-NC | 2.95 | 112.74 | 109.97 |
| 25 | 7 | 604 | CLA | C2C-C1C-NC | 2.95 | 112.74 | 109.97 |
| 25 | 2 | 615 | CLA | C2C-C1C-NC | 2.95 | 112.74 | 109.97 |
| 25 | O | 1803 | CLA | CAA-C2A-C3A | -2.95 | 109.21 | 116.10 |
| 25 | a | 611 | CLA | CMA-C3A-C4A | 2.95 | 119.70 | 111.77 |
| 26 | 8 | 613 | CHL | C1-O2A-CGA | 2.95 | 124.18 | 116.44 |
| 25 | 4 | 616 | CLA | CMA-C3A-C4A | 2.95 | 119.69 | 111.77 |
| 25 | A | 1102 | CLA | CMB-C2B-C3B | 2.95 | 130.19 | 124.68 |
| 43 | a | 502 | LUT | C11-C10-C9 | -2.94 | 123.11 | 127.31 |
| 26 | 9 | 613 | CHL | C2C-C3C-C4C | 2.94 | 108.59 | 106.49 |
| 25 | B | 1232 | CLA | C2C-C1C-NC | 2.94 | 112.73 | 109.97 |
| 25 | 8 | 605 | CLA | CHD-C1D-ND | -2.94 | 121.75 | 124.45 |
| 25 | A | 1102 | CLA | C2C-C1C-NC | 2.94 | 112.73 | 109.97 |
| 25 | 5 | 612 | CLA | C2C-C1C-NC | 2.94 | 112.73 | 109.97 |
| 25 | A | 1125 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 44 | 7 | 504 | AXT | C15-C35-C34 | 2.94 | 129.50 | 123.47 |
| 43 | 9 | 501 | LUT | C22-C23-C24 | -2.94 | 108.39 | 111.74 |
| 25 | 3 | 616 | CLA | CMA-C3A-C4A | 2.94 | 119.67 | 111.77 |
| 40 | J | 4002 | RRX | C12-C13-C14 | 2.94 | 123.45 | 118.94 |
| 43 | 1 | 503 | LUT | C20-C13-C12 | 2.94 | 122.71 | 118.08 |
| 29 | J | 4001 | BCR | C33-C5-C6 | -2.94 | 121.23 | 124.53 |
| 25 | 4 | 602 | CLA | C1-C2-C3 | -2.94 | 120.96 | 126.04 |
| 25 | A | 1121 | CLA | C2C-C1C-NC | 2.94 | 112.72 | 109.97 |
| 26 | 7 | 617 | CHL | CMA-C3A-C4A | 2.94 | 119.67 | 111.77 |
| 25 | A | 1105 | CLA | C2D-C1D-ND | 2.94 | 112.27 | 110.10 |
| 29 | A | 4001 | BCR | C35-C13-C12 | 2.94 | 122.70 | 118.08 |
| 25 | 5 | 608 | CLA | CHD-C1D-ND | -2.94 | 121.76 | 124.45 |
| 25 | B | 1237 | CLA | C2C-C1C-NC | 2.94 | 112.72 | 109.97 |
| 29 | 5 | 503 | BCR | C33-C5-C4 | 2.93 | 119.25 | 113.62 |
| 26 | 7 | 613 | CHL | C2C-C3C-C4C | 2.93 | 108.58 | 106.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 7 | 615 | CHL | C3C-C4C-NC | -2.93 | 107.28 | 110.57 |
| 25 | 3 | 605 | CLA | C2C-C1C-NC | 2.93 | 112.72 | 109.97 |
| 25 | 8 | 609 | CLA | O2D-CGD-O1D | -2.93 | 118.10 | 123.84 |
| 25 | a | 602 | CLA | C2D-C1D-ND | 2.93 | 112.27 | 110.10 |
| 26 | 3 | 608 | CHL | CMA-C3A-C4A | 2.93 | 119.66 | 111.77 |
| 25 | B | 1217 | CLA | C2D-C1D-ND | 2.93 | 112.27 | 110.10 |
| 25 | 2 | 604 | CLA | C2C-C1C-NC | 2.93 | 112.72 | 109.97 |
| 25 | 2 | 605 | CLA | C2C-C1C-NC | 2.93 | 112.72 | 109.97 |
| 25 | A | 1101 | CLA | C2C-C1C-NC | 2.93 | 112.72 | 109.97 |
| 25 | 3 | 601 | CLA | C2C-C1C-NC | 2.93 | 112.72 | 109.97 |
| 25 | A | 1116 | CLA | C2D-C1D-ND | 2.93 | 112.26 | 110.10 |
| 25 | 8 | 620 | CLA | CMA-C3A-C4A | 2.93 | 119.64 | 111.77 |
| 25 | A | 1109 | CLA | C2C-C1C-NC | 2.93 | 112.72 | 109.97 |
| 25 | 7 | 607 | CLA | CMA-C3A-C4A | 2.93 | 119.64 | 111.77 |
| 25 | A | 1133 | CLA | C1C-C2C-C3C | -2.93 | 103.88 | 106.96 |
| 26 | 9 | 603 | CHL | CMA-C3A-C4A | 2.93 | 119.64 | 111.77 |
| 25 | 2 | 601 | CLA | C2C-C1C-NC | 2.93 | 112.71 | 109.97 |
| 25 | B | 1201 | CLA | C2C-C1C-NC | 2.92 | 112.71 | 109.97 |
| 25 | A | 1101 | CLA | C1-C2-C3 | -2.92 | 120.98 | 126.04 |
| 25 | A | 1108 | CLA | CMA-C3A-C4A | 2.92 | 119.63 | 111.77 |
| 25 | 2 | 615 | CLA | CMA-C3A-C4A | 2.92 | 119.63 | 111.77 |
| 25 | 5 | 609 | CLA | CMA-C3A-C4A | 2.92 | 119.63 | 111.77 |
| 25 | 5 | 603 | CLA | C2C-C1C-NC | 2.92 | 112.71 | 109.97 |
| 25 | A | 1118 | CLA | C2D-C1D-ND | 2.92 | 112.26 | 110.10 |
| 25 | B | 1222 | CLA | C2D-C1D-ND | 2.92 | 112.26 | 110.10 |
| 43 | 4 | 502 | LUT | C22-C23-C24 | -2.92 | 108.42 | 111.74 |
| 25 | A | 1117 | CLA | CMA-C3A-C4A | 2.92 | 119.62 | 111.77 |
| 43 | 5 | 505 | LUT | C31-C30-C29 | -2.92 | 123.14 | 127.31 |
| 25 | 2 | 602 | CLA | C2D-C1D-ND | 2.92 | 112.26 | 110.10 |
| 25 | B | 1202 | CLA | C2C-C1C-NC | 2.92 | 112.71 | 109.97 |
| 29 | H | 4001 | BCR | C28-C27-C26 | -2.92 | 108.86 | 114.08 |
| 25 | G | 1601 | CLA | CHD-C1D-ND | -2.92 | 121.77 | 124.45 |
| 25 | B | 1212 | CLA | C2C-C1C-NC | 2.92 | 112.71 | 109.97 |
| 25 | 2 | 607 | CLA | CMA-C3A-C4A | 2.92 | 119.62 | 111.77 |
| 25 | 7 | 612 | CLA | C1-C2-C3 | -2.92 | 121.00 | 126.04 |
| 25 | 5 | 607 | CLA | CMA-C3A-C4A | 2.92 | 119.61 | 111.77 |
| 43 | 6 | 501 | LUT | C22-C23-C24 | -2.92 | 108.42 | 111.74 |
| 25 | A | 1107 | CLA | CMA-C3A-C4A | 2.92 | 119.61 | 111.77 |
| 26 | 7 | 611 | CHL | CMA-C3A-C4A | 2.92 | 119.61 | 111.77 |
| 25 | A | 1124 | CLA | C2C-C1C-NC | 2.92 | 112.70 | 109.97 |
| 26 | 9 | 603 | CHL | C3C-C4C-NC | -2.91 | 107.30 | 110.57 |
| 25 | A | 1013 | CLA | CMB-C2B-C3B | 2.91 | 130.13 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1220 | CLA | CMA-C3A-C4A | 2.91 | 119.60 | 111.77 |
| 25 | O | 1802 | CLA | C2D-C1D-ND | 2.91 | 112.25 | 110.10 |
| 26 | 8 | 604 | CHL | CMA-C3A-C4A | 2.91 | 119.60 | 111.77 |
| 26 | A | 1114 | CHL | C4A-NA-C1A | 2.91 | 108.01 | 106.71 |
| 26 | 9 | 608 | CHL | CMA-C3A-C4A | 2.91 | 119.59 | 111.77 |
| 50 | 9 | 507 | XAT | C38-C25-C26 | -2.91 | 117.39 | 122.26 |
| 25 | A | 1120 | CLA | C2C-C1C-NC | 2.91 | 112.70 | 109.97 |
| 40 | J | 4002 | RRX | C38-C26-C27 | 2.91 | 119.74 | 114.36 |
| 30 | 3 | 801 | LHG | C5-O7-C7 | -2.91 | 110.63 | 117.79 |
| 25 | O | 1802 | CLA | CMA-C3A-C4A | 2.91 | 119.59 | 111.77 |
| 25 | 4 | 604 | CLA | CMA-C3A-C4A | 2.91 | 119.59 | 111.77 |
| 26 | 9 | 610 | CHL | CMA-C3A-C4A | 2.91 | 119.58 | 111.77 |
| 25 | A | 1123 | CLA | CMA-C3A-C4A | 2.91 | 119.58 | 111.77 |
| 25 | 6 | 607 | CLA | CMA-C3A-C4A | 2.91 | 119.58 | 111.77 |
| 25 | 8 | 609 | CLA | CMA-C3A-C4A | 2.91 | 119.58 | 111.77 |
| 26 | 5 | 613 | CHL | C2C-C3C-C4C | 2.91 | 108.56 | 106.49 |
| 25 | 4 | 602 | CLA | C6-C5-C3 | -2.90 | 109.87 | 114.62 |
| 25 | 9 | 612 | CLA | CMA-C3A-C4A | 2.90 | 119.58 | 111.77 |
| 26 | 2 | 609 | CHL | CMA-C3A-C4A | 2.90 | 119.58 | 111.77 |
| 26 | 5 | 610 | CHL | C4A-NA-C1A | 2.90 | 108.01 | 106.71 |
| 25 | A | 1101 | CLA | O2D-CGD-O1D | -2.90 | 118.16 | 123.84 |
| 25 | B | 1202 | CLA | O2D-CGD-O1D | -2.90 | 118.16 | 123.84 |
| 25 | 5 | 615 | CLA | C2D-C1D-ND | 2.90 | 112.24 | 110.10 |
| 25 | A | 1105 | CLA | C2C-C1C-NC | 2.90 | 112.69 | 109.97 |
| 25 | B | 1216 | CLA | C1-C2-C3 | -2.90 | 121.02 | 126.04 |
| 25 | 2 | 602 | CLA | C6-C5-C3 | -2.90 | 109.88 | 114.62 |
| 25 | K | 1401 | CLA | CHD-C1D-ND | -2.90 | 121.79 | 124.45 |
| 25 | B | 1220 | CLA | C2D-C1D-ND | 2.90 | 112.24 | 110.10 |
| 40 | J | 4002 | RRX | C35-C13-C14 | -2.90 | 118.86 | 122.92 |
| 25 | 5 | 615 | CLA | CMA-C3A-C4A | 2.90 | 119.56 | 111.77 |
| 25 | B | 1226 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 26 | 9 | 603 | CHL | C1-C2-C3 | -2.90 | 121.03 | 126.04 |
| 25 | A | 1128 | CLA | CHD-C1D-ND | -2.90 | 121.79 | 124.45 |
| 25 | 4 | 605 | CLA | CHD-C1D-ND | -2.90 | 121.79 | 124.45 |
| 43 | 5 | 502 | LUT | C10-C11-C12 | -2.89 | 114.18 | 123.22 |
| 25 | 4 | 607 | CLA | CMA-C3A-C4A | 2.89 | 119.55 | 111.77 |
| 26 | 8 | 610 | CHL | C1-O2A-CGA | 2.89 | 124.04 | 116.44 |
| 25 | A | 1110 | CLA | CMA-C3A-C4A | 2.89 | 119.55 | 111.77 |
| 25 | 1 | 605 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 25 | A | 1140 | CLA | C2C-C1C-NC | 2.89 | 112.68 | 109.97 |
| 25 | G | 1602 | CLA | O2A-CGA-CBA | 2.89 | 120.98 | 111.91 |
| 25 | 9 | 602 | CLA | C2D-C1D-ND | 2.89 | 112.23 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 3 | 503 | BCR | C33-C5-C4 | 2.89 | 119.17 | 113.62 |
| 25 | a | 612 | CLA | C1-C2-C3 | -2.89 | 121.04 | 126.04 |
| 25 | B | 1235 | CLA | C2D-C1D-ND | 2.89 | 112.23 | 110.10 |
| 25 | A | 1012 | CLA | O2A-CGA-CBA | 2.89 | 120.98 | 111.91 |
| 25 | 2 | 615 | CLA | CHD-C1D-ND | -2.89 | 121.80 | 124.45 |
| 25 | A | 1138 | CLA | C2C-C1C-NC | 2.89 | 112.68 | 109.97 |
| 25 | B | 1223 | CLA | C2C-C1C-NC | 2.89 | 112.68 | 109.97 |
| 25 | A | 1102 | CLA | O2A-CGA-CBA | 2.89 | 120.96 | 111.91 |
| 29 | K | 4001 | BCR | C19-C18-C17 | 2.88 | 123.37 | 118.94 |
| 25 | 1 | 605 | CLA | C1-O2A-CGA | 2.88 | 124.01 | 116.44 |
| 25 | A | 1140 | CLA | C2D-C1D-ND | 2.88 | 112.23 | 110.10 |
| 25 | 7 | 607 | CLA | O2D-CGD-O1D | -2.88 | 118.20 | 123.84 |
| 25 | A | 1122 | CLA | C2C-C1C-NC | 2.88 | 112.67 | 109.97 |
| 25 | A | 1122 | CLA | CMA-C3A-C4A | 2.88 | 119.52 | 111.77 |
| 25 | A | 1105 | CLA | C1-C2-C3 | -2.88 | 121.06 | 126.04 |
| 25 | 5 | 604 | CLA | C2C-C1C-NC | 2.88 | 112.67 | 109.97 |
| 43 | 1 | 503 | LUT | C40-C33-C32 | 2.88 | 122.61 | 118.08 |
| 24 | A | 1011 | CL0 | CMB-C2B-C3B | 2.88 | 130.06 | 124.68 |
| 25 | 5 | 607 | CLA | C2D-C1D-ND | 2.88 | 112.22 | 110.10 |
| 25 | B | 1223 | CLA | O2D-CGD-O1D | -2.88 | 118.21 | 123.84 |
| 29 | H | 4001 | BCR | C36-C18-C17 | -2.88 | 118.89 | 122.92 |
| 25 | B | 1205 | CLA | O2D-CGD-O1D | -2.88 | 118.21 | 123.84 |
| 43 | 3 | 502 | LUT | C11-C10-C9 | -2.88 | 123.20 | 127.31 |
| 25 | 5 | 602 | CLA | CHD-C1D-ND | -2.88 | 121.81 | 124.45 |
| 25 | a | 601 | CLA | C2C-C1C-NC | 2.88 | 112.67 | 109.97 |
| 25 | G | 1602 | CLA | C2C-C1C-NC | 2.87 | 112.67 | 109.97 |
| 26 | 6 | 619 | CHL | C2C-C3C-C4C | 2.87 | 108.54 | 106.49 |
| 40 | J | 4002 | RRX | C30-C25-C26 | -2.87 | 118.56 | 122.61 |
| 25 | B | 1021 | CLA | C2D-C1D-ND | 2.87 | 112.22 | 110.10 |
| 35 | A | 5008 | LMT | C1'-O5'-C5' | -2.87 | 108.05 | 113.69 |
| 43 | 8 | 502 | LUT | C35-C15-C14 | -2.87 | 117.59 | 123.47 |
| 43 | 5 | 501 | LUT | C35-C15-C14 | -2.87 | 117.59 | 123.47 |
| 26 | 4 | 613 | CHL | C2C-C3C-C4C | 2.87 | 108.54 | 106.49 |
| 25 | B | 1239 | CLA | C2D-C1D-ND | 2.87 | 112.22 | 110.10 |
| 25 | B | 1228 | CLA | C1-C2-C3 | -2.87 | 121.08 | 126.04 |
| 25 | A | 1113 | CLA | C2C-C1C-NC | 2.87 | 112.66 | 109.97 |
| 25 | B | 1221 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 25 | 2 | 621 | CLA | CMA-C3A-C4A | 2.87 | 119.48 | 111.77 |
| 25 | B | 1230 | CLA | C2C-C1C-NC | 2.87 | 112.66 | 109.97 |
| 25 | 1 | 601 | CLA | C2C-C1C-NC | 2.87 | 112.66 | 109.97 |
| 26 | 7 | 613 | CHL | C1-O2A-CGA | 2.87 | 123.97 | 116.44 |
| 26 | 8 | 613 | CHL | CMA-C3A-C4A | 2.87 | 119.48 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1106 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 25 | 6 | 612 | CLA | C2D-C1D-ND | 2.87 | 112.22 | 110.10 |
| 25 | 1 | 608 | CLA | C1C-C2C-C3C | -2.87 | 103.94 | 106.96 |
| 25 | L | 1502 | CLA | C2C-C1C-NC | 2.86 | 112.66 | 109.97 |
| 25 | 3 | 612 | CLA | C2C-C1C-NC | 2.86 | 112.66 | 109.97 |
| 25 | 9 | 606 | CLA | C2C-C1C-NC | 2.86 | 112.66 | 109.97 |
| 25 | B | 1215 | CLA | CMA-C3A-C4A | 2.86 | 119.47 | 111.77 |
| 29 | I | 4001 | BCR | C38-C26-C27 | 2.86 | 119.12 | 113.62 |
| 43 | 4 | 501 | LUT | C31-C32-C33 | -2.86 | 118.37 | 126.42 |
| 26 | a | 606 | CHL | C1-C2-C3 | -2.86 | 121.09 | 126.04 |
| 26 | 3 | 603 | CHL | C2C-C3C-C4C | 2.86 | 108.53 | 106.49 |
| 25 | B | 1229 | CLA | C2C-C1C-NC | 2.86 | 112.65 | 109.97 |
| 29 | B | 4002 | BCR | C33-C5-C4 | 2.86 | 119.11 | 113.62 |
| 25 | 9 | 605 | CLA | CHD-C1D-ND | -2.86 | 121.83 | 124.45 |
| 25 | A | 1130 | CLA | C2C-C1C-NC | 2.86 | 112.65 | 109.97 |
| 25 | 8 | 605 | CLA | C2D-C1D-ND | 2.86 | 112.21 | 110.10 |
| 25 | 2 | 603 | CLA | CMA-C3A-C4A | 2.86 | 119.46 | 111.77 |
| 30 | 2 | 802 | LHG | O8-C23-C24 | 2.86 | 120.88 | 111.91 |
| 26 | 8 | 601 | CHL | CMA-C3A-C4A | 2.86 | 119.45 | 111.77 |
| 29 | 8 | 503 | BCR | C36-C18-C17 | -2.86 | 118.92 | 122.92 |
| 43 | 7 | 501 | LUT | C7-C8-C9 | -2.86 | 121.92 | 126.23 |
| 25 | B | 1212 | CLA | C2D-C1D-ND | 2.86 | 112.21 | 110.10 |
| 29 | B | 4006 | BCR | C35-C13-C12 | 2.85 | 122.57 | 118.08 |
| 25 | B | 1201 | CLA | C2D-C1D-ND | 2.85 | 112.21 | 110.10 |
| 25 | J | 1901 | CLA | CMA-C3A-C4A | 2.85 | 119.44 | 111.77 |
| 25 | 8 | 615 | CLA | C1C-C2C-C3C | -2.85 | 103.96 | 106.96 |
| 26 | 7 | 615 | CHL | CMA-C3A-C4A | 2.85 | 119.44 | 111.77 |
| 25 | B | 1021 | CLA | CHD-C1D-ND | -2.85 | 121.83 | 124.45 |
| 25 | 8 | 607 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 25 | 1 | 607 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 25 | A | 1119 | CLA | C2C-C1C-NC | 2.85 | 112.64 | 109.97 |
| 26 | 9 | 610 | CHL | C3C-C4C-NC | -2.85 | 107.38 | 110.57 |
| 25 | 4 | 602 | CLA | C2D-C1D-ND | 2.85 | 112.20 | 110.10 |
| 25 | A | 1110 | CLA | C2C-C1C-NC | 2.85 | 112.64 | 109.97 |
| 26 | a | 613 | CHL | C3C-C4C-NC | -2.85 | 107.38 | 110.57 |
| 29 | B | 4006 | BCR | C12-C13-C14 | -2.85 | 114.57 | 118.94 |
| 29 | K | 4002 | BCR | C19-C18-C17 | 2.85 | 123.31 | 118.94 |
| 25 | 2 | 607 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 25 | 2 | 603 | CLA | C2D-C1D-ND | 2.85 | 112.20 | 110.10 |
| 25 | B | 1208 | CLA | C2C-C1C-NC | 2.85 | 112.64 | 109.97 |
| 25 | B | 1226 | CLA | C1C-C2C-C3C | -2.85 | 103.96 | 106.96 |
| 25 | 9 | 605 | CLA | C2D-C1D-ND | 2.85 | 112.20 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 4 | 501 | LUT | C15-C14-C13 | -2.85 | 123.25 | 127.31 |
| 26 | 9 | 610 | CHL | CHC-C1C-NC | 2.85 | 128.52 | 124.20 |
| 29 | B | 4006 | BCR | C23-C24-C25 | -2.84 | 119.21 | 127.20 |
| 25 | 4 | 610 | CLA | CMA-C3A-C4A | 2.84 | 119.42 | 111.77 |
| 25 | 1 | 602 | CLA | CMA-C3A-C4A | 2.84 | 119.42 | 111.77 |
| 25 | B | 1225 | CLA | CMA-C3A-C4A | 2.84 | 119.42 | 111.77 |
| 25 | G | 1603 | CLA | C2D-C1D-ND | 2.84 | 112.20 | 110.10 |
| 25 | 3 | 616 | CLA | C2D-C1D-ND | 2.84 | 112.20 | 110.10 |
| 25 | 5 | 601 | CLA | C2D-C1D-ND | 2.84 | 112.20 | 110.10 |
| 29 | J | 4001 | BCR | C19-C18-C17 | 2.84 | 123.30 | 118.94 |
| 43 | 6 | 502 | LUT | C22-C23-C24 | -2.84 | 108.51 | 111.74 |
| 25 | A | 1137 | CLA | C2C-C1C-NC | 2.84 | 112.63 | 109.97 |
| 25 | 3 | 607 | CLA | CMA-C3A-C4A | 2.84 | 119.41 | 111.77 |
| 25 | B | 1203 | CLA | C2D-C1D-ND | 2.84 | 112.20 | 110.10 |
| 25 | A | 1123 | CLA | CHD-C1D-ND | -2.84 | 121.84 | 124.45 |
| 25 | A | 1115 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 25 | A | 1132 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 25 | 8 | 608 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 25 | 7 | 603 | CLA | C2D-C1D-ND | 2.84 | 112.19 | 110.10 |
| 25 | 9 | 609 | CLA | CMB-C2B-C3B | 2.84 | 129.98 | 124.68 |
| 43 | 6 | 501 | LUT | C7-C8-C9 | -2.84 | 121.95 | 126.23 |
| 26 | 7 | 617 | CHL | C1-O2A-CGA | 2.84 | 123.88 | 116.44 |
| 26 | 5 | 618 | CHL | C2C-C3C-C4C | 2.84 | 108.51 | 106.49 |
| 25 | B | 1201 | CLA | O2D-CGD-O1D | -2.84 | 118.30 | 123.84 |
| 25 | 2 | 602 | CLA | C1-C2-C3 | -2.83 | 121.14 | 126.04 |
| 25 | B | 1235 | CLA | CMA-C3A-C4A | 2.83 | 119.38 | 111.77 |
| 25 | B | 1223 | CLA | CMA-C3A-C4A | 2.83 | 119.38 | 111.77 |
| 25 | 3 | 602 | CLA | C2D-C1D-ND | 2.83 | 112.19 | 110.10 |
| 25 | B | 1226 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 25 | B | 1234 | CLA | O2A-CGA-CBA | 2.83 | 120.78 | 111.91 |
| 25 | 9 | 612 | CLA | C1C-C2C-C3C | -2.83 | 103.98 | 106.96 |
| 25 | B | 1209 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 43 | 5 | 505 | LUT | C18-C5-C6 | -2.82 | 121.36 | 124.53 |
| 25 | 4 | 603 | CLA | C2C-C1C-NC | 2.82 | 112.62 | 109.97 |
| 26 | a | 609 | CHL | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 25 | 8 | 618 | CLA | C1C-C2C-C3C | -2.82 | 103.99 | 106.96 |
| 25 | 1 | 605 | CLA | C1C-C2C-C3C | -2.82 | 103.99 | 106.96 |
| 25 | B | 1021 | CLA | C2C-C1C-NC | 2.82 | 112.61 | 109.97 |
| 25 | A | 1124 | CLA | C2D-C1D-ND | 2.82 | 112.18 | 110.10 |
| 25 | H | 1702 | CLA | O2D-CGD-O1D | -2.82 | 118.32 | 123.84 |
| 29 | A | 4005 | BCR | C34-C9-C10 | -2.82 | 118.97 | 122.92 |
| 25 | B | 1215 | CLA | C2D-C1D-ND | 2.82 | 112.18 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1139 | CLA | C2C-C1C-NC | 2.82 | 112.61 | 109.97 |
| 25 | 5 | 614 | CLA | C2D-C1D-ND | 2.82 | 112.18 | 110.10 |
| 25 | B | 1215 | CLA | C1C-C2C-C3C | -2.82 | 103.99 | 106.96 |
| 25 | K | 1403 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 25 | 7 | 601 | CLA | C2D-C1D-ND | 2.82 | 112.18 | 110.10 |
| 29 | L | 4003 | BCR | C27-C26-C25 | -2.82 | 118.64 | 122.73 |
| 25 | A | 1110 | CLA | O2D-CGD-O1D | -2.81 | 118.33 | 123.84 |
| 25 | A | 1112 | CLA | CMA-C3A-C4A | 2.81 | 119.34 | 111.77 |
| 43 | 3 | 502 | LUT | C10-C11-C12 | -2.81 | 114.44 | 123.22 |
| 25 | 8 | 605 | CLA | CMA-C3A-C4A | 2.81 | 119.34 | 111.77 |
| 25 | 4 | 607 | CLA | O2A-CGA-CBA | 2.81 | 120.74 | 111.91 |
| 25 | B | 1022 | CLA | OBD-CAD-C3D | -2.81 | 121.75 | 128.52 |
| 31 | A | 5004 | LMG | O8-C28-C29 | 2.81 | 120.73 | 111.91 |
| 25 | A | 1120 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 25 | B | 1235 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 43 | 9 | 502 | LUT | C35-C15-C14 | -2.81 | 117.72 | 123.47 |
| 25 | F | 1302 | CLA | CMA-C3A-C4A | 2.81 | 119.33 | 111.77 |
| 26 | 7 | 609 | CHL | C1-C2-C3 | -2.81 | 121.19 | 126.04 |
| 25 | A | 1134 | CLA | C2D-C1D-ND | 2.81 | 112.17 | 110.10 |
| 25 | 1 | 605 | CLA | C2D-C1D-ND | 2.81 | 112.17 | 110.10 |
| 25 | 9 | 607 | CLA | C2D-C1D-ND | 2.81 | 112.17 | 110.10 |
| 51 | 7 | 807 | 4RF | O18-C16-C15 | 2.81 | 120.71 | 111.91 |
| 25 | 4 | 608 | CLA | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 25 | 4 | 615 | CLA | CHD-C1D-ND | -2.81 | 121.88 | 124.45 |
| 25 | A | 1141 | CLA | C2D-C1D-ND | 2.80 | 112.17 | 110.10 |
| 25 | A | 1115 | CLA | C2D-C1D-ND | 2.80 | 112.17 | 110.10 |
| 43 | 1 | 503 | LUT | C32-C33-C34 | -2.80 | 114.64 | 118.94 |
| 25 | A | 1103 | CLA | C2C-C1C-NC | 2.80 | 112.60 | 109.97 |
| 25 | B | 1238 | CLA | C2C-C1C-NC | 2.80 | 112.60 | 109.97 |
| 26 | 6 | 613 | CHL | C2C-C3C-C4C | 2.80 | 108.49 | 106.49 |
| 25 | B | 1218 | CLA | C1C-C2C-C3C | -2.80 | 104.01 | 106.96 |
| 25 | A | 1122 | CLA | C2D-C1D-ND | 2.80 | 112.17 | 110.10 |
| 25 | B | 1224 | CLA | C2D-C1D-ND | 2.80 | 112.17 | 110.10 |
| 25 | 2 | 605 | CLA | C2D-C1D-ND | 2.80 | 112.17 | 110.10 |
| 25 | 5 | 612 | CLA | CMA-C3A-C4A | 2.80 | 119.30 | 111.77 |
| 25 | B | 1230 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 30 | 4 | 802 | LHG | O8-C23-C24 | 2.80 | 120.69 | 111.91 |
| 26 | 5 | 613 | CHL | CMA-C3A-C4A | 2.80 | 119.29 | 111.77 |
| 25 | A | 1129 | CLA | O2D-CGD-O1D | -2.80 | 118.37 | 123.84 |
| 25 | 2 | 608 | CLA | CMA-C3A-C4A | 2.80 | 119.29 | 111.77 |
| 26 | 3 | 611 | CHL | CMA-C3A-C4A | 2.80 | 119.29 | 111.77 |
| 25 | 8 | 606 | CLA | CMB-C2B-C3B | 2.80 | 129.91 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | O | 4001 | BCR | C33-C5-C4 | 2.80 | 118.99 | 113.62 |
| 29 | 8 | 503 | BCR | C33-C5-C4 | 2.80 | 118.99 | 113.62 |
| 30 | 2 | 801 | LHG | O8-C23-C24 | 2.80 | 120.68 | 111.91 |
| 25 | B | 1214 | CLA | C1-O2A-CGA | 2.80 | 123.78 | 116.44 |
| 26 | 6 | 619 | CHL | C1-C2-C3 | -2.79 | 121.21 | 126.04 |
| 29 | A | 4001 | BCR | C36-C18-C17 | -2.79 | 119.01 | 122.92 |
| 26 | 6 | 611 | CHL | C1-C2-C3 | -2.79 | 122.23 | 126.75 |
| 25 | 1 | 615 | CLA | CMA-C3A-C4A | 2.79 | 119.28 | 111.77 |
| 25 | A | 1139 | CLA | CMA-C3A-C4A | 2.79 | 119.28 | 111.77 |
| 25 | 8 | 602 | CLA | C6-C5-C3 | -2.79 | 110.05 | 114.62 |
| 50 | 9 | 504 | XAT | C38-C25-C26 | -2.79 | 117.58 | 122.26 |
| 25 | L | 1502 | CLA | CMA-C3A-C4A | 2.79 | 119.28 | 111.77 |
| 25 | A | 1135 | CLA | C2D-C1D-ND | 2.79 | 112.16 | 110.10 |
| 25 | a | 601 | CLA | C2D-C1D-ND | 2.79 | 112.16 | 110.10 |
| 25 | B | 1221 | CLA | C1-C2-C3 | -2.79 | 121.22 | 126.04 |
| 25 | B | 1023 | CLA | C2D-C1D-ND | 2.79 | 112.16 | 110.10 |
| 25 | 2 | 601 | CLA | CMA-C3A-C4A | 2.79 | 119.27 | 111.77 |
| 25 | B | 1240 | CLA | CMA-C3A-C4A | 2.79 | 119.27 | 111.77 |
| 25 | 1 | 608 | CLA | C2C-C1C-NC | 2.79 | 112.58 | 109.97 |
| 25 | B | 1220 | CLA | C1C-C2C-C3C | -2.79 | 104.02 | 106.96 |
| 25 | 7 | 608 | CLA | CMA-C3A-C4A | 2.79 | 119.27 | 111.77 |
| 25 | 5 | 607 | CLA | C1C-C2C-C3C | -2.79 | 104.03 | 106.96 |
| 25 | B | 1205 | CLA | C1C-C2C-C3C | -2.79 | 104.03 | 106.96 |
| 25 | 2 | 604 | CLA | CMB-C2B-C3B | 2.79 | 129.89 | 124.68 |
| 25 | a | 615 | CLA | CHD-C1D-ND | -2.79 | 121.89 | 124.45 |
| 25 | B | 1212 | CLA | CMA-C3A-C4A | 2.79 | 119.26 | 111.77 |
| 25 | A | 1110 | CLA | C2D-C1D-ND | 2.79 | 112.16 | 110.10 |
| 25 | 3 | 618 | CLA | C2D-C1D-ND | 2.79 | 112.16 | 110.10 |
| 25 | A | 1127 | CLA | CHD-C1D-ND | -2.79 | 121.89 | 124.45 |
| 25 | 1 | 605 | CLA | C2C-C1C-NC | 2.78 | 112.58 | 109.97 |
| 26 | 1 | 609 | CHL | C3C-C4C-NC | -2.78 | 107.45 | 110.57 |
| 25 | 9 | 604 | CLA | CMB-C2B-C3B | 2.78 | 129.89 | 124.68 |
| 25 | B | 1202 | CLA | C1-C2-C3 | -2.78 | 121.23 | 126.04 |
| 25 | G | 1602 | CLA | C2D-C1D-ND | 2.78 | 112.16 | 110.10 |
| 43 | 5 | 502 | LUT | C22-C23-C24 | -2.78 | 108.57 | 111.74 |
| 25 | 5 | 605 | CLA | CHD-C1D-ND | -2.78 | 121.90 | 124.45 |
| 26 | 7 | 615 | CHL | C1-O2A-CGA | 2.78 | 123.75 | 116.44 |
| 25 | B | 1202 | CLA | O2A-CGA-CBA | 2.78 | 120.64 | 111.91 |
| 25 | 8 | 611 | CLA | CMA-C3A-C4A | 2.78 | 119.25 | 111.77 |
| 25 | 4 | 606 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 25 | B | 1227 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 25 | 8 | 615 | CLA | CMA-C3A-C4A | 2.78 | 119.24 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1121 | CLA | CMD-C2D-C3D | -2.78 | 121.22 | 127.61 |
| 25 | 6 | 602 | CLA | C6-C5-C3 | -2.78 | 110.08 | 114.62 |
| 26 | 8 | 603 | CHL | C1-C2-C3 | -2.78 | 121.24 | 126.04 |
| 39 | F | 4001 | NEX | C16-C1-C2 | 2.77 | 121.51 | 109.05 |
| 25 | 3 | 613 | CLA | C2C-C1C-NC | 2.77 | 112.57 | 109.97 |
| 25 | A | 1124 | CLA | CMA-C3A-C4A | 2.77 | 119.23 | 111.77 |
| 29 | A | 4003 | BCR | C37-C22-C21 | -2.77 | 119.04 | 122.92 |
| 26 | 8 | 610 | CHL | C1B-CHB-C4A | -2.77 | 124.62 | 130.12 |
| 29 | O | 4001 | BCR | C27-C26-C25 | -2.77 | 118.71 | 122.73 |
| 29 | A | 4004 | BCR | C12-C13-C14 | -2.77 | 114.69 | 118.94 |
| 25 | A | 1131 | CLA | C1C-C2C-C3C | -2.77 | 104.04 | 106.96 |
| 25 | 5 | 603 | CLA | C1-C2-C3 | -2.77 | 121.25 | 126.04 |
| 25 | 2 | 615 | CLA | C1-C2-C3 | -2.77 | 121.25 | 126.04 |
| 25 | A | 1115 | CLA | CMA-C3A-C4A | 2.77 | 119.22 | 111.77 |
| 26 | 9 | 601 | CHL | C4D-CHA-C1A | 2.77 | 124.62 | 121.25 |
| 25 | A | 1136 | CLA | C2D-C1D-ND | 2.77 | 112.14 | 110.10 |
| 25 | B | 1235 | CLA | C2C-C1C-NC | 2.77 | 112.56 | 109.97 |
| 25 | 4 | 606 | CLA | C2C-C1C-NC | 2.77 | 112.56 | 109.97 |
| 29 | B | 4001 | BCR | C36-C18-C17 | -2.77 | 119.05 | 122.92 |
| 25 | L | 1504 | CLA | C1C-C2C-C3C | -2.77 | 104.05 | 106.96 |
| 25 | H | 1701 | CLA | CMA-C3A-C4A | 2.77 | 119.20 | 111.77 |
| 25 | A | 1013 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 25 | 5 | 601 | CLA | C2C-C1C-NC | 2.76 | 112.56 | 109.97 |
| 25 | 5 | 612 | CLA | C1C-C2C-C3C | -2.76 | 104.05 | 106.96 |
| 29 | A | 4004 | BCR | C34-C9-C10 | -2.76 | 119.05 | 122.92 |
| 25 | 4 | 606 | CLA | CMB-C2B-C3B | 2.76 | 129.85 | 124.68 |
| 29 | B | 4007 | BCR | C36-C18-C17 | -2.76 | 119.05 | 122.92 |
| 26 | 6 | 610 | CHL | C2C-C3C-C4C | 2.76 | 108.46 | 106.49 |
| 25 | 5 | 603 | CLA | O2A-CGA-CBA | 2.76 | 120.57 | 111.91 |
| 25 | H | 1703 | CLA | C2D-C1D-ND | 2.76 | 112.14 | 110.10 |
| 30 | 9 | 801 | LHG | O8-C23-C24 | 2.76 | 120.56 | 111.91 |
| 25 | 2 | 621 | CLA | C1C-C2C-C3C | -2.76 | 104.06 | 106.96 |
| 26 | 4 | 609 | CHL | CMA-C3A-C4A | 2.76 | 119.19 | 111.77 |
| 25 | 8 | 618 | CLA | CMD-C2D-C3D | -2.76 | 121.27 | 127.61 |
| 25 | 4 | 612 | CLA | C1C-C2C-C3C | -2.76 | 104.06 | 106.96 |
| 25 | A | 1118 | CLA | CMA-C3A-C4A | 2.76 | 119.18 | 111.77 |
| 25 | 8 | 612 | CLA | C2C-C1C-NC | 2.76 | 112.55 | 109.97 |
| 25 | 4 | 611 | CLA | C2D-C1D-ND | 2.76 | 112.14 | 110.10 |
| 25 | a | 608 | CLA | C1C-C2C-C3C | -2.76 | 104.06 | 106.96 |
| 25 | 8 | 609 | CLA | C1C-C2C-C3C | -2.76 | 104.06 | 106.96 |
| 25 | B | 1211 | CLA | O2D-CGD-O1D | -2.76 | 118.45 | 123.84 |
| 26 | 4 | 618 | CHL | CMA-C3A-C4A | 2.76 | 119.18 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1108 | CLA | C2C-C1C-NC | 2.76 | 112.55 | 109.97 |
| 25 | B | 1210 | CLA | O2D-CGD-O1D | -2.75 | 118.45 | 123.84 |
| 25 | 4 | 601 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | A | 1115 | CLA | C2C-C1C-NC | 2.75 | 112.55 | 109.97 |
| 25 | B | 1211 | CLA | C2C-C1C-NC | 2.75 | 112.55 | 109.97 |
| 25 | O | 1803 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | B | 1209 | CLA | C2C-C1C-NC | 2.75 | 112.55 | 109.97 |
| 25 | B | 1217 | CLA | CMA-C3A-C4A | 2.75 | 119.17 | 111.77 |
| 29 | L | 4002 | BCR | C34-C9-C10 | -2.75 | 119.07 | 122.92 |
| 25 | F | 1301 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | 7 | 610 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | 4 | 610 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | A | 1109 | CLA | O2D-CGD-O1D | -2.75 | 118.46 | 123.84 |
| 25 | 7 | 605 | CLA | CHD-C1D-ND | -2.75 | 121.93 | 124.45 |
| 25 | 6 | 608 | CLA | C1C-C2C-C3C | -2.75 | 104.07 | 106.96 |
| 25 | A | 1104 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 29 | 5 | 504 | BCR | C33-C5-C6 | -2.75 | 121.44 | 124.53 |
| 25 | A | 1012 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | A | 1126 | CLA | C2D-C1D-ND | 2.75 | 112.13 | 110.10 |
| 25 | A | 1128 | CLA | CMB-C2B-C3B | 2.75 | 129.82 | 124.68 |
| 25 | B | 1203 | CLA | C1C-C2C-C3C | -2.75 | 104.07 | 106.96 |
| 25 | B | 1219 | CLA | CMA-C3A-C4A | 2.74 | 119.15 | 111.77 |
| 25 | 9 | 606 | CLA | C1-C2-C3 | -2.74 | 121.30 | 126.04 |
| 25 | 9 | 606 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 25 | B | 1227 | CLA | C2D-C1D-ND | 2.74 | 112.12 | 110.10 |
| 25 | B | 1229 | CLA | CMA-C3A-C4A | 2.74 | 119.14 | 111.77 |
| 25 | 3 | 613 | CLA | C2D-C1D-ND | 2.74 | 112.12 | 110.10 |
| 29 | G | 4001 | BCR | C37-C22-C21 | -2.74 | 119.08 | 122.92 |
| 25 | B | 1232 | CLA | CMA-C3A-C4A | 2.74 | 119.14 | 111.77 |
| 26 | 6 | 609 | CHL | C4D-CHA-C1A | 2.74 | 124.58 | 121.25 |
| 25 | A | 1127 | CLA | C2C-C1C-NC | 2.74 | 112.54 | 109.97 |
| 25 | 8 | 611 | CLA | C2C-C1C-NC | 2.74 | 112.54 | 109.97 |
| 26 | 9 | 610 | CHL | C4D-CHA-C1A | 2.74 | 124.58 | 121.25 |
| 25 | F | 1302 | CLA | C2D-C1D-ND | 2.74 | 112.12 | 110.10 |
| 25 | 8 | 602 | CLA | C2D-C1D-ND | 2.74 | 112.12 | 110.10 |
| 36 | 7 | 806 | DGD | O1G-C1A-C2A | 2.74 | 120.50 | 111.91 |
| 26 | a | 604 | CHL | C4D-CHA-C1A | 2.74 | 124.58 | 121.25 |
| 25 | G | 1601 | CLA | C2D-C1D-ND | 2.74 | 112.12 | 110.10 |
| 25 | A | 1105 | CLA | CMA-C3A-C4A | 2.73 | 119.12 | 111.77 |
| 43 | 1 | 503 | LUT | C39-C29-C30 | -2.73 | 119.09 | 122.92 |
| 25 | B | 1211 | CLA | CMB-C2B-C3B | 2.73 | 129.79 | 124.68 |
| 25 | L | 1501 | CLA | C1C-C2C-C3C | -2.73 | 104.08 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1205 | CLA | C2D-C1D-ND | 2.73 | 112.12 | 110.10 |
| 25 | 8 | 609 | CLA | C1-C2-C3 | -2.73 | 121.32 | 126.04 |
| 25 | B | 1207 | CLA | C1C-C2C-C3C | -2.73 | 104.08 | 106.96 |
| 25 | 2 | 607 | CLA | C2D-C1D-ND | 2.73 | 112.12 | 110.10 |
| 33 | 9 | 803 | PTY | O4-C30-C31 | 2.73 | 120.48 | 111.91 |
| 25 | 3 | 612 | CLA | C1C-C2C-C3C | -2.73 | 104.08 | 106.96 |
| 38 | F | 5003 | LPX | O3-P1-O4 | 2.73 | 125.74 | 112.24 |
| 30 | 9 | 802 | LHG | O8-C23-C24 | 2.73 | 120.48 | 111.91 |
| 25 | 9 | 609 | CLA | C2D-C1D-ND | 2.73 | 112.12 | 110.10 |
| 25 | 7 | 612 | CLA | C1C-C2C-C3C | -2.73 | 104.09 | 106.96 |
| 25 | B | 1208 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 25 | B | 1208 | CLA | CMA-C3A-C4A | 2.73 | 119.11 | 111.77 |
| 25 | 4 | 603 | CLA | C2D-C1D-ND | 2.73 | 112.11 | 110.10 |
| 25 | 1 | 615 | CLA | CMB-C2B-C3B | 2.73 | 129.78 | 124.68 |
| 25 | 7 | 608 | CLA | C1C-C2C-C3C | -2.73 | 104.09 | 106.96 |
| 30 | F | 5001 | LHG | O8-C23-C24 | 2.73 | 120.47 | 111.91 |
| 25 | 7 | 612 | CLA | CAA-C2A-C3A | -2.73 | 105.31 | 112.78 |
| 50 | 7 | 502 | XAT | C38-C25-C26 | -2.73 | 117.69 | 122.26 |
| 34 | A | 5007 | 3PH | O31-C31-C32 | 2.73 | 120.46 | 111.91 |
| 25 | A | 1108 | CLA | C2D-C1D-ND | 2.73 | 112.11 | 110.10 |
| 25 | 2 | 621 | CLA | O2D-CGD-O1D | -2.73 | 118.51 | 123.84 |
| 25 | 8 | 606 | CLA | C1C-C2C-C3C | -2.73 | 104.09 | 106.96 |
| 25 | A | 1121 | CLA | CMA-C3A-C4A | 2.72 | 119.10 | 111.77 |
| 25 | 4 | 617 | CLA | C2D-C1D-ND | 2.72 | 112.11 | 110.10 |
| 43 | 2 | 507 | LUT | C19-C9-C8 | 2.72 | 122.37 | 118.08 |
| 25 | 1 | 612 | CLA | C1-C2-C3 | -2.72 | 121.33 | 126.04 |
| 26 | 7 | 615 | CHL | C2C-C3C-C4C | 2.72 | 108.43 | 106.49 |
| 29 | B | 4007 | BCR | C34-C9-C10 | -2.72 | 119.11 | 122.92 |
| 25 | 1 | 602 | CLA | C2D-C1D-ND | 2.72 | 112.11 | 110.10 |
| 25 | 2 | 607 | CLA | C1-C2-C3 | -2.72 | 121.33 | 126.04 |
| 25 | 4 | 611 | CLA | C1C-C2C-C3C | -2.72 | 104.09 | 106.96 |
| 25 | A | 1117 | CLA | CMB-C2B-C1B | -2.72 | 124.28 | 128.46 |
| 43 | 4 | 501 | LUT | C35-C15-C14 | -2.72 | 117.90 | 123.47 |
| 29 | L | 4002 | BCR | C19-C18-C17 | 2.72 | 123.12 | 118.94 |
| 25 | K | 1403 | CLA | C2D-C1D-ND | 2.72 | 112.11 | 110.10 |
| 43 | 3 | 501 | LUT | C35-C15-C14 | -2.72 | 117.90 | 123.47 |
| 25 | B | 1235 | CLA | O2A-CGA-CBA | 2.72 | 120.44 | 111.91 |
| 25 | A | 1103 | CLA | CMA-C3A-C4A | 2.72 | 119.08 | 111.77 |
| 50 | 9 | 504 | XAT | C18-C5-C6 | -2.72 | 117.71 | 122.26 |
| 26 | 7 | 611 | CHL | C1-C2-C3 | -2.72 | 121.34 | 126.04 |
| 30 | 9 | 802 | LHG | C5-O7-C7 | -2.72 | 111.10 | 117.79 |
| 29 | A | 4003 | BCR | C33-C5-C4 | 2.72 | 118.84 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 9 | 504 | XAT | C6-C7-C8 | -2.72 | 120.25 | 125.99 |
| 25 | B | 1221 | CLA | C1C-C2C-C3C | -2.72 | 104.10 | 106.96 |
| 25 | 1 | 612 | CLA | C1C-C2C-C3C | -2.72 | 104.10 | 106.96 |
| 25 | B | 1214 | CLA | CMA-C3A-C4A | 2.72 | 119.08 | 111.77 |
| 40 | 3 | 506 | RRX | C33-C5-C4 | 2.72 | 118.83 | 113.62 |
| 26 | 9 | 601 | CHL | C1B-CHB-C4A | -2.72 | 124.74 | 130.12 |
| 25 | 6 | 604 | CLA | O2A-CGA-CBA | 2.72 | 120.43 | 111.91 |
| 50 | 9 | 507 | XAT | C20-C13-C14 | -2.72 | 119.12 | 122.92 |
| 50 | 9 | 507 | XAT | C7-C8-C9 | -2.72 | 121.32 | 125.53 |
| 43 | 6 | 502 | LUT | C11-C10-C9 | -2.72 | 123.44 | 127.31 |
| 25 | A | 1104 | CLA | C1C-C2C-C3C | -2.71 | 104.10 | 106.96 |
| 39 | F | 4001 | NEX | C40-C33-C34 | -2.71 | 119.12 | 122.92 |
| 37 | K | 5001 | PCW | O3-C11-C12 | 2.71 | 120.42 | 111.91 |
| 25 | B | 1212 | CLA | O2D-CGD-O1D | -2.71 | 118.53 | 123.84 |
| 30 | A | 5001 | LHG | O8-C23-C24 | 2.71 | 120.42 | 111.91 |
| 51 | 7 | 807 | 4RF | O40-C41-C43 | 2.71 | 120.42 | 111.91 |
| 25 | B | 1231 | CLA | CMD-C2D-C3D | -2.71 | 121.37 | 127.61 |
| 25 | A | 1134 | CLA | CMA-C3A-C4A | 2.71 | 119.06 | 111.77 |
| 30 | F | 5002 | LHG | O8-C23-C24 | 2.71 | 120.42 | 111.91 |
| 25 | A | 1103 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 25 | H | 1701 | CLA | C1C-C2C-C3C | -2.71 | 104.11 | 106.96 |
| 25 | B | 1215 | CLA | O2D-CGD-O1D | -2.71 | 118.54 | 123.84 |
| 26 | 5 | 610 | CHL | C2C-C3C-C4C | 2.71 | 108.42 | 106.49 |
| 43 | 4 | 501 | LUT | C22-C23-C24 | -2.71 | 108.66 | 111.74 |
| 25 | A | 1130 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 25 | L | 1501 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 30 | B | 5002 | LHG | O8-C23-C24 | 2.71 | 120.42 | 111.91 |
| 25 | 8 | 618 | CLA | O2D-CGD-O1D | -2.71 | 118.54 | 123.84 |
| 25 | B | 1226 | CLA | C1-C2-C3 | -2.71 | 121.36 | 126.04 |
| 42 | M | 4001 | ECH | C8-C7-C6 | -2.71 | 119.59 | 127.20 |
| 36 | B | 5003 | DGD | O1G-C1A-C2A | 2.71 | 120.41 | 111.91 |
| 25 | B | 1216 | CLA | C1C-C2C-C3C | -2.71 | 104.11 | 106.96 |
| 29 | B | 4004 | BCR | C35-C13-C12 | 2.71 | 122.35 | 118.08 |
| 25 | A | 1139 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 25 | A | 1107 | CLA | C1-C2-C3 | -2.71 | 121.36 | 126.04 |
| 25 | A | 1130 | CLA | CMA-C3A-C4A | 2.71 | 119.06 | 111.77 |
| 25 | L | 1503 | CLA | C1C-C2C-C3C | -2.71 | 104.11 | 106.96 |
| 25 | A | 1116 | CLA | C2C-C1C-NC | 2.71 | 112.51 | 109.97 |
| 25 | 5 | 605 | CLA | C2C-C1C-NC | 2.71 | 112.51 | 109.97 |
| 25 | 5 | 612 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 25 | 6 | 601 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 26 | 9 | 608 | CHL | C4D-CHA-C1A | 2.71 | 124.55 | 121.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1228 | CLA | CMB-C2B-C3B | 2.71 | 129.74 | 124.68 |
| 25 | L | 1502 | CLA | C1D-ND-C4D | -2.71 | 104.41 | 106.33 |
| 29 | L | 4002 | BCR | C35-C13-C12 | 2.71 | 122.34 | 118.08 |
| 44 | 7 | 504 | AXT | C30-C31-C32 | 2.71 | 131.66 | 123.22 |
| 25 | 6 | 607 | CLA | C2D-C1D-ND | 2.71 | 112.10 | 110.10 |
| 25 | 6 | 612 | CLA | C1C-C2C-C3C | -2.71 | 104.11 | 106.96 |
| 25 | B | 1238 | CLA | C1-C2-C3 | -2.70 | 121.36 | 126.04 |
| 29 | A | 4001 | BCR | C27-C26-C25 | -2.70 | 118.80 | 122.73 |
| 25 | H | 1702 | CLA | C1C-C2C-C3C | -2.70 | 104.11 | 106.96 |
| 26 | 6 | 610 | CHL | C1B-CHB-C4A | -2.70 | 124.76 | 130.12 |
| 25 | 6 | 604 | CLA | C1D-ND-C4D | -2.70 | 104.41 | 106.33 |
| 25 | 6 | 606 | CLA | C1C-C2C-C3C | -2.70 | 104.11 | 106.96 |
| 25 | 7 | 608 | CLA | C2D-C1D-ND | 2.70 | 112.10 | 110.10 |
| 25 | A | 1106 | CLA | C2C-C1C-NC | 2.70 | 112.50 | 109.97 |
| 35 | 1 | 804 | LMT | C1'-O5'-C5' | -2.70 | 108.39 | 113.69 |
| 25 | B | 1217 | CLA | O2A-CGA-CBA | 2.70 | 120.38 | 111.91 |
| 25 | a | 611 | CLA | C1C-C2C-C3C | -2.70 | 104.12 | 106.96 |
| 25 | B | 1219 | CLA | C2D-C1D-ND | 2.70 | 112.09 | 110.10 |
| 25 | 3 | 601 | CLA | C2D-C1D-ND | 2.70 | 112.09 | 110.10 |
| 29 | H | 4001 | BCR | C34-C9-C10 | -2.70 | 119.14 | 122.92 |
| 25 | 7 | 602 | CLA | C2D-C1D-ND | 2.70 | 112.09 | 110.10 |
| 43 | 2 | 502 | LUT | C39-C29-C28 | 2.70 | 122.33 | 118.08 |
| 25 | a | 603 | CLA | O2A-CGA-CBA | 2.70 | 120.38 | 111.91 |
| 29 | A | 4005 | BCR | C12-C13-C14 | -2.70 | 114.80 | 118.94 |
| 25 | B | 1223 | CLA | CHD-C1D-ND | -2.70 | 121.98 | 124.45 |
| 25 | 1 | 601 | CLA | CAA-C2A-C3A | -2.70 | 105.40 | 112.78 |
| 29 | J | 4001 | BCR | C27-C26-C25 | -2.70 | 118.82 | 122.73 |
| 25 | 7 | 604 | CLA | CMA-C3A-C4A | 2.69 | 119.02 | 111.77 |
| 25 | 3 | 605 | CLA | C2D-C1D-ND | 2.69 | 112.09 | 110.10 |
| 40 | 3 | 506 | RRX | C4-C5-C6 | -2.69 | 118.82 | 122.73 |
| 25 | 4 | 617 | CLA | C1C-C2C-C3C | -2.69 | 104.12 | 106.96 |
| 25 | 2 | 601 | CLA | C1C-C2C-C3C | -2.69 | 104.12 | 106.96 |
| 25 | B | 1213 | CLA | C2D-C1D-ND | 2.69 | 112.09 | 110.10 |
| 26 | 6 | 610 | CHL | C4D-CHA-C1A | 2.69 | 124.53 | 121.25 |
| 25 | B | 1240 | CLA | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 25 | A | 1127 | CLA | CMA-C3A-C4A | 2.69 | 119.01 | 111.77 |
| 25 | a | 612 | CLA | C1C-C2C-C3C | -2.69 | 104.13 | 106.96 |
| 26 | 9 | 603 | CHL | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 25 | B | 1222 | CLA | C2C-C1C-NC | 2.69 | 112.49 | 109.97 |
| 25 | 4 | 604 | CLA | C2D-C1D-ND | 2.69 | 112.09 | 110.10 |
| 25 | H | 1703 | CLA | OBD-CAD-C3D | -2.69 | 122.05 | 128.52 |
| 25 | 7 | 605 | CLA | CMA-C3A-C4A | 2.69 | 119.00 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1123 | CLA | C1C-C2C-C3C | -2.69 | 104.13 | 106.96 |
| 25 | H | 1702 | CLA | C2D-C1D-ND | 2.69 | 112.08 | 110.10 |
| 25 | B | 1228 | CLA | C2D-C1D-ND | 2.69 | 112.08 | 110.10 |
| 25 | K | 1404 | CLA | C1C-C2C-C3C | -2.69 | 104.13 | 106.96 |
| 25 | 3 | 602 | CLA | CMB-C2B-C3B | 2.69 | 129.70 | 124.68 |
| 25 | A | 1110 | CLA | C1-C2-C3 | -2.69 | 121.40 | 126.04 |
| 25 | B | 1231 | CLA | C1-C2-C3 | -2.69 | 121.40 | 126.04 |
| 25 | B | 1226 | CLA | CMD-C2D-C3D | -2.68 | 121.44 | 127.61 |
| 25 | B | 1023 | CLA | C2C-C1C-NC | 2.68 | 112.49 | 109.97 |
| 25 | A | 1117 | CLA | C1C-C2C-C3C | -2.68 | 104.13 | 106.96 |
| 25 | 7 | 608 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 25 | 6 | 602 | CLA | C2D-C1D-ND | 2.68 | 112.08 | 110.10 |
| 25 | A | 1102 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 43 | 2 | 502 | LUT | C38-C25-C24 | -2.68 | 117.82 | 123.56 |
| 29 | O | 4001 | BCR | C38-C26-C27 | 2.68 | 118.77 | 113.62 |
| 25 | 6 | 601 | CLA | C2C-C1C-NC | 2.68 | 112.48 | 109.97 |
| 25 | 2 | 603 | CLA | O2A-CGA-CBA | 2.68 | 120.32 | 111.91 |
| 25 | B | 1022 | CLA | C1C-C2C-C3C | -2.68 | 104.14 | 106.96 |
| 25 | 1 | 615 | CLA | C1C-C2C-C3C | -2.68 | 104.14 | 106.96 |
| 25 | A | 1113 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 25 | A | 1128 | CLA | CMA-C3A-C4A | 2.68 | 118.98 | 111.77 |
| 33 | 3 | 802 | PTY | O4-C30-C31 | 2.68 | 120.32 | 111.91 |
| 25 | 2 | 604 | CLA | CMA-C3A-C4A | 2.68 | 118.98 | 111.77 |
| 25 | a | 605 | CLA | C1C-C2C-C3C | -2.68 | 104.14 | 106.96 |
| 30 | 1 | 801 | LHG | O8-C23-C24 | 2.68 | 120.31 | 111.91 |
| 48 | 3 | 803 | DGA | OG1-CA1-CA2 | 2.68 | 120.31 | 111.91 |
| 26 | 8 | 610 | CHL | C2C-C3C-C4C | 2.68 | 108.40 | 106.49 |
| 50 | 7 | 502 | XAT | C6-C7-C8 | -2.68 | 120.33 | 125.99 |
| 25 | 2 | 601 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 26 | 3 | 608 | CHL | C1B-CHB-C4A | -2.68 | 124.81 | 130.12 |
| 26 | a | 609 | CHL | C2C-C3C-C4C | 2.68 | 108.40 | 106.49 |
| 25 | K | 1401 | CLA | CMA-C3A-C4A | 2.68 | 118.97 | 111.77 |
| 25 | L | 1503 | CLA | CMB-C2B-C3B | 2.68 | 129.69 | 124.68 |
| 24 | A | 1011 | CL0 | CMC-C2C-C1C | 2.68 | 129.11 | 125.04 |
| 26 | 7 | 613 | CHL | CHD-C4C-C3C | 2.68 | 128.77 | 124.84 |
| 25 | G | 1602 | CLA | C1-O2A-CGA | 2.68 | 123.46 | 116.44 |
| 25 | A | 1105 | CLA | O2D-CGD-O1D | -2.68 | 118.61 | 123.84 |
| 25 | 9 | 605 | CLA | CHA-C4D-ND | 2.68 | 138.09 | 132.50 |
| 25 | 6 | 602 | CLA | C1C-C2C-C3C | -2.67 | 104.14 | 106.96 |
| 29 | L | 4003 | BCR | C36-C18-C17 | -2.67 | 119.18 | 122.92 |
| 25 | 5 | 604 | CLA | C2D-C1D-ND | 2.67 | 112.08 | 110.10 |
| 25 | A | 1136 | CLA | O2D-CGD-O1D | -2.67 | 118.61 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 607 | CLA | C2D-C1D-ND | 2.67 | 112.07 | 110.10 |
| 25 | 7 | 607 | CLA | C2D-C1D-ND | 2.67 | 112.07 | 110.10 |
| 25 | 8 | 608 | CLA | C1C-C2C-C3C | -2.67 | 104.15 | 106.96 |
| 25 | a | 607 | CLA | O2D-CGD-O1D | -2.67 | 118.61 | 123.84 |
| 25 | 1 | 608 | CLA | C2D-C1D-ND | 2.67 | 112.07 | 110.10 |
| 50 | 9 | 504 | XAT | O4-C5-C4 | -2.67 | 111.38 | 113.38 |
| 25 | G | 1603 | CLA | C1C-C2C-C3C | -2.67 | 104.15 | 106.96 |
| 42 | M | 4001 | ECH | C7-C8-C9 | -2.67 | 122.20 | 126.23 |
| 25 | 3 | 613 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 25 | 4 | 610 | CLA | C1C-C2C-C3C | -2.67 | 104.15 | 106.96 |
| 25 | 6 | 612 | CLA | CMA-C3A-C4A | 2.67 | 118.95 | 111.77 |
| 26 | 6 | 613 | CHL | CMA-C3A-C4A | 2.67 | 118.95 | 111.77 |
| 26 | 1 | 609 | CHL | C2C-C3C-C4C | 2.67 | 108.39 | 106.49 |
| 25 | B | 1225 | CLA | C2D-C1D-ND | 2.67 | 112.07 | 110.10 |
| 25 | 3 | 602 | CLA | C1C-C2C-C3C | -2.67 | 104.15 | 106.96 |
| 25 | 2 | 607 | CLA | C1C-C2C-C3C | -2.67 | 104.15 | 106.96 |
| 25 | 6 | 601 | CLA | CMA-C3A-C4A | 2.67 | 118.94 | 111.77 |
| 33 | 7 | 804 | PTY | O4-C30-C31 | 2.67 | 120.27 | 111.91 |
| 43 | a | 503 | LUT | C7-C8-C9 | -2.67 | 122.21 | 126.23 |
| 43 | 8 | 502 | LUT | C10-C11-C12 | -2.66 | 114.90 | 123.22 |
| 25 | B | 1228 | CLA | O2A-CGA-CBA | 2.66 | 120.27 | 111.91 |
| 25 | A | 1121 | CLA | O2D-CGD-O1D | -2.66 | 118.63 | 123.84 |
| 25 | 2 | 604 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 29 | A | 4004 | BCR | C36-C18-C17 | -2.66 | 119.19 | 122.92 |
| 26 | 8 | 613 | CHL | C1-C2-C3 | -2.66 | 122.44 | 126.75 |
| 25 | B | 1209 | CLA | O2A-CGA-CBA | 2.66 | 120.27 | 111.91 |
| 29 | K | 4002 | BCR | C34-C9-C10 | -2.66 | 119.19 | 122.92 |
| 43 | 2 | 507 | LUT | C18-C5-C4 | 2.66 | 119.28 | 114.36 |
| 29 | A | 4005 | BCR | C35-C13-C12 | 2.66 | 122.27 | 118.08 |
| 26 | a | 610 | CHL | C2C-C3C-C4C | 2.66 | 108.39 | 106.49 |
| 25 | A | 1134 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 26 | 9 | 610 | CHL | C1-O2A-CGA | 2.66 | 123.42 | 116.44 |
| 43 | 2 | 507 | LUT | C39-C29-C30 | -2.66 | 119.20 | 122.92 |
| 25 | 3 | 616 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 25 | 2 | 612 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 25 | 3 | 610 | CLA | C2D-C1D-ND | 2.66 | 112.06 | 110.10 |
| 25 | 4 | 608 | CLA | C2D-C1D-ND | 2.66 | 112.06 | 110.10 |
| 25 | 6 | 606 | CLA | C2D-C1D-ND | 2.66 | 112.06 | 110.10 |
| 29 | I | 4001 | BCR | C35-C13-C12 | 2.66 | 122.27 | 118.08 |
| 25 | 9 | 609 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 26 | 7 | 611 | CHL | C1-O2A-CGA | 2.66 | 123.42 | 116.44 |
| 25 | A | 1133 | CLA | C2D-C1D-ND | 2.66 | 112.06 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | K | 1404 | CLA | C2D-C1D-ND | 2.66 | 112.06 | 110.10 |
| 33 | 5 | 802 | PTY | O4-C30-C31 | 2.66 | 120.25 | 111.91 |
| 25 | A | 1134 | CLA | O2D-CGD-O1D | -2.66 | 118.64 | 123.84 |
| 25 | 5 | 607 | CLA | O2D-CGD-O1D | -2.66 | 118.64 | 123.84 |
| 25 | a | 602 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 25 | 7 | 604 | CLA | C1C-C2C-C3C | -2.66 | 104.16 | 106.96 |
| 25 | 8 | 618 | CLA | CMA-C3A-C4A | 2.66 | 118.91 | 111.77 |
| 29 | K | 4001 | BCR | C37-C22-C21 | -2.66 | 119.20 | 122.92 |
| 25 | 9 | 606 | CLA | C2D-C1D-ND | 2.66 | 112.06 | 110.10 |
| 25 | 7 | 603 | CLA | C1C-C2C-C3C | -2.65 | 104.17 | 106.96 |
| 25 | 1 | 612 | CLA | C2D-C1D-ND | 2.65 | 112.06 | 110.10 |
| 25 | O | 1803 | CLA | C1C-C2C-C3C | -2.65 | 104.17 | 106.96 |
| 43 | 1 | 503 | LUT | C31-C30-C29 | -2.65 | 123.52 | 127.31 |
| 25 | 2 | 602 | CLA | CMA-C3A-C4A | 2.65 | 118.90 | 111.77 |
| 33 | B | 5005 | PTY | O4-C30-C31 | 2.65 | 120.23 | 111.91 |
| 25 | A | 1118 | CLA | C1C-C2C-C3C | -2.65 | 104.17 | 106.96 |
| 25 | A | 1130 | CLA | C1C-C2C-C3C | -2.65 | 104.17 | 106.96 |
| 25 | 6 | 605 | CLA | CMA-C3A-C4A | 2.65 | 118.90 | 111.77 |
| 43 | a | 503 | LUT | C35-C15-C14 | -2.65 | 118.04 | 123.47 |
| 25 | 5 | 603 | CLA | C1-O2A-CGA | 2.65 | 123.40 | 116.44 |
| 25 | A | 1123 | CLA | C2D-C1D-ND | 2.65 | 112.06 | 110.10 |
| 25 | 2 | 601 | CLA | C2D-C1D-ND | 2.65 | 112.06 | 110.10 |
| 25 | 1 | 606 | CLA | CMB-C2B-C3B | 2.65 | 129.63 | 124.68 |
| 25 | K | 1403 | CLA | C1C-C2C-C3C | -2.65 | 104.17 | 106.96 |
| 25 | 4 | 601 | CLA | C1C-C2C-C3C | -2.65 | 104.17 | 106.96 |
| 25 | 7 | 602 | CLA | O2D-CGD-O1D | -2.65 | 118.66 | 123.84 |
| 25 | B | 1238 | CLA | C2D-C1D-ND | 2.65 | 112.06 | 110.10 |
| 25 | 5 | 608 | CLA | C2D-C1D-ND | 2.65 | 112.06 | 110.10 |
| 26 | 2 | 609 | CHL | C1B-CHB-C4A | -2.65 | 124.88 | 130.12 |
| 36 | 8 | 803 | DGD | O1G-C1A-C2A | 2.65 | 120.21 | 111.91 |
| 25 | B | 1231 | CLA | C2C-C1C-NC | 2.65 | 112.45 | 109.97 |
| 26 | 6 | 613 | CHL | C1-O2A-CGA | 2.65 | 123.39 | 116.44 |
| 25 | A | 1113 | CLA | CMB-C2B-C3B | 2.65 | 129.63 | 124.68 |
| 48 | 5 | 803 | DGA | OG1-CA1-CA2 | 2.64 | 120.21 | 111.91 |
| 40 | 3 | 506 | RRX | C16-C15-C14 | 2.64 | 128.89 | 123.47 |
| 25 | L | 1503 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 25 | 4 | 607 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 25 | 5 | 608 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 25 | A | 1105 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 43 | 6 | 501 | LUT | C10-C11-C12 | -2.64 | 114.97 | 123.22 |
| 25 | B | 1208 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | 1 | 603 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 616 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | 5 | 608 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 26 | 5 | 618 | CHL | C4D-CHA-C1A | 2.64 | 124.47 | 121.25 |
| 30 | A | 5002 | LHG | O8-C23-C24 | 2.64 | 120.20 | 111.91 |
| 25 | 8 | 611 | CLA | C2D-C1D-ND | 2.64 | 112.05 | 110.10 |
| 26 | 2 | 609 | CHL | C4D-CHA-C1A | 2.64 | 124.46 | 121.25 |
| 25 | B | 1229 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | A | 1101 | CLA | CMA-C3A-C4A | 2.64 | 118.87 | 111.77 |
| 25 | 7 | 602 | CLA | CMA-C3A-C4A | 2.64 | 118.87 | 111.77 |
| 29 | 4 | 503 | BCR | C38-C26-C25 | -2.64 | 121.56 | 124.53 |
| 29 | A | 4001 | BCR | C19-C18-C17 | 2.64 | 122.99 | 118.94 |
| 25 | B | 1236 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 25 | A | 1141 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | B | 1206 | CLA | C2D-C1D-ND | 2.64 | 112.05 | 110.10 |
| 25 | A | 1132 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | 7 | 607 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | 4 | 612 | CLA | C2D-C1D-ND | 2.64 | 112.05 | 110.10 |
| 25 | 6 | 601 | CLA | CAA-C2A-C3A | -2.64 | 105.55 | 112.78 |
| 25 | 4 | 607 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 36 | 8 | 802 | DGD | C3G-O3G-C1D | -2.64 | 108.59 | 113.74 |
| 33 | a | 802 | PTY | O4-C30-C31 | 2.64 | 120.18 | 111.91 |
| 25 | B | 1209 | CLA | CMA-C3A-C4A | 2.64 | 118.86 | 111.77 |
| 25 | L | 1502 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 25 | 1 | 602 | CLA | C1C-C2C-C3C | -2.64 | 104.18 | 106.96 |
| 29 | A | 4004 | BCR | C35-C13-C12 | 2.64 | 122.23 | 118.08 |
| 25 | 1 | 607 | CLA | C1C-C2C-C3C | -2.64 | 104.19 | 106.96 |
| 25 | 7 | 601 | CLA | O2A-CGA-CBA | 2.64 | 120.18 | 111.91 |
| 30 | 4 | 802 | LHG | C5-O7-C7 | -2.64 | 111.30 | 117.79 |
| 25 | B | 1219 | CLA | C1C-C2C-C3C | -2.64 | 104.19 | 106.96 |
| 50 | 9 | 507 | XAT | C6-C7-C8 | -2.63 | 120.42 | 125.99 |
| 25 | B | 1217 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |
| 25 | a | 601 | CLA | O2A-CGA-CBA | 2.63 | 120.17 | 111.91 |
| 25 | B | 1204 | CLA | C1D-ND-C4D | -2.63 | 104.47 | 106.33 |
| 25 | 6 | 607 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |
| 48 | 8 | 804 | DGA | OG1-CA1-CA2 | 2.63 | 120.17 | 111.91 |
| 25 | 3 | 606 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |
| 25 | B | 1232 | CLA | C2D-C1D-ND | 2.63 | 112.04 | 110.10 |
| 25 | A | 1107 | CLA | CMB-C2B-C1B | -2.63 | 124.42 | 128.46 |
| 25 | L | 1502 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 25 | 8 | 602 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 25 | B | 1228 | CLA | CMA-C3A-C4A | 2.63 | 118.84 | 111.77 |
| 25 | 4 | 615 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1131 | CLA | C2D-C1D-ND | 2.63 | 112.04 | 110.10 |
| 25 | B | 1213 | CLA | O2A-CGA-CBA | 2.63 | 120.16 | 111.91 |
| 29 | L | 4003 | BCR | C38-C26-C27 | 2.63 | 118.67 | 113.62 |
| 29 | 3 | 504 | BCR | C38-C26-C27 | 2.63 | 118.67 | 113.62 |
| 25 | 6 | 605 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |
| 25 | 9 | 602 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |
| 25 | B | 1210 | CLA | O2A-CGA-CBA | 2.63 | 120.16 | 111.91 |
| 25 | A | 1102 | CLA | C2D-C1D-ND | 2.63 | 112.04 | 110.10 |
| 25 | A | 1120 | CLA | C1C-C2C-C3C | -2.63 | 104.19 | 106.96 |
| 25 | 5 | 605 | CLA | CHA-C4D-ND | 2.63 | 138.00 | 132.50 |
| 29 | B | 4003 | BCR | C35-C13-C12 | 2.63 | 122.22 | 118.08 |
| 25 | 6 | 608 | CLA | O2A-CGA-CBA | 2.63 | 120.15 | 111.91 |
| 25 | 3 | 618 | CLA | CMA-C3A-C4A | 2.63 | 118.83 | 111.77 |
| 25 | B | 1204 | CLA | C1C-C2C-C3C | -2.63 | 104.20 | 106.96 |
| 25 | B | 1227 | CLA | C1C-C2C-C3C | -2.63 | 104.20 | 106.96 |
| 25 | 9 | 607 | CLA | C1C-C2C-C3C | -2.63 | 104.20 | 106.96 |
| 25 | A | 1012 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | 6 | 615 | CLA | CMA-C3A-C4A | 2.62 | 118.83 | 111.77 |
| 29 | J | 4001 | BCR | C28-C27-C26 | -2.62 | 109.39 | 114.08 |
| 29 | 6 | 504 | BCR | C27-C26-C25 | -2.62 | 118.92 | 122.73 |
| 25 | B | 1204 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 25 | B | 1217 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 25 | 4 | 602 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 25 | 8 | 612 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 25 | 9 | 607 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 25 | B | 1021 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | 2 | 602 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | B | 1207 | CLA | C2D-C1D-ND | 2.62 | 112.04 | 110.10 |
| 43 | a | 501 | LUT | C35-C15-C14 | -2.62 | 118.10 | 123.47 |
| 43 | a | 502 | LUT | C35-C15-C14 | -2.62 | 118.10 | 123.47 |
| 25 | 9 | 605 | CLA | O2A-CGA-CBA | 2.62 | 120.13 | 111.91 |
| 29 | 6 | 504 | BCR | C34-C9-C10 | -2.62 | 119.25 | 122.92 |
| 25 | a | 603 | CLA | CMB-C2B-C3B | 2.62 | 129.58 | 124.68 |
| 25 | 2 | 603 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | 9 | 602 | CLA | CMA-C3A-C4A | 2.62 | 118.81 | 111.77 |
| 25 | 5 | 609 | CLA | C2D-C1D-ND | 2.62 | 112.03 | 110.10 |
| 25 | 1 | 601 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | 6 | 618 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 37 | B | 5004 | PCW | O3-C11-C12 | 2.62 | 120.12 | 111.91 |
| 25 | A | 1109 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | A | 1140 | CLA | C1C-C2C-C3C | -2.62 | 104.20 | 106.96 |
| 25 | 6 | 603 | CLA | C2D-C1D-ND | 2.62 | 112.03 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 7 | 612 | CLA | C2D-C1D-ND | 2.62 | 112.03 | 110.10 |
| 25 | G | 1601 | CLA | C1C-C2C-C3C | -2.62 | 104.21 | 106.96 |
| 25 | 7 | 601 | CLA | CMA-C3A-C4A | 2.62 | 118.80 | 111.77 |
| 25 | B | 1223 | CLA | CHA-C4D-ND | 2.62 | 137.97 | 132.50 |
| 25 | L | 1504 | CLA | C2D-C1D-ND | 2.61 | 112.03 | 110.10 |
| 25 | a | 608 | CLA | C2D-C1D-ND | 2.61 | 112.03 | 110.10 |
| 25 | G | 1603 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 25 | 8 | 605 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 25 | A | 1120 | CLA | CMA-C3A-C4A | 2.61 | 118.80 | 111.77 |
| 25 | A | 1131 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 25 | 8 | 607 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 25 | 2 | 604 | CLA | CMD-C2D-C3D | -2.61 | 121.60 | 127.61 |
| 25 | 9 | 604 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 25 | 1 | 603 | CLA | C2D-C1D-ND | 2.61 | 112.03 | 110.10 |
| 25 | a | 607 | CLA | C2D-C1D-ND | 2.61 | 112.03 | 110.10 |
| 25 | 5 | 612 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 25 | A | 1116 | CLA | O2A-CGA-CBA | 2.61 | 120.10 | 111.91 |
| 25 | 6 | 602 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 25 | 6 | 603 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 29 | L | 4001 | BCR | C34-C9-C10 | -2.61 | 119.27 | 122.92 |
| 25 | B | 1204 | CLA | O2A-CGA-CBA | 2.61 | 120.10 | 111.91 |
| 26 | 1 | 610 | CHL | C1B-CHB-C4A | -2.61 | 124.95 | 130.12 |
| 25 | F | 1302 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 25 | 3 | 601 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 26 | a | 613 | CHL | C2C-C3C-C4C | 2.61 | 108.35 | 106.49 |
| 25 | 4 | 604 | CLA | C1C-C2C-C3C | -2.61 | 104.21 | 106.96 |
| 25 | A | 1116 | CLA | CMA-C3A-C4A | 2.61 | 118.78 | 111.77 |
| 25 | 2 | 605 | CLA | CMA-C3A-C4A | 2.61 | 118.78 | 111.77 |
| 25 | 2 | 608 | CLA | C2D-C1D-ND | 2.61 | 112.03 | 110.10 |
| 25 | 3 | 607 | CLA | C1-C2-C3 | -2.61 | 121.53 | 126.04 |
| 25 | 1 | 607 | CLA | CMA-C3A-C4A | 2.61 | 118.78 | 111.77 |
| 25 | A | 1139 | CLA | O2D-CGD-O1D | -2.61 | 118.74 | 123.84 |
| 25 | 5 | 602 | CLA | C1C-C2C-C3C | -2.61 | 104.22 | 106.96 |
| 25 | 7 | 604 | CLA | O2A-CGA-CBA | 2.61 | 120.09 | 111.91 |
| 25 | B | 1231 | CLA | O2D-CGD-O1D | -2.61 | 118.74 | 123.84 |
| 25 | 7 | 601 | CLA | C1D-ND-C4D | -2.61 | 104.48 | 106.33 |
| 43 | 2 | 507 | LUT | C3-C4-C5 | -2.60 | 106.67 | 111.85 |
| 25 | a | 601 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | A | 1107 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | 3 | 605 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | A | 1113 | CLA | O2A-CGA-CBA | 2.60 | 120.08 | 111.91 |
| 25 | 1 | 615 | CLA | C2D-C1D-ND | 2.60 | 112.02 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 2 | 502 | LUT | C15-C35-C34 | -2.60 | 118.14 | 123.47 |
| 30 | a | 801 | LHG | O8-C23-C24 | 2.60 | 120.07 | 111.91 |
| 48 | 2 | 803 | DGA | OG1-CA1-CA2 | 2.60 | 120.07 | 111.91 |
| 29 | L | 4002 | BCR | C33-C5-C4 | 2.60 | 118.61 | 113.62 |
| 25 | 5 | 606 | CLA | C2D-C1D-ND | 2.60 | 112.02 | 110.10 |
| 25 | A | 1135 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | 3 | 618 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | 5 | 615 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | B | 1238 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 25 | a | 605 | CLA | C2D-C1D-ND | 2.60 | 112.02 | 110.10 |
| 25 | K | 1402 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 25 | 6 | 601 | CLA | C1-O2A-CGA | 2.60 | 123.27 | 116.44 |
| 25 | 9 | 602 | CLA | CMB-C2B-C3B | 2.60 | 129.54 | 124.68 |
| 25 | B | 1201 | CLA | C1C-C2C-C3C | -2.60 | 104.22 | 106.96 |
| 25 | B | 1222 | CLA | O2D-CGD-O1D | -2.60 | 118.76 | 123.84 |
| 25 | H | 1703 | CLA | C2C-C1C-NC | 2.60 | 112.41 | 109.97 |
| 25 | a | 603 | CLA | C2D-C1D-ND | 2.60 | 112.02 | 110.10 |
| 25 | H | 1701 | CLA | C2D-C1D-ND | 2.60 | 112.02 | 110.10 |
| 25 | 5 | 603 | CLA | C2D-C1D-ND | 2.60 | 112.02 | 110.10 |
| 25 | 1 | 606 | CLA | C1C-C2C-C3C | -2.60 | 104.23 | 106.96 |
| 25 | 7 | 605 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 26 | a | 613 | CHL | C4A-NA-C1A | 2.59 | 107.87 | 106.71 |
| 26 | 1 | 611 | CHL | C1-C2-C3 | -2.59 | 121.56 | 126.04 |
| 25 | K | 1402 | CLA | C2D-C1D-ND | 2.59 | 112.02 | 110.10 |
| 25 | 8 | 612 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 26 | 3 | 611 | CHL | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 25 | A | 1138 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | a | 603 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | 3 | 612 | CLA | C2D-C1D-ND | 2.59 | 112.01 | 110.10 |
| 25 | 3 | 610 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | A | 1123 | CLA | O2D-CGD-O1D | -2.59 | 118.77 | 123.84 |
| 43 | 1 | 501 | LUT | C7-C8-C9 | -2.59 | 122.32 | 126.23 |
| 25 | 6 | 618 | CLA | C2D-C1D-ND | 2.59 | 112.01 | 110.10 |
| 25 | A | 1128 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | A | 1129 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | 2 | 606 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | B | 1207 | CLA | CAA-C2A-C3A | -2.59 | 105.69 | 112.78 |
| 25 | B | 1023 | CLA | O2D-CGD-O1D | -2.59 | 118.78 | 123.84 |
| 25 | A | 1102 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | a | 607 | CLA | C1C-C2C-C3C | -2.59 | 104.23 | 106.96 |
| 25 | B | 1218 | CLA | C2D-C1D-ND | 2.59 | 112.01 | 110.10 |
| 25 | 4 | 616 | CLA | C2D-C1D-ND | 2.59 | 112.01 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | I | 4001 | BCR | C34-C9-C10 | -2.59 | 119.30 | 122.92 |
| 29 | A | 4002 | BCR | C33-C5-C4 | 2.59 | 118.59 | 113.62 |
| 25 | 9 | 604 | CLA | O2A-CGA-CBA | 2.59 | 120.03 | 111.91 |
| 26 | 5 | 610 | CHL | CMA-C3A-C4A | 2.59 | 118.72 | 111.77 |
| 25 | K | 1402 | CLA | C1C-C2C-C3C | -2.59 | 104.24 | 106.96 |
| 25 | A | 1126 | CLA | CMA-C3A-C4A | 2.59 | 118.72 | 111.77 |
| 25 | 3 | 616 | CLA | O2D-CGD-O1D | -2.59 | 118.78 | 123.84 |
| 26 | 6 | 610 | CHL | C1-C2-C3 | -2.59 | 121.57 | 126.04 |
| 29 | K | 4002 | BCR | C37-C22-C21 | -2.58 | 119.30 | 122.92 |
| 25 | 4 | 608 | CLA | C1C-C2C-C3C | -2.58 | 104.24 | 106.96 |
| 25 | A | 1013 | CLA | CMB-C2B-C1B | -2.58 | 124.49 | 128.46 |
| 25 | 5 | 614 | CLA | C1C-C2C-C3C | -2.58 | 104.24 | 106.96 |
| 25 | B | 1236 | CLA | C1C-C2C-C3C | -2.58 | 104.24 | 106.96 |
| 25 | 9 | 605 | CLA | C1C-C2C-C3C | -2.58 | 104.24 | 106.96 |
| 29 | 7 | 503 | BCR | C33-C5-C4 | 2.58 | 118.58 | 113.62 |
| 25 | A | 1112 | CLA | O2D-CGD-O1D | -2.58 | 118.79 | 123.84 |
| 25 | A | 1012 | CLA | OBD-CAD-C3D | -2.58 | 122.31 | 128.52 |
| 26 | 7 | 609 | CHL | CMA-C3A-C4A | 2.58 | 118.71 | 111.77 |
| 25 | 8 | 607 | CLA | C2D-C1D-ND | 2.58 | 112.01 | 110.10 |
| 25 | 5 | 604 | CLA | O2A-CGA-CBA | 2.58 | 120.00 | 111.91 |
| 30 | 5 | 801 | LHG | O8-C23-C24 | 2.58 | 120.00 | 111.91 |
| 25 | A | 1141 | CLA | CHA-C4D-ND | 2.58 | 137.90 | 132.50 |
| 25 | 2 | 615 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 25 | 4 | 606 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 25 | 5 | 606 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 25 | B | 1213 | CLA | C2C-C1C-NC | 2.58 | 112.39 | 109.97 |
| 25 | A | 1131 | CLA | CMA-C3A-C4A | 2.58 | 118.70 | 111.77 |
| 25 | 6 | 605 | CLA | O2D-CGD-O1D | -2.58 | 118.80 | 123.84 |
| 25 | 5 | 601 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 25 | A | 1129 | CLA | C2D-C1D-ND | 2.58 | 112.00 | 110.10 |
| 25 | a | 611 | CLA | O2D-CGD-O1D | -2.58 | 118.80 | 123.84 |
| 25 | B | 1205 | CLA | O2A-CGA-CBA | 2.58 | 119.99 | 111.91 |
| 25 | B | 1224 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 29 | B | 4007 | BCR | C19-C18-C17 | 2.58 | 122.89 | 118.94 |
| 25 | 4 | 605 | CLA | CHA-C4D-ND | 2.58 | 137.89 | 132.50 |
| 25 | B | 1231 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 25 | 2 | 608 | CLA | C1C-C2C-C3C | -2.58 | 104.25 | 106.96 |
| 30 | 7 | 803 | LHG | O8-C23-C24 | 2.57 | 119.99 | 111.91 |
| 25 | 9 | 605 | CLA | O2D-CGD-O1D | -2.57 | 118.80 | 123.84 |
| 25 | 7 | 605 | CLA | CHA-C4D-ND | 2.57 | 137.88 | 132.50 |
| 26 | 1 | 610 | CHL | C2C-C3C-C4C | 2.57 | 108.32 | 106.49 |
| 30 | 8 | 801 | LHG | O8-C23-C24 | 2.57 | 119.99 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 601 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 25 | 5 | 609 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | A | 1112 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | 7 | 610 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | B | 1240 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 25 | A | 1116 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 25 | 4 | 604 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 25 | 1 | 607 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 26 | 9 | 610 | CHL | C4A-NA-C1A | 2.57 | 107.86 | 106.71 |
| 25 | A | 1136 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | B | 1228 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | B | 1229 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 25 | B | 1210 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 25 | 5 | 605 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 25 | 4 | 610 | CLA | C1-C2-C3 | -2.57 | 121.60 | 126.04 |
| 25 | B | 1237 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | 3 | 607 | CLA | C1C-C2C-C3C | -2.57 | 104.25 | 106.96 |
| 25 | A | 1137 | CLA | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 29 | A | 4001 | BCR | C38-C26-C27 | 2.57 | 118.55 | 113.62 |
| 25 | A | 1126 | CLA | C1C-C2C-C3C | -2.57 | 104.26 | 106.96 |
| 25 | A | 1138 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 25 | 8 | 606 | CLA | C2D-C1D-ND | 2.57 | 112.00 | 110.10 |
| 26 | a | 606 | CHL | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 26 | 5 | 617 | CHL | C4D-CHA-C1A | 2.57 | 124.37 | 121.25 |
| 25 | L | 1501 | CLA | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 25 | 7 | 610 | CLA | CMA-C3A-C4A | 2.57 | 118.67 | 111.77 |
| 25 | A | 1111 | CLA | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 33 | A | 5006 | PTY | O4-C30-C31 | 2.57 | 119.96 | 111.91 |
| 30 | 5 | 801 | LHG | C5-O7-C7 | -2.57 | 111.48 | 117.79 |
| 25 | 6 | 603 | CLA | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 25 | A | 1107 | CLA | O2A-CGA-CBA | 2.56 | 119.96 | 111.91 |
| 29 | B | 4005 | BCR | C33-C5-C4 | 2.56 | 118.54 | 113.62 |
| 29 | 7 | 503 | BCR | C35-C13-C12 | 2.56 | 122.12 | 118.08 |
| 25 | G | 1602 | CLA | C1C-C2C-C3C | -2.56 | 104.26 | 106.96 |
| 25 | 8 | 611 | CLA | C1C-C2C-C3C | -2.56 | 104.26 | 106.96 |
| 25 | A | 1124 | CLA | C1C-C2C-C3C | -2.56 | 104.26 | 106.96 |
| 25 | 9 | 612 | CLA | O2D-CGD-O1D | -2.56 | 118.83 | 123.84 |
| 25 | 8 | 609 | CLA | C1D-ND-C4D | -2.56 | 104.51 | 106.33 |
| 37 | 6 | 803 | PCW | O3-C11-C12 | 2.56 | 119.95 | 111.91 |
| 26 | 5 | 613 | CHL | C1-C2-C3 | -2.56 | 121.61 | 126.04 |
| 25 | 4 | 603 | CLA | C1C-C2C-C3C | -2.56 | 104.26 | 106.96 |
| 29 | O | 4001 | BCR | C34-C9-C10 | -2.56 | 119.33 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 603 | CLA | O2D-CGD-O1D | -2.56 | 118.83 | 123.84 |
| 26 | 5 | 610 | CHL | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 25 | 2 | 605 | CLA | CHA-C4D-ND | 2.56 | 137.86 | 132.50 |
| 25 | B | 1214 | CLA | C2D-C1D-ND | 2.56 | 111.99 | 110.10 |
| 25 | K | 1401 | CLA | C1C-C2C-C3C | -2.56 | 104.27 | 106.96 |
| 25 | 6 | 615 | CLA | C1C-C2C-C3C | -2.56 | 104.27 | 106.96 |
| 30 | A | 5003 | LHG | O8-C23-C24 | 2.56 | 119.94 | 111.91 |
| 25 | B | 1219 | CLA | CMB-C2B-C3B | 2.56 | 129.47 | 124.68 |
| 25 | O | 1802 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 25 | 8 | 612 | CLA | C2D-C1D-ND | 2.56 | 111.99 | 110.10 |
| 25 | 9 | 609 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 26 | 6 | 610 | CHL | C1-O2A-CGA | 2.56 | 123.15 | 116.44 |
| 30 | 6 | 802 | LHG | O8-C23-C24 | 2.56 | 119.93 | 111.91 |
| 25 | G | 1601 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 25 | B | 1203 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 26 | 8 | 601 | CHL | C1-O2A-CGA | 2.56 | 123.15 | 116.44 |
| 25 | A | 1112 | CLA | C2D-C1D-ND | 2.56 | 111.99 | 110.10 |
| 43 | 1 | 503 | LUT | C8-C7-C6 | -2.55 | 120.03 | 127.20 |
| 25 | B | 1215 | CLA | C1-C2-C3 | -2.55 | 121.63 | 126.04 |
| 25 | 4 | 606 | CLA | C2D-C1D-ND | 2.55 | 111.99 | 110.10 |
| 25 | a | 612 | CLA | C2D-C1D-ND | 2.55 | 111.98 | 110.10 |
| 25 | 2 | 602 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 25 | 4 | 608 | CLA | CMA-C3A-C4A | 2.55 | 118.63 | 111.77 |
| 25 | B | 1216 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 25 | A | 1112 | CLA | CMB-C2B-C3B | 2.55 | 129.45 | 124.68 |
| 25 | 5 | 604 | CLA | C1C-C2C-C3C | -2.55 | 104.27 | 106.96 |
| 33 | a | 803 | PTY | O4-C30-C31 | 2.55 | 119.91 | 111.91 |
| 25 | 9 | 612 | CLA | C2D-C1D-ND | 2.55 | 111.98 | 110.10 |
| 25 | A | 1101 | CLA | C1C-C2C-C3C | -2.55 | 104.28 | 106.96 |
| 26 | 7 | 609 | CHL | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 25 | 3 | 612 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 25 | 6 | 604 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 26 | 3 | 611 | CHL | C4D-CHA-C1A | 2.55 | 124.35 | 121.25 |
| 25 | B | 1234 | CLA | C2C-C1C-NC | 2.55 | 113.64 | 109.79 |
| 52 | 8 | 805 | P5S | O19-C17-C20 | 2.55 | 119.91 | 111.91 |
| 25 | A | 1104 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 25 | 6 | 606 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 25 | B | 1208 | CLA | C2D-C1D-ND | 2.55 | 111.98 | 110.10 |
| 25 | 6 | 606 | CLA | CMA-C3A-C4A | 2.55 | 118.62 | 111.77 |
| 25 | A | 1106 | CLA | C1C-C2C-C3C | -2.55 | 104.28 | 106.96 |
| 30 | B | 5002 | LHG | C5-O7-C7 | -2.55 | 111.52 | 117.79 |
| 24 | A | 1011 | CL0 | C4-C3-C5 | 2.55 | 119.56 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | H | 1703 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 25 | 2 | 605 | CLA | C1C-C2C-C3C | -2.55 | 104.28 | 106.96 |
| 25 | 7 | 604 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 25 | 5 | 614 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 25 | 6 | 608 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 25 | 4 | 604 | CLA | O2A-CGA-CBA | 2.55 | 119.90 | 111.91 |
| 50 | 9 | 507 | XAT | C27-C28-C29 | 2.55 | 129.48 | 125.53 |
| 42 | M | 4001 | ECH | C29-C30-C25 | -2.54 | 106.56 | 110.48 |
| 25 | 6 | 605 | CLA | C2D-C1D-ND | 2.54 | 111.98 | 110.10 |
| 25 | B | 1201 | CLA | CMB-C2B-C3B | 2.54 | 129.44 | 124.68 |
| 25 | A | 1124 | CLA | O2D-CGD-O1D | -2.54 | 118.86 | 123.84 |
| 25 | 2 | 606 | CLA | O2D-CGD-O1D | -2.54 | 118.86 | 123.84 |
| 29 | 4 | 503 | BCR | C33-C5-C4 | 2.54 | 118.50 | 113.62 |
| 25 | B | 1205 | CLA | CMA-C3A-C4A | 2.54 | 118.61 | 111.77 |
| 25 | B | 1206 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 25 | 7 | 604 | CLA | CMD-C2D-C3D | -2.54 | 121.76 | 127.61 |
| 29 | 3 | 504 | BCR | C23-C24-C25 | -2.54 | 120.06 | 127.20 |
| 25 | 1 | 606 | CLA | CHA-C4D-ND | 2.54 | 137.82 | 132.50 |
| 25 | B | 1230 | CLA | C1C-C2C-C3C | -2.54 | 104.28 | 106.96 |
| 36 | 7 | 806 | DGD | O6D-C5D-C6D | 2.54 | 111.80 | 106.67 |
| 25 | 6 | 608 | CLA | C2D-C1D-ND | 2.54 | 111.98 | 110.10 |
| 25 | B | 1213 | CLA | CMB-C2B-C3B | 2.54 | 129.43 | 124.68 |
| 37 | K | 5002 | PCW | O3-C11-C12 | 2.54 | 119.88 | 111.91 |
| 25 | A | 1130 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 25 | 5 | 602 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 25 | 5 | 605 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 29 | B | 4004 | BCR | C38-C26-C25 | -2.54 | 121.68 | 124.53 |
| 43 | 7 | 501 | LUT | C31-C32-C33 | -2.54 | 119.28 | 126.42 |
| 25 | 6 | 612 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 25 | B | 1222 | CLA | C1C-C2C-C3C | -2.54 | 104.29 | 106.96 |
| 25 | 7 | 605 | CLA | C2D-C1D-ND | 2.54 | 111.97 | 110.10 |
| 26 | 6 | 609 | CHL | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 25 | B | 1225 | CLA | C1C-C2C-C3C | -2.54 | 104.29 | 106.96 |
| 25 | K | 1401 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 25 | A | 1013 | CLA | C2C-C1C-NC | 2.54 | 112.35 | 109.97 |
| 26 | a | 609 | CHL | C1-C2-C3 | -2.54 | 121.66 | 126.04 |
| 24 | A | 1011 | CL0 | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 25 | A | 1012 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 25 | A | 1013 | CLA | C1C-C2C-C3C | -2.54 | 104.29 | 106.96 |
| 25 | B | 1240 | CLA | C1C-C2C-C3C | -2.54 | 104.29 | 106.96 |
| 25 | B | 1240 | CLA | O2A-CGA-CBA | 2.54 | 119.86 | 111.91 |
| 25 | K | 1404 | CLA | CHA-C4D-ND | 2.54 | 137.80 | 132.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 605 | CLA | CHA-C4D-ND | 2.54 | 137.80 | 132.50 |
| 25 | A | 1125 | CLA | CMA-C3A-C4A | 2.54 | 118.59 | 111.77 |
| 25 | B | 1022 | CLA | CHA-C4D-ND | 2.54 | 137.80 | 132.50 |
| 25 | 1 | 606 | CLA | C2D-C1D-ND | 2.53 | 111.97 | 110.10 |
| 25 | A | 1119 | CLA | C1C-C2C-C3C | -2.53 | 104.29 | 106.96 |
| 26 | a | 610 | CHL | C4D-CHA-C1A | 2.53 | 124.33 | 121.25 |
| 29 | 6 | 503 | BCR | C33-C5-C4 | 2.53 | 118.48 | 113.62 |
| 43 | 4 | 502 | LUT | C10-C11-C12 | -2.53 | 115.31 | 123.22 |
| 43 | 9 | 502 | LUT | C38-C25-C24 | -2.53 | 118.14 | 123.56 |
| 25 | 8 | 618 | CLA | CHA-C4D-ND | 2.53 | 137.80 | 132.50 |
| 25 | B | 1219 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 25 | 3 | 610 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 25 | B | 1202 | CLA | C1C-C2C-C3C | -2.53 | 104.29 | 106.96 |
| 44 | 7 | 504 | AXT | C38-C25-C26 | -2.53 | 120.04 | 124.11 |
| 25 | B | 1209 | CLA | C2D-C1D-ND | 2.53 | 111.97 | 110.10 |
| 26 | 9 | 610 | CHL | C1B-CHB-C4A | -2.53 | 125.10 | 130.12 |
| 25 | 5 | 601 | CLA | O2A-CGA-CBA | 2.53 | 119.85 | 111.91 |
| 25 | G | 1602 | CLA | C1-C2-C3 | -2.53 | 121.67 | 126.04 |
| 25 | 2 | 612 | CLA | C2D-C1D-ND | 2.53 | 111.97 | 110.10 |
| 25 | 6 | 605 | CLA | CHA-C4D-ND | 2.53 | 137.79 | 132.50 |
| 26 | a | 606 | CHL | C4D-CHA-C1A | 2.53 | 124.33 | 121.25 |
| 25 | 1 | 602 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 30 | 6 | 801 | LHG | O8-C23-C24 | 2.53 | 119.84 | 111.91 |
| 26 | 6 | 609 | CHL | C4A-NA-C1A | 2.53 | 107.84 | 106.71 |
| 25 | A | 1108 | CLA | C1C-C2C-C3C | -2.53 | 104.30 | 106.96 |
| 25 | 4 | 602 | CLA | C1C-C2C-C3C | -2.53 | 104.30 | 106.96 |
| 25 | 6 | 608 | CLA | CMD-C2D-C3D | -2.53 | 121.80 | 127.61 |
| 25 | 2 | 606 | CLA | CMB-C2B-C3B | 2.53 | 129.41 | 124.68 |
| 25 | B | 1022 | CLA | O2D-CGD-O1D | -2.53 | 118.90 | 123.84 |
| 25 | B | 1226 | CLA | CHA-C4D-ND | 2.53 | 137.78 | 132.50 |
| 33 | J | 5001 | PTY | O4-C30-C31 | 2.53 | 119.84 | 111.91 |
| 25 | 7 | 612 | CLA | O2D-CGD-O1D | -2.53 | 118.90 | 123.84 |
| 25 | B | 1218 | CLA | O2A-CGA-CBA | 2.53 | 119.84 | 111.91 |
| 25 | 8 | 602 | CLA | CMA-C3A-C4A | 2.53 | 118.56 | 111.77 |
| 25 | 2 | 605 | CLA | O2A-CGA-CBA | 2.53 | 119.83 | 111.91 |
| 25 | 8 | 602 | CLA | C1C-C2C-C3C | -2.53 | 104.30 | 106.96 |
| 26 | 6 | 611 | CHL | C1-O2A-CGA | 2.52 | 123.07 | 116.44 |
| 26 | 5 | 613 | CHL | C4A-NA-C1A | 2.52 | 107.84 | 106.71 |
| 25 | A | 1012 | CLA | CHA-C4D-ND | 2.52 | 137.78 | 132.50 |
| 25 | 2 | 621 | CLA | O2A-CGA-CBA | 2.52 | 119.83 | 111.91 |
| 25 | 1 | 612 | CLA | CMA-C3A-C4A | 2.52 | 118.56 | 111.77 |
| 25 | F | 1302 | CLA | O2A-CGA-CBA | 2.52 | 119.83 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1013 | CLA | C1-C2-C3 | -2.52 | 121.68 | 126.04 |
| 25 | 4 | 605 | CLA | C1C-C2C-C3C | -2.52 | 104.30 | 106.96 |
| 29 | 6 | 504 | BCR | C28-C27-C26 | -2.52 | 109.57 | 114.08 |
| 25 | B | 1209 | CLA | C1C-C2C-C3C | -2.52 | 104.30 | 106.96 |
| 25 | B | 1223 | CLA | OBD-CAD-C3D | -2.52 | 122.45 | 128.52 |
| 44 | 1 | 502 | AXT | C8-C7-C6 | 2.52 | 134.29 | 127.20 |
| 25 | B | 1214 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 25 | 3 | 606 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 26 | 9 | 603 | CHL | C4A-NA-C1A | 2.52 | 107.84 | 106.71 |
| 25 | 3 | 618 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 25 | A | 1113 | CLA | C2D-C1D-ND | 2.52 | 111.96 | 110.10 |
| 30 | 6 | 801 | LHG | C5-O7-C7 | -2.52 | 111.59 | 117.79 |
| 25 | B | 1228 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 25 | A | 1111 | CLA | CMB-C2B-C3B | 2.52 | 129.39 | 124.68 |
| 25 | B | 1238 | CLA | C1C-C2C-C3C | -2.52 | 104.31 | 106.96 |
| 25 | 6 | 606 | CLA | O2A-CGA-CBA | 2.52 | 119.81 | 111.91 |
| 26 | 5 | 613 | CHL | C4D-CHA-C1A | 2.52 | 124.31 | 121.25 |
| 25 | B | 1237 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 25 | A | 1140 | CLA | O2D-CGD-O1D | -2.52 | 118.92 | 123.84 |
| 25 | B | 1213 | CLA | CMA-C3A-C4A | 2.52 | 118.54 | 111.77 |
| 25 | B | 1207 | CLA | O2D-CGD-O1D | -2.52 | 118.92 | 123.84 |
| 25 | B | 1021 | CLA | CHA-C4D-ND | 2.52 | 137.76 | 132.50 |
| 25 | 7 | 604 | CLA | C2D-C1D-ND | 2.52 | 111.96 | 110.10 |
| 25 | B | 1235 | CLA | C1C-C2C-C3C | -2.52 | 104.31 | 106.96 |
| 26 | 1 | 610 | CHL | C1-O2A-CGA | 2.52 | 124.04 | 116.73 |
| 26 | 2 | 613 | CHL | C1-O2A-CGA | 2.52 | 123.05 | 116.44 |
| 29 | 3 | 505 | BCR | C19-C18-C17 | 2.52 | 122.80 | 118.94 |
| 25 | 3 | 605 | CLA | CHA-C4D-ND | 2.52 | 137.76 | 132.50 |
| 25 | A | 1107 | CLA | C2D-C1D-ND | 2.52 | 111.96 | 110.10 |
| 25 | 2 | 621 | CLA | C2D-C1D-ND | 2.52 | 111.96 | 110.10 |
| 25 | A | 1122 | CLA | O2A-CGA-CBA | 2.52 | 119.80 | 111.91 |
| 25 | B | 1211 | CLA | C1C-C2C-C3C | -2.51 | 104.31 | 106.96 |
| 25 | B | 1213 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 43 | 1 | 501 | LUT | C10-C11-C12 | -2.51 | 115.38 | 123.22 |
| 25 | A | 1140 | CLA | CMA-C3A-C4A | 2.51 | 118.52 | 111.77 |
| 25 | A | 1115 | CLA | C1C-C2C-C3C | -2.51 | 104.32 | 106.96 |
| 25 | J | 1901 | CLA | C1C-C2C-C3C | -2.51 | 104.32 | 106.96 |
| 25 | A | 1111 | CLA | C2D-C1D-ND | 2.51 | 111.95 | 110.10 |
| 25 | 2 | 606 | CLA | C2D-C1D-ND | 2.51 | 111.95 | 110.10 |
| 26 | 9 | 613 | CHL | C4D-CHA-C1A | 2.51 | 124.30 | 121.25 |
| 25 | B | 1022 | CLA | CMA-C3A-C4A | 2.51 | 118.52 | 111.77 |
| 25 | 7 | 601 | CLA | C2C-C1C-NC | 2.51 | 112.32 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1118 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 29 | 7 | 503 | BCR | C27-C26-C25 | -2.51 | 119.09 | 122.73 |
| 25 | a | 603 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 25 | 8 | 608 | CLA | O2A-CGA-CBA | 2.51 | 119.78 | 111.91 |
| 25 | 2 | 612 | CLA | O2D-CGD-O1D | -2.51 | 118.94 | 123.84 |
| 25 | 3 | 607 | CLA | O2D-CGD-O1D | -2.51 | 118.94 | 123.84 |
| 29 | O | 4001 | BCR | C23-C24-C25 | -2.51 | 120.17 | 127.20 |
| 26 | a | 606 | CHL | C1B-CHB-C4A | -2.51 | 125.16 | 130.12 |
| 25 | A | 1110 | CLA | C1C-C2C-C3C | -2.50 | 104.32 | 106.96 |
| 25 | 9 | 604 | CLA | O2D-CGD-O1D | -2.50 | 118.94 | 123.84 |
| 25 | J | 1901 | CLA | CHA-C4D-ND | 2.50 | 137.74 | 132.50 |
| 25 | B | 1237 | CLA | C2D-C1D-ND | 2.50 | 111.95 | 110.10 |
| 25 | A | 1125 | CLA | CHA-C4D-ND | 2.50 | 137.73 | 132.50 |
| 25 | A | 1109 | CLA | CMD-C2D-C3D | -2.50 | 121.86 | 127.61 |
| 30 | 1 | 802 | LHG | C5-O7-C7 | -2.50 | 111.63 | 117.79 |
| 25 | B | 1230 | CLA | C1D-ND-C4D | -2.50 | 104.56 | 106.33 |
| 29 | 3 | 504 | BCR | C34-C9-C10 | -2.50 | 119.42 | 122.92 |
| 29 | B | 4003 | BCR | C12-C13-C14 | -2.50 | 115.11 | 118.94 |
| 25 | 1 | 601 | CLA | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 25 | A | 1104 | CLA | CHA-C4D-ND | 2.50 | 137.73 | 132.50 |
| 25 | B | 1211 | CLA | C2D-C1D-ND | 2.50 | 111.95 | 110.10 |
| 25 | J | 1901 | CLA | C2D-C1D-ND | 2.50 | 111.95 | 110.10 |
| 25 | 1 | 601 | CLA | O2A-CGA-CBA | 2.50 | 119.75 | 111.91 |
| 26 | 5 | 618 | CHL | C4A-NA-C1A | 2.50 | 107.83 | 106.71 |
| 29 | A | 4002 | BCR | C19-C18-C17 | 2.50 | 122.77 | 118.94 |
| 26 | 7 | 609 | CHL | C1-O2A-CGA | 2.50 | 123.00 | 116.44 |
| 25 | 7 | 601 | CLA | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 25 | 4 | 606 | CLA | CHA-C4D-ND | 2.50 | 137.72 | 132.50 |
| 25 | A | 1119 | CLA | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 50 | 2 | 501 | XAT | C25-C24-C23 | -2.50 | 107.81 | 112.75 |
| 50 | 2 | 501 | XAT | O24-C25-C38 | -2.50 | 112.06 | 115.06 |
| 26 | a | 606 | CHL | CMA-C3A-C4A | 2.50 | 118.48 | 111.77 |
| 25 | 1 | 615 | CLA | CHA-C4D-ND | 2.49 | 137.72 | 132.50 |
| 25 | B | 1209 | CLA | C1-O2A-CGA | 2.49 | 122.99 | 116.44 |
| 25 | 3 | 607 | CLA | C2D-C1D-ND | 2.49 | 111.94 | 110.10 |
| 25 | 3 | 602 | CLA | O2D-CGD-O1D | -2.49 | 118.96 | 123.84 |
| 25 | 6 | 605 | CLA | CMD-C2D-C3D | -2.49 | 121.88 | 127.61 |
| 25 | 2 | 607 | CLA | CHA-C4D-ND | 2.49 | 137.72 | 132.50 |
| 25 | B | 1216 | CLA | CMB-C2B-C3B | 2.49 | 129.34 | 124.68 |
| 25 | A | 1113 | CLA | C1C-C2C-C3C | -2.49 | 104.33 | 106.96 |
| 25 | A | 1104 | CLA | O2A-CGA-CBA | 2.49 | 119.73 | 111.91 |
| 29 | O | 4001 | BCR | C30-C25-C26 | -2.49 | 119.10 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1122 | CLA | C1C-C2C-C3C | -2.49 | 104.34 | 106.96 |
| 25 | B | 1201 | CLA | CMA-C3A-C4A | 2.49 | 118.47 | 111.77 |
| 29 | B | 4006 | BCR | C36-C18-C17 | -2.49 | 119.43 | 122.92 |
| 25 | 9 | 604 | CLA | C2D-C1D-ND | 2.49 | 111.94 | 110.10 |
| 25 | 6 | 601 | CLA | C1C-C2C-C3C | -2.49 | 104.34 | 106.96 |
| 29 | J | 4001 | BCR | C23-C24-C25 | -2.49 | 120.20 | 127.20 |
| 25 | B | 1206 | CLA | CMA-C3A-C4A | 2.49 | 118.47 | 111.77 |
| 25 | B | 1221 | CLA | CMB-C2B-C3B | 2.49 | 129.34 | 124.68 |
| 25 | 7 | 612 | CLA | CMA-C3A-C4A | 2.49 | 118.47 | 111.77 |
| 25 | A | 1106 | CLA | C1D-ND-C4D | -2.49 | 104.57 | 106.33 |
| 25 | 8 | 605 | CLA | C1D-ND-C4D | -2.49 | 104.57 | 106.33 |
| 26 | 9 | 603 | CHL | C2C-C3C-C4C | 2.49 | 108.26 | 106.49 |
| 29 | H | 4001 | BCR | C33-C5-C6 | -2.49 | 121.73 | 124.53 |
| 26 | 2 | 610 | CHL | C4D-CHA-C1A | 2.49 | 124.28 | 121.25 |
| 43 | 1 | 501 | LUT | C38-C25-C24 | -2.49 | 118.23 | 123.56 |
| 25 | 4 | 601 | CLA | CMB-C2B-C3B | 2.49 | 129.34 | 124.68 |
| 25 | 5 | 604 | CLA | O2D-CGD-O1D | -2.49 | 118.97 | 123.84 |
| 25 | B | 1229 | CLA | C1D-ND-C4D | -2.49 | 104.57 | 106.33 |
| 25 | 4 | 608 | CLA | O2A-CGA-CBA | 2.49 | 119.72 | 111.91 |
| 50 | 2 | 501 | XAT | O4-C5-C18 | -2.49 | 112.08 | 115.06 |
| 25 | B | 1221 | CLA | CHA-C4D-ND | 2.49 | 137.70 | 132.50 |
| 25 | A | 1113 | CLA | CAA-C2A-C3A | -2.49 | 105.97 | 112.78 |
| 25 | 5 | 605 | CLA | CMA-C3A-C4A | 2.49 | 118.46 | 111.77 |
| 29 | L | 4001 | BCR | C36-C18-C17 | -2.49 | 119.44 | 122.92 |
| 43 | a | 503 | LUT | C31-C32-C33 | -2.49 | 119.43 | 126.42 |
| 25 | A | 1112 | CLA | O1D-CGD-CBD | -2.49 | 119.40 | 124.48 |
| 25 | 9 | 602 | CLA | O2D-CGD-O1D | -2.49 | 118.98 | 123.84 |
| 25 | B | 1214 | CLA | C1C-C2C-C3C | -2.48 | 104.34 | 106.96 |
| 25 | a | 605 | CLA | CHA-C4D-ND | 2.48 | 137.70 | 132.50 |
| 25 | 4 | 612 | CLA | CHA-C4D-ND | 2.48 | 137.69 | 132.50 |
| 25 | A | 1102 | CLA | CHA-C4D-ND | 2.48 | 137.69 | 132.50 |
| 25 | K | 1403 | CLA | CHA-C4D-ND | 2.48 | 137.69 | 132.50 |
| 25 | 9 | 605 | CLA | C1-C2-C3 | -2.48 | 121.75 | 126.04 |
| 26 | 6 | 619 | CHL | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 25 | B | 1231 | CLA | CHA-C4D-ND | 2.48 | 137.69 | 132.50 |
| 25 | H | 1702 | CLA | CHA-C4D-ND | 2.48 | 137.69 | 132.50 |
| 25 | a | 605 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 25 | 7 | 603 | CLA | O2A-CGA-CBA | 2.48 | 119.70 | 111.91 |
| 25 | 2 | 604 | CLA | O2D-CGD-O1D | -2.48 | 118.99 | 123.84 |
| 29 | L | 4002 | BCR | C12-C13-C14 | -2.48 | 115.13 | 118.94 |
| 25 | 6 | 608 | CLA | CHA-C4D-ND | 2.48 | 137.69 | 132.50 |
| 25 | 2 | 604 | CLA | C2D-C1D-ND | 2.48 | 111.93 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 5 | 501 | LUT | C11-C10-C9 | -2.48 | 123.77 | 127.31 |
| 26 | a | 609 | CHL | C1-O2A-CGA | 2.48 | 122.95 | 116.44 |
| 25 | A | 1117 | CLA | O1D-CGD-CBD | -2.48 | 119.41 | 124.48 |
| 43 | 4 | 502 | LUT | C35-C15-C14 | -2.48 | 118.40 | 123.47 |
| 43 | 8 | 501 | LUT | C11-C10-C9 | -2.48 | 123.77 | 127.31 |
| 25 | B | 1238 | CLA | C1-O2A-CGA | 2.48 | 122.95 | 116.44 |
| 29 | 3 | 505 | BCR | C33-C5-C4 | 2.48 | 118.38 | 113.62 |
| 25 | A | 1126 | CLA | CHA-C4D-ND | 2.48 | 137.68 | 132.50 |
| 25 | A | 1132 | CLA | C2D-C1D-ND | 2.48 | 111.93 | 110.10 |
| 30 | 7 | 802 | LHG | O8-C23-C24 | 2.48 | 119.68 | 111.91 |
| 25 | 6 | 607 | CLA | O2D-CGD-O1D | -2.48 | 119.00 | 123.84 |
| 43 | a | 502 | LUT | C10-C11-C12 | -2.47 | 115.50 | 123.22 |
| 25 | A | 1132 | CLA | CHA-C4D-ND | 2.47 | 137.68 | 132.50 |
| 25 | L | 1503 | CLA | CHA-C4D-ND | 2.47 | 137.68 | 132.50 |
| 25 | O | 1802 | CLA | C1C-C2C-C3C | -2.47 | 104.36 | 106.96 |
| 30 | 3 | 801 | LHG | O8-C23-C24 | 2.47 | 119.67 | 111.91 |
| 25 | 6 | 601 | CLA | O2A-CGA-CBA | 2.47 | 119.67 | 111.91 |
| 25 | B | 1232 | CLA | C1C-C2C-C3C | -2.47 | 104.36 | 106.96 |
| 26 | 2 | 609 | CHL | C1-C2-C3 | -2.47 | 121.77 | 126.04 |
| 35 | 1 | 804 | LMT | O5B-C5B-C4B | 2.47 | 114.18 | 109.69 |
| 25 | 5 | 604 | CLA | C1D-ND-C4D | -2.47 | 104.58 | 106.33 |
| 25 | 9 | 609 | CLA | CMB-C2B-C1B | -2.47 | 124.67 | 128.46 |
| 25 | 5 | 614 | CLA | CMA-C3A-C4A | 2.47 | 118.42 | 111.77 |
| 25 | 4 | 601 | CLA | O2A-CGA-CBA | 2.47 | 119.66 | 111.91 |
| 40 | J | 4002 | RRX | C20-C21-C22 | -2.47 | 123.78 | 127.31 |
| 25 | 6 | 602 | CLA | CMA-C3A-C4A | 2.47 | 118.41 | 111.77 |
| 25 | B | 1239 | CLA | O2D-CGD-O1D | -2.47 | 119.01 | 123.84 |
| 25 | A | 1101 | CLA | CHA-C4D-ND | 2.47 | 137.66 | 132.50 |
| 25 | 2 | 621 | CLA | CHA-C4D-ND | 2.47 | 137.66 | 132.50 |
| 25 | B | 1211 | CLA | CHA-C4D-ND | 2.47 | 137.66 | 132.50 |
| 25 | A | 1137 | CLA | C1C-C2C-C3C | -2.47 | 104.36 | 106.96 |
| 25 | L | 1502 | CLA | CAA-C2A-C3A | -2.47 | 106.02 | 112.78 |
| 30 | 1 | 802 | LHG | O8-C23-C24 | 2.47 | 119.65 | 111.91 |
| 43 | 7 | 501 | LUT | C10-C11-C12 | -2.47 | 115.52 | 123.22 |
| 26 | 6 | 613 | CHL | CHB-C4A-NA | 2.47 | 127.92 | 124.51 |
| 25 | A | 1107 | CLA | O2D-CGD-O1D | -2.47 | 119.02 | 123.84 |
| 25 | 8 | 615 | CLA | C1D-ND-C4D | -2.47 | 104.58 | 106.33 |
| 25 | B | 1203 | CLA | CHA-C4D-ND | 2.47 | 137.66 | 132.50 |
| 25 | A | 1109 | CLA | C2D-C1D-ND | 2.47 | 111.92 | 110.10 |
| 29 | 6 | 503 | BCR | C19-C18-C17 | 2.47 | 122.72 | 118.94 |
| 25 | A | 1117 | CLA | CHA-C4D-ND | 2.47 | 137.66 | 132.50 |
| 25 | a | 611 | CLA | O2A-CGA-CBA | 2.47 | 119.64 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | G | 1602 | CLA | O2D-CGD-O1D | -2.46 | 119.02 | 123.84 |
| 25 | A | 1111 | CLA | CHA-C4D-ND | 2.46 | 137.66 | 132.50 |
| 25 | A | 1119 | CLA | C2D-C1D-ND | 2.46 | 111.92 | 110.10 |
| 25 | 4 | 610 | CLA | CHA-C4D-ND | 2.46 | 137.65 | 132.50 |
| 25 | B | 1224 | CLA | O2A-CGA-CBA | 2.46 | 119.63 | 111.91 |
| 25 | B | 1236 | CLA | CHA-C4D-ND | 2.46 | 137.65 | 132.50 |
| 26 | 7 | 615 | CHL | CHB-C4A-NA | 2.46 | 127.92 | 124.51 |
| 25 | A | 1107 | CLA | CHA-C4D-ND | 2.46 | 137.65 | 132.50 |
| 25 | F | 1302 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 25 | L | 1503 | CLA | C2D-C1D-ND | 2.46 | 111.92 | 110.10 |
| 25 | 4 | 605 | CLA | C2D-C1D-ND | 2.46 | 111.92 | 110.10 |
| 30 | 7 | 801 | LHG | O8-C23-C24 | 2.46 | 119.63 | 111.91 |
| 25 | A | 1133 | CLA | O2D-CGD-O1D | -2.46 | 119.03 | 123.84 |
| 25 | 6 | 606 | CLA | CHA-C4D-ND | 2.46 | 137.64 | 132.50 |
| 25 | B | 1210 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 46 | a | 504 | QTB | C13-C12-C14 | 2.46 | 115.55 | 111.04 |
| 25 | 5 | 604 | CLA | CMD-C2D-C3D | -2.46 | 121.96 | 127.61 |
| 25 | 1 | 603 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 25 | 7 | 603 | CLA | O2D-CGD-O1D | -2.46 | 119.03 | 123.84 |
| 25 | A | 1129 | CLA | CHA-C4D-ND | 2.46 | 137.64 | 132.50 |
| 29 | A | 4003 | BCR | C23-C24-C25 | -2.46 | 120.30 | 127.20 |
| 25 | H | 1701 | CLA | O2D-CGD-O1D | -2.46 | 119.03 | 123.84 |
| 25 | A | 1113 | CLA | CMA-C3A-C4A | 2.46 | 118.38 | 111.77 |
| 25 | B | 1230 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 25 | A | 1131 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 25 | 4 | 617 | CLA | CHA-C4D-ND | 2.46 | 137.64 | 132.50 |
| 29 | 6 | 503 | BCR | C38-C26-C25 | -2.46 | 121.77 | 124.53 |
| 25 | 3 | 610 | CLA | CMA-C3A-C4A | 2.46 | 118.37 | 111.77 |
| 25 | B | 1220 | CLA | C1D-ND-C4D | -2.45 | 104.59 | 106.33 |
| 43 | 3 | 501 | LUT | C10-C11-C12 | -2.45 | 115.56 | 123.22 |
| 25 | 8 | 607 | CLA | CHA-C4D-ND | 2.45 | 137.63 | 132.50 |
| 25 | A | 1139 | CLA | C1C-C2C-C3C | -2.45 | 104.38 | 106.96 |
| 25 | F | 1301 | CLA | C1C-C2C-C3C | -2.45 | 104.38 | 106.96 |
| 25 | 1 | 602 | CLA | CHA-C4D-ND | 2.45 | 137.63 | 132.50 |
| 25 | 3 | 618 | CLA | CHA-C4D-ND | 2.45 | 137.63 | 132.50 |
| 25 | 8 | 609 | CLA | O2A-CGA-CBA | 2.45 | 119.60 | 111.91 |
| 25 | a | 611 | CLA | C2D-C1D-ND | 2.45 | 111.91 | 110.10 |
| 29 | 6 | 504 | BCR | C19-C18-C17 | 2.45 | 122.70 | 118.94 |
| 43 | 5 | 502 | LUT | C35-C15-C14 | -2.45 | 118.45 | 123.47 |
| 25 | a | 605 | CLA | O2A-CGA-CBA | 2.45 | 119.60 | 111.91 |
| 25 | A | 1121 | CLA | C1C-C2C-C3C | -2.45 | 104.38 | 106.96 |
| 25 | B | 1229 | CLA | O2A-CGA-CBA | 2.45 | 119.60 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 605 | CLA | CMA-C3A-C4A | 2.45 | 118.36 | 111.77 |
| 25 | 2 | 606 | CLA | CMA-C3A-C4A | 2.45 | 118.36 | 111.77 |
| 25 | 5 | 602 | CLA | CHA-C4D-ND | 2.45 | 137.63 | 132.50 |
| 25 | 8 | 620 | CLA | CHA-C4D-ND | 2.45 | 137.63 | 132.50 |
| 26 | a | 613 | CHL | CHB-C4A-NA | 2.45 | 127.90 | 124.51 |
| 25 | B | 1023 | CLA | O2A-CGA-CBA | 2.45 | 119.60 | 111.91 |
| 25 | B | 1234 | CLA | O2D-CGD-O1D | -2.45 | 119.05 | 123.84 |
| 25 | L | 1504 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | 4 | 615 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | 2 | 603 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | A | 1102 | CLA | CMB-C2B-C1B | -2.45 | 124.70 | 128.46 |
| 25 | a | 615 | CLA | C1C-C2C-C3C | -2.45 | 104.38 | 106.96 |
| 25 | 1 | 605 | CLA | C1D-ND-C4D | -2.45 | 104.59 | 106.33 |
| 25 | A | 1117 | CLA | C2D-C1D-ND | 2.45 | 111.91 | 110.10 |
| 25 | K | 1403 | CLA | O2A-CGA-CBA | 2.45 | 119.59 | 111.91 |
| 25 | 4 | 605 | CLA | CMA-C3A-C4A | 2.45 | 118.36 | 111.77 |
| 43 | 7 | 501 | LUT | C38-C25-C24 | -2.45 | 118.32 | 123.56 |
| 25 | 1 | 612 | CLA | O2D-CGD-O1D | -2.45 | 119.05 | 123.84 |
| 25 | 7 | 610 | CLA | O2D-CGD-O1D | -2.45 | 119.05 | 123.84 |
| 25 | 7 | 605 | CLA | CMB-C2B-C3B | 2.45 | 129.26 | 124.68 |
| 25 | F | 1301 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | 2 | 612 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | A | 1111 | CLA | O2A-CGA-CBA | 2.45 | 119.59 | 111.91 |
| 25 | 1 | 608 | CLA | O2A-CGA-CBA | 2.45 | 119.59 | 111.91 |
| 25 | 3 | 605 | CLA | CMB-C2B-C3B | 2.45 | 129.25 | 124.68 |
| 25 | A | 1134 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | 4 | 604 | CLA | CHA-C4D-ND | 2.45 | 137.62 | 132.50 |
| 25 | A | 1121 | CLA | CHA-C4D-ND | 2.45 | 137.61 | 132.50 |
| 25 | 2 | 605 | CLA | CMD-C2D-C3D | -2.44 | 121.99 | 127.61 |
| 25 | 8 | 602 | CLA | CHA-C4D-ND | 2.44 | 137.61 | 132.50 |
| 25 | K | 1402 | CLA | CHA-C4D-ND | 2.44 | 137.61 | 132.50 |
| 26 | 6 | 611 | CHL | C4D-CHA-C1A | 2.44 | 124.22 | 121.25 |
| 25 | 4 | 616 | CLA | O2D-CGD-O1D | -2.44 | 119.06 | 123.84 |
| 25 | 7 | 606 | CLA | C2D-C1D-ND | 2.44 | 111.90 | 110.10 |
| 25 | A | 1109 | CLA | CHA-C4D-ND | 2.44 | 137.60 | 132.50 |
| 40 | J | 4002 | RRX | C24-C25-C26 | -2.44 | 115.55 | 121.46 |
| 25 | A | 1109 | CLA | CAA-C2A-C3A | -2.44 | 106.10 | 112.78 |
| 43 | 5 | 505 | LUT | C38-C25-C24 | -2.44 | 118.34 | 123.56 |
| 26 | 8 | 613 | CHL | CHB-C4A-NA | 2.44 | 127.89 | 124.51 |
| 30 | A | 5003 | LHG | C5-O7-C7 | -2.44 | 111.79 | 117.79 |
| 29 | 8 | 503 | BCR | C19-C18-C17 | 2.44 | 122.68 | 118.94 |
| 25 | B | 1224 | CLA | O1D-CGD-CBD | -2.44 | 119.50 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 603 | CLA | C1C-C2C-C3C | -2.44 | 104.39 | 106.96 |
| 29 | 3 | 504 | BCR | C37-C22-C21 | -2.44 | 119.51 | 122.92 |
| 43 | 1 | 503 | LUT | C19-C9-C8 | 2.44 | 121.92 | 118.08 |
| 25 | 4 | 615 | CLA | O2D-CGD-O1D | -2.44 | 119.07 | 123.84 |
| 25 | a | 612 | CLA | CHA-C4D-ND | 2.44 | 137.60 | 132.50 |
| 25 | B | 1222 | CLA | C1D-ND-C4D | -2.44 | 104.60 | 106.33 |
| 25 | F | 1301 | CLA | O2D-CGD-O1D | -2.44 | 119.07 | 123.84 |
| 43 | 2 | 502 | LUT | C40-C33-C32 | 2.44 | 121.92 | 118.08 |
| 46 | a | 504 | QTB | C03-C04-C05 | -2.44 | 115.61 | 123.22 |
| 25 | a | 601 | CLA | CMA-C3A-C4A | 2.44 | 118.32 | 111.77 |
| 25 | 8 | 608 | CLA | C2D-C1D-ND | 2.44 | 111.90 | 110.10 |
| 26 | 2 | 610 | CHL | C4A-NA-C1A | 2.44 | 107.80 | 106.71 |
| 25 | H | 1701 | CLA | CHA-C4D-ND | 2.44 | 137.59 | 132.50 |
| 25 | a | 612 | CLA | CMA-C3A-C4A | 2.44 | 118.32 | 111.77 |
| 43 | 4 | 501 | LUT | C31-C30-C29 | -2.43 | 123.83 | 127.31 |
| 26 | 5 | 613 | CHL | CHB-C4A-NA | 2.43 | 127.88 | 124.51 |
| 26 | 4 | 609 | CHL | C1-O2A-CGA | 2.43 | 122.83 | 116.44 |
| 25 | B | 1231 | CLA | C1D-ND-C4D | -2.43 | 104.61 | 106.33 |
| 25 | A | 1123 | CLA | CHA-C4D-ND | 2.43 | 137.59 | 132.50 |
| 25 | 7 | 603 | CLA | CHA-C4D-ND | 2.43 | 137.59 | 132.50 |
| 25 | 7 | 601 | CLA | CAA-C2A-C3A | -2.43 | 106.11 | 112.78 |
| 25 | 4 | 602 | CLA | CHA-C4D-ND | 2.43 | 137.59 | 132.50 |
| 25 | 8 | 609 | CLA | CHA-C4D-ND | 2.43 | 137.59 | 132.50 |
| 25 | 9 | 612 | CLA | CHA-C4D-ND | 2.43 | 137.59 | 132.50 |
| 25 | B | 1214 | CLA | CHA-C4D-ND | 2.43 | 137.59 | 132.50 |
| 25 | a | 602 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 25 | 7 | 601 | CLA | CMD-C2D-C3D | -2.43 | 122.02 | 127.61 |
| 25 | B | 1231 | CLA | C2D-C1D-ND | 2.43 | 111.90 | 110.10 |
| 25 | A | 1105 | CLA | C1D-ND-C4D | -2.43 | 104.61 | 106.33 |
| 29 | H | 4001 | BCR | C15-C14-C13 | -2.43 | 123.84 | 127.31 |
| 25 | B | 1208 | CLA | C1-O2A-CGA | 2.43 | 122.82 | 116.44 |
| 25 | 6 | 618 | CLA | O2D-CGD-O1D | -2.43 | 119.09 | 123.84 |
| 25 | B | 1212 | CLA | C1C-C2C-C3C | -2.43 | 104.40 | 106.96 |
| 25 | A | 1113 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 25 | 9 | 604 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 25 | 3 | 607 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 26 | 7 | 613 | CHL | CMA-C3A-C4A | 2.43 | 118.30 | 111.77 |
| 25 | B | 1210 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 25 | B | 1223 | CLA | C3D-C2D-C1D | -2.43 | 102.52 | 105.83 |
| 29 | B | 4001 | BCR | C33-C5-C4 | 2.43 | 118.28 | 113.62 |
| 43 | 9 | 501 | LUT | C10-C11-C12 | -2.43 | 115.64 | 123.22 |
| 25 | B | 1208 | CLA | O2A-CGA-CBA | 2.43 | 119.53 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 2 | 615 | CLA | O2A-CGA-CBA | 2.43 | 119.53 | 111.91 |
| 30 | 9 | 801 | LHG | C5-O7-C7 | -2.43 | 111.81 | 117.79 |
| 25 | A | 1139 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 36 | 8 | 802 | DGD | O1G-C1A-C2A | 2.43 | 119.53 | 111.91 |
| 43 | 6 | 502 | LUT | C31-C30-C29 | -2.43 | 123.84 | 127.31 |
| 25 | a | 605 | CLA | CMB-C2B-C3B | 2.43 | 129.22 | 124.68 |
| 25 | 5 | 606 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 29 | J | 4001 | BCR | C35-C13-C12 | 2.43 | 121.90 | 118.08 |
| 25 | 6 | 602 | CLA | CHA-C4D-ND | 2.43 | 137.58 | 132.50 |
| 26 | 4 | 609 | CHL | CHB-C4A-NA | 2.43 | 127.87 | 124.51 |
| 26 | 7 | 617 | CHL | C1-C2-C3 | -2.43 | 121.85 | 126.04 |
| 29 | 8 | 503 | BCR | C38-C26-C25 | -2.43 | 121.80 | 124.53 |
| 25 | A | 1128 | CLA | CHA-C4D-ND | 2.43 | 137.57 | 132.50 |
| 43 | 8 | 502 | LUT | C31-C30-C29 | -2.43 | 123.85 | 127.31 |
| 25 | 1 | 605 | CLA | C1-C2-C3 | -2.43 | 121.85 | 126.04 |
| 25 | 2 | 602 | CLA | CHA-C4D-ND | 2.43 | 137.57 | 132.50 |
| 25 | 9 | 605 | CLA | CMA-C3A-C4A | 2.43 | 118.29 | 111.77 |
| 25 | 7 | 601 | CLA | CHA-C4D-ND | 2.42 | 137.57 | 132.50 |
| 25 | 4 | 606 | CLA | CMD-C2D-C3D | -2.42 | 122.04 | 127.61 |
| 25 | 7 | 610 | CLA | CHA-C4D-ND | 2.42 | 137.57 | 132.50 |
| 25 | A | 1135 | CLA | O2D-CGD-O1D | -2.42 | 119.10 | 123.84 |
| 29 | 3 | 503 | BCR | C36-C18-C17 | -2.42 | 119.53 | 122.92 |
| 25 | B | 1213 | CLA | C1C-C2C-C3C | -2.42 | 104.41 | 106.96 |
| 25 | 3 | 605 | CLA | O2D-CGD-O1D | -2.42 | 119.10 | 123.84 |
| 25 | A | 1135 | CLA | CHA-C4D-ND | 2.42 | 137.57 | 132.50 |
| 25 | B | 1213 | CLA | CHA-C4D-ND | 2.42 | 137.57 | 132.50 |
| 25 | 7 | 606 | CLA | CHA-C4D-ND | 2.42 | 137.57 | 132.50 |
| 25 | A | 1137 | CLA | CAA-CBA-CGA | -2.42 | 106.17 | 113.25 |
| 29 | L | 4003 | BCR | C30-C25-C26 | -2.42 | 119.20 | 122.61 |
| 25 | O | 1801 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | 5 | 606 | CLA | CMA-C3A-C4A | 2.42 | 118.28 | 111.77 |
| 25 | A | 1131 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | G | 1602 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | 3 | 602 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 26 | 2 | 613 | CHL | CMA-C3A-C4A | 2.42 | 118.28 | 111.77 |
| 43 | a | 501 | LUT | C8-C7-C6 | -2.42 | 120.41 | 127.20 |
| 25 | 9 | 606 | CLA | C1C-C2C-C3C | -2.42 | 104.41 | 106.96 |
| 25 | A | 1125 | CLA | C2C-C1C-NC | 2.42 | 112.24 | 109.97 |
| 25 | 1 | 601 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | 7 | 603 | CLA | C1-O2A-CGA | 2.42 | 122.79 | 116.44 |
| 44 | 7 | 504 | AXT | C20-C13-C14 | -2.42 | 119.53 | 122.92 |
| 43 | 6 | 502 | LUT | C10-C11-C12 | -2.42 | 115.67 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 1 | 612 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | 5 | 603 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | B | 1202 | CLA | CMA-C3A-C4A | 2.42 | 118.27 | 111.77 |
| 25 | 4 | 615 | CLA | CMA-C3A-C4A | 2.42 | 118.27 | 111.77 |
| 25 | 1 | 607 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | 9 | 607 | CLA | CHA-C4D-ND | 2.42 | 137.56 | 132.50 |
| 25 | A | 1127 | CLA | O2D-CGD-O1D | -2.42 | 119.11 | 123.84 |
| 25 | A | 1140 | CLA | CHA-C4D-ND | 2.42 | 137.55 | 132.50 |
| 43 | 3 | 501 | LUT | C38-C25-C24 | -2.42 | 118.39 | 123.56 |
| 25 | O | 1803 | CLA | CHA-C4D-ND | 2.41 | 137.55 | 132.50 |
| 25 | A | 1116 | CLA | CHA-C4D-ND | 2.41 | 137.55 | 132.50 |
| 25 | 2 | 606 | CLA | CHA-C4D-ND | 2.41 | 137.55 | 132.50 |
| 25 | 9 | 606 | CLA | CHA-C4D-ND | 2.41 | 137.55 | 132.50 |
| 25 | 8 | 618 | CLA | C2D-C1D-ND | 2.41 | 111.88 | 110.10 |
| 25 | G | 1601 | CLA | CHA-C4D-ND | 2.41 | 137.55 | 132.50 |
| 25 | 2 | 608 | CLA | CHA-C4D-ND | 2.41 | 137.55 | 132.50 |
| 25 | 5 | 603 | CLA | CMD-C2D-C3D | -2.41 | 122.06 | 127.61 |
| 25 | A | 1108 | CLA | C1D-ND-C4D | -2.41 | 104.62 | 106.33 |
| 29 | 6 | 504 | BCR | C38-C26-C27 | 2.41 | 118.25 | 113.62 |
| 25 | A | 1116 | CLA | C1C-C2C-C3C | -2.41 | 104.42 | 106.96 |
| 25 | B | 1205 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 25 | 7 | 607 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 25 | B | 1223 | CLA | O2A-CGA-CBA | 2.41 | 119.48 | 111.91 |
| 25 | 6 | 603 | CLA | O2A-CGA-CBA | 2.41 | 119.47 | 111.91 |
| 25 | B | 1213 | CLA | C1-O2A-CGA | 2.41 | 122.77 | 116.44 |
| 25 | 5 | 608 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 25 | O | 1801 | CLA | CMD-C2D-C3D | -2.41 | 122.07 | 127.61 |
| 43 | 3 | 502 | LUT | C31-C30-C29 | -2.41 | 123.87 | 127.31 |
| 25 | a | 615 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 29 | B | 4002 | BCR | C36-C18-C17 | -2.41 | 119.55 | 122.92 |
| 25 | A | 1137 | CLA | C1D-ND-C4D | -2.41 | 104.62 | 106.33 |
| 25 | B | 1239 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 25 | 9 | 602 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 29 | 3 | 505 | BCR | C38-C26-C27 | 2.41 | 118.25 | 113.62 |
| 25 | B | 1212 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 26 | a | 610 | CHL | C1B-CHB-C4A | -2.41 | 125.35 | 130.12 |
| 25 | 1 | 605 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 25 | 5 | 614 | CLA | CHA-C4D-ND | 2.41 | 137.54 | 132.50 |
| 25 | 3 | 612 | CLA | CHA-C4D-ND | 2.41 | 137.53 | 132.50 |
| 25 | 4 | 616 | CLA | CHA-C4D-ND | 2.41 | 137.53 | 132.50 |
| 43 | 8 | 502 | LUT | C38-C25-C24 | -2.41 | 118.41 | 123.56 |
| 25 | 4 | 615 | CLA | C2D-C1D-ND | 2.41 | 111.88 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 8 | 610 | CHL | C1-C2-C3 | -2.41 | 121.88 | 126.04 |
| 25 | 2 | 608 | CLA | O2D-CGD-O1D | -2.41 | 119.13 | 123.84 |
| 25 | B | 1240 | CLA | CHA-C4D-ND | 2.41 | 137.53 | 132.50 |
| 24 | A | 1011 | CL0 | CAA-C2A-C3A | -2.41 | 106.19 | 112.78 |
| 25 | 2 | 604 | CLA | CMB-C2B-C1B | -2.41 | 124.77 | 128.46 |
| 25 | B | 1231 | CLA | O2A-CGA-CBA | 2.41 | 119.46 | 111.91 |
| 25 | 7 | 606 | CLA | CMB-C2B-C3B | 2.41 | 129.18 | 124.68 |
| 25 | 2 | 604 | CLA | C1-O2A-CGA | 2.41 | 122.76 | 116.44 |
| 25 | 4 | 607 | CLA | CHA-C4D-ND | 2.41 | 137.53 | 132.50 |
| 25 | B | 1221 | CLA | C2D-C1D-ND | 2.40 | 111.88 | 110.10 |
| 25 | 2 | 604 | CLA | CHA-C4D-ND | 2.40 | 137.53 | 132.50 |
| 29 | 6 | 503 | BCR | C8-C7-C6 | -2.40 | 120.45 | 127.20 |
| 29 | 5 | 503 | BCR | C38-C26-C27 | 2.40 | 118.23 | 113.62 |
| 25 | B | 1216 | CLA | CAA-C2A-C3A | -2.40 | 106.19 | 112.78 |
| 25 | L | 1503 | CLA | CMA-C3A-C4A | 2.40 | 118.23 | 111.77 |
| 25 | B | 1224 | CLA | CHA-C4D-ND | 2.40 | 137.53 | 132.50 |
| 25 | 7 | 607 | CLA | O2A-CGA-CBA | 2.40 | 119.45 | 111.91 |
| 25 | 7 | 612 | CLA | CHA-C4D-ND | 2.40 | 137.53 | 132.50 |
| 25 | B | 1232 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 25 | B | 1207 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 25 | 6 | 612 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 25 | 7 | 612 | CLA | O2A-CGA-CBA | 2.40 | 119.44 | 111.91 |
| 25 | 2 | 605 | CLA | O2D-CGD-O1D | -2.40 | 119.14 | 123.84 |
| 25 | K | 1404 | CLA | CMA-C3A-C4A | 2.40 | 118.23 | 111.77 |
| 25 | B | 1235 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 25 | B | 1222 | CLA | CMB-C2B-C3B | 2.40 | 129.17 | 124.68 |
| 25 | B | 1239 | CLA | O2A-CGA-CBA | 2.40 | 119.44 | 111.91 |
| 25 | 1 | 615 | CLA | O2D-CGD-O1D | -2.40 | 119.14 | 123.84 |
| 25 | B | 1209 | CLA | CMD-C2D-C3D | -2.40 | 122.09 | 127.61 |
| 29 | 3 | 503 | BCR | C35-C13-C12 | 2.40 | 121.86 | 118.08 |
| 29 | 5 | 503 | BCR | C27-C26-C25 | -2.40 | 119.25 | 122.73 |
| 25 | 7 | 606 | CLA | CMD-C2D-C3D | -2.40 | 122.09 | 127.61 |
| 25 | B | 1216 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 25 | 7 | 604 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 25 | A | 1115 | CLA | CHA-C4D-ND | 2.40 | 137.52 | 132.50 |
| 43 | 1 | 501 | LUT | C11-C10-C9 | -2.40 | 123.89 | 127.31 |
| 25 | 9 | 609 | CLA | CHA-C4D-ND | 2.40 | 137.51 | 132.50 |
| 25 | 5 | 601 | CLA | O2D-CGD-O1D | -2.40 | 119.15 | 123.84 |
| 25 | A | 1134 | CLA | O2A-CGA-CBA | 2.40 | 119.43 | 111.91 |
| 25 | B | 1217 | CLA | CHA-C4D-ND | 2.40 | 137.51 | 132.50 |
| 25 | A | 1103 | CLA | CHA-C4D-ND | 2.40 | 137.51 | 132.50 |
| 46 | a | 504 | QTB | C11-C10-C09 | 2.40 | 130.67 | 125.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | B | 4004 | BCR | C12-C13-C14 | -2.40 | 115.26 | 118.94 |
| 25 | a | 611 | CLA | CHA-C4D-ND | 2.40 | 137.51 | 132.50 |
| 26 | 4 | 613 | CHL | C4D-CHA-C1A | 2.40 | 124.16 | 121.25 |
| 26 | 6 | 619 | CHL | C4D-CHA-C1A | 2.40 | 124.16 | 121.25 |
| 25 | a | 605 | CLA | CMD-C2D-C3D | -2.40 | 122.10 | 127.61 |
| 25 | A | 1130 | CLA | CHA-C4D-ND | 2.39 | 137.51 | 132.50 |
| 25 | 3 | 616 | CLA | O2A-CGA-CBA | 2.39 | 119.42 | 111.91 |
| 26 | 7 | 613 | CHL | CHB-C4A-NA | 2.39 | 127.82 | 124.51 |
| 25 | 3 | 613 | CLA | C1C-C2C-C3C | -2.39 | 104.44 | 106.96 |
| 25 | B | 1204 | CLA | CMA-C3A-C4A | 2.39 | 118.21 | 111.77 |
| 25 | A | 1119 | CLA | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 25 | 5 | 609 | CLA | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 25 | 8 | 605 | CLA | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 29 | 5 | 503 | BCR | C15-C14-C13 | -2.39 | 123.89 | 127.31 |
| 25 | B | 1023 | CLA | CHA-C4D-ND | 2.39 | 137.51 | 132.50 |
| 26 | 7 | 611 | CHL | C4A-NA-C1A | 2.39 | 107.78 | 106.71 |
| 25 | a | 602 | CLA | C1D-ND-C4D | -2.39 | 104.64 | 106.33 |
| 43 | 8 | 502 | LUT | C15-C14-C13 | -2.39 | 123.89 | 127.31 |
| 25 | 8 | 615 | CLA | CHA-C4D-ND | 2.39 | 137.50 | 132.50 |
| 30 | A | 5001 | LHG | C5-O7-C7 | -2.39 | 111.90 | 117.79 |
| 25 | B | 1022 | CLA | C2D-C1D-ND | 2.39 | 111.87 | 110.10 |
| 25 | B | 1239 | CLA | CMA-C3A-C4A | 2.39 | 118.20 | 111.77 |
| 26 | 7 | 617 | CHL | CHB-C4A-NA | 2.39 | 127.82 | 124.51 |
| 25 | A | 1137 | CLA | CHA-C4D-ND | 2.39 | 137.50 | 132.50 |
| 25 | B | 1236 | CLA | O2A-CGA-CBA | 2.39 | 119.41 | 111.91 |
| 25 | 8 | 615 | CLA | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 25 | B | 1236 | CLA | C1D-ND-C4D | -2.39 | 104.64 | 106.33 |
| 25 | 4 | 611 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 25 | B | 1220 | CLA | O2A-CGA-CBA | 2.39 | 119.41 | 111.91 |
| 25 | B | 1209 | CLA | CHA-C4D-ND | 2.39 | 137.50 | 132.50 |
| 25 | B | 1219 | CLA | CHA-C4D-ND | 2.39 | 137.50 | 132.50 |
| 25 | B | 1228 | CLA | CHA-C4D-ND | 2.39 | 137.50 | 132.50 |
| 25 | B | 1225 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 25 | 8 | 620 | CLA | C1C-C2C-C3C | -2.39 | 104.44 | 106.96 |
| 26 | A | 1114 | CHL | C4D-CHA-C1A | 2.39 | 124.16 | 121.25 |
| 25 | 4 | 601 | CLA | CMA-C3A-C4A | 2.39 | 118.19 | 111.77 |
| 25 | a | 608 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 25 | A | 1106 | CLA | CHA-C4D-ND | 2.39 | 137.49 | 132.50 |
| 25 | B | 1227 | CLA | CHA-C4D-ND | 2.39 | 137.49 | 132.50 |
| 25 | A | 1136 | CLA | CHA-C4D-ND | 2.39 | 137.49 | 132.50 |
| 25 | 3 | 606 | CLA | CHA-C4D-ND | 2.38 | 137.49 | 132.50 |
| 30 | 8 | 801 | LHG | C5-O7-C7 | -2.38 | 111.92 | 117.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 1 | 501 | LUT | C35-C15-C14 | -2.38 | 118.59 | 123.47 |
| 25 | 3 | 606 | CLA | C2D-C1D-ND | 2.38 | 111.86 | 110.10 |
| 25 | 4 | 603 | CLA | C1-O2A-CGA | 2.38 | 122.70 | 116.44 |
| 25 | a | 603 | CLA | CHA-C4D-ND | 2.38 | 137.49 | 132.50 |
| 25 | B | 1238 | CLA | CHA-C4D-ND | 2.38 | 137.49 | 132.50 |
| 25 | 6 | 607 | CLA | CHA-C4D-ND | 2.38 | 137.49 | 132.50 |
| 25 | 8 | 606 | CLA | O2D-CGD-O1D | -2.38 | 119.18 | 123.84 |
| 43 | 5 | 501 | LUT | C10-C11-C12 | -2.38 | 115.78 | 123.22 |
| 25 | 5 | 601 | CLA | CHA-C4D-ND | 2.38 | 137.48 | 132.50 |
| 25 | B | 1023 | CLA | CMB-C2B-C3B | 2.38 | 129.14 | 124.68 |
| 25 | 5 | 607 | CLA | CHA-C4D-ND | 2.38 | 137.48 | 132.50 |
| 25 | O | 1802 | CLA | C1-O2A-CGA | 2.38 | 122.69 | 116.44 |
| 25 | a | 612 | CLA | O2D-CGD-O1D | -2.38 | 119.18 | 123.84 |
| 25 | 8 | 606 | CLA | CHA-C4D-ND | 2.38 | 137.48 | 132.50 |
| 25 | a | 607 | CLA | O2A-CGA-CBA | 2.38 | 119.38 | 111.91 |
| 25 | 8 | 606 | CLA | CMB-C2B-C1B | -2.38 | 124.81 | 128.46 |
| 25 | B | 1201 | CLA | O1D-CGD-CBD | -2.38 | 119.61 | 124.48 |
| 25 | A | 1116 | CLA | C1D-ND-C4D | -2.38 | 104.64 | 106.33 |
| 25 | A | 1133 | CLA | CHA-C4D-ND | 2.38 | 137.48 | 132.50 |
| 25 | B | 1229 | CLA | CHA-C4D-ND | 2.38 | 137.48 | 132.50 |
| 26 | 5 | 610 | CHL | C4D-CHA-C1A | 2.38 | 124.14 | 121.25 |
| 25 | 4 | 605 | CLA | O2D-CGD-O1D | -2.38 | 119.19 | 123.84 |
| 25 | A | 1112 | CLA | CHA-C4D-ND | 2.38 | 137.48 | 132.50 |
| 25 | A | 1138 | CLA | O2A-CGA-CBA | 2.38 | 119.37 | 111.91 |
| 25 | A | 1121 | CLA | C2D-C1D-ND | 2.38 | 111.86 | 110.10 |
| 25 | B | 1218 | CLA | O1D-CGD-CBD | -2.38 | 119.62 | 124.48 |
| 25 | A | 1119 | CLA | CHA-C4D-ND | 2.38 | 137.47 | 132.50 |
| 25 | O | 1802 | CLA | CHA-C4D-ND | 2.38 | 137.47 | 132.50 |
| 26 | 4 | 618 | CHL | CHB-C4A-NA | 2.38 | 127.80 | 124.51 |
| 25 | 3 | 613 | CLA | CHA-C4D-ND | 2.38 | 137.47 | 132.50 |
| 25 | B | 1208 | CLA | CHA-C4D-ND | 2.38 | 137.47 | 132.50 |
| 25 | 8 | 608 | CLA | CHA-C4D-ND | 2.38 | 137.47 | 132.50 |
| 25 | 5 | 606 | CLA | O2D-CGD-O1D | -2.38 | 119.19 | 123.84 |
| 25 | 1 | 605 | CLA | CMD-C2D-C3D | -2.38 | 122.15 | 127.61 |
| 30 | 7 | 803 | LHG | C5-O7-C7 | -2.37 | 111.94 | 117.79 |
| 30 | 4 | 801 | LHG | O8-C23-C24 | 2.37 | 119.36 | 111.91 |
| 25 | A | 1127 | CLA | CHA-C4D-ND | 2.37 | 137.47 | 132.50 |
| 25 | 4 | 615 | CLA | O2A-CGA-CBA | 2.37 | 119.36 | 111.91 |
| 25 | A | 1108 | CLA | CAA-C2A-C3A | -2.37 | 106.28 | 112.78 |
| 25 | B | 1201 | CLA | CHA-C4D-ND | 2.37 | 137.47 | 132.50 |
| 25 | a | 602 | CLA | CHA-C4D-ND | 2.37 | 137.47 | 132.50 |
| 25 | a | 607 | CLA | CHA-C4D-ND | 2.37 | 137.47 | 132.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 6 | 615 | CLA | CHA-C4D-ND | 2.37 | 137.47 | 132.50 |
| 25 | B | 1202 | CLA | CHA-C4D-ND | 2.37 | 137.46 | 132.50 |
| 25 | 6 | 605 | CLA | CMB-C2B-C3B | 2.37 | 129.12 | 124.68 |
| 25 | 6 | 601 | CLA | CHA-C4D-ND | 2.37 | 137.46 | 132.50 |
| 30 | B | 5001 | LHG | O8-C23-C24 | 2.37 | 119.35 | 111.91 |
| 25 | 5 | 605 | CLA | C1C-C2C-C3C | -2.37 | 104.46 | 106.96 |
| 25 | B | 1203 | CLA | C1D-ND-C4D | -2.37 | 104.65 | 106.33 |
| 29 | B | 4005 | BCR | C8-C7-C6 | -2.37 | 120.54 | 127.20 |
| 26 | 5 | 610 | CHL | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 25 | 5 | 615 | CLA | CHA-C4D-ND | 2.37 | 137.46 | 132.50 |
| 25 | 3 | 605 | CLA | CMA-C3A-C4A | 2.37 | 118.14 | 111.77 |
| 25 | J | 1901 | CLA | O2D-CGD-O1D | -2.37 | 119.20 | 123.84 |
| 25 | G | 1603 | CLA | CHA-C4D-ND | 2.37 | 137.46 | 132.50 |
| 25 | 6 | 618 | CLA | CHA-C4D-ND | 2.37 | 137.46 | 132.50 |
| 25 | 5 | 612 | CLA | CHA-C4D-ND | 2.37 | 137.46 | 132.50 |
| 26 | 6 | 617 | CHL | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 40 | 3 | 506 | RRX | C37-C22-C21 | -2.37 | 119.60 | 122.92 |
| 25 | 8 | 620 | CLA | C1D-ND-C4D | -2.37 | 104.65 | 106.33 |
| 29 | I | 4001 | BCR | C33-C5-C4 | 2.37 | 118.17 | 113.62 |
| 25 | 7 | 602 | CLA | CHA-C4D-ND | 2.37 | 137.45 | 132.50 |
| 26 | 2 | 610 | CHL | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 25 | B | 1219 | CLA | O2A-CGA-CBA | 2.37 | 119.34 | 111.91 |
| 25 | a | 601 | CLA | CHA-C4D-ND | 2.37 | 137.45 | 132.50 |
| 25 | 4 | 608 | CLA | CHA-C4D-ND | 2.37 | 137.45 | 132.50 |
| 25 | 5 | 604 | CLA | CHA-C4D-ND | 2.37 | 137.45 | 132.50 |
| 43 | 8 | 501 | LUT | C10-C11-C12 | -2.37 | 115.83 | 123.22 |
| 26 | 8 | 610 | CHL | C4A-NA-C1A | 2.37 | 107.77 | 106.71 |
| 25 | B | 1205 | CLA | O1D-CGD-CBD | -2.37 | 119.64 | 124.48 |
| 25 | 5 | 601 | CLA | C1D-ND-C4D | -2.37 | 104.65 | 106.33 |
| 29 | B | 4006 | BCR | C33-C5-C4 | 2.37 | 118.16 | 113.62 |
| 25 | 3 | 602 | CLA | CMA-C3A-C4A | 2.37 | 118.13 | 111.77 |
| 25 | O | 1801 | CLA | C2D-C1D-ND | 2.37 | 111.85 | 110.10 |
| 25 | B | 1221 | CLA | CMA-C3A-C4A | 2.36 | 118.13 | 111.77 |
| 25 | 8 | 618 | CLA | O2A-CGA-CBA | 2.36 | 119.33 | 111.91 |
| 25 | F | 1302 | CLA | CHA-C4D-ND | 2.36 | 137.44 | 132.50 |
| 25 | 1 | 606 | CLA | CMD-C2D-C3D | -2.36 | 122.18 | 127.61 |
| 25 | 5 | 609 | CLA | CHA-C4D-ND | 2.36 | 137.44 | 132.50 |
| 29 | B | 4005 | BCR | C37-C22-C23 | 2.36 | 121.80 | 118.08 |
| 25 | H | 1703 | CLA | CHA-C4D-ND | 2.36 | 137.44 | 132.50 |
| 24 | A | 1011 | CL0 | C3D-C4D-ND | 2.36 | 114.06 | 110.24 |
| 25 | 1 | 603 | CLA | CMB-C2B-C3B | 2.36 | 129.10 | 124.68 |
| 29 | 5 | 504 | BCR | C1-C6-C5 | -2.36 | 119.29 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1138 | CLA | CHA-C4D-ND | 2.36 | 137.44 | 132.50 |
| 25 | 4 | 603 | CLA | CHA-C4D-ND | 2.36 | 137.44 | 132.50 |
| 25 | 1 | 601 | CLA | CMD-C2D-C3D | -2.36 | 122.18 | 127.61 |
| 25 | 7 | 601 | CLA | C1C-C2C-C3C | -2.36 | 104.47 | 106.96 |
| 25 | B | 1021 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 25 | A | 1138 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 26 | 1 | 609 | CHL | CHB-C4A-NA | 2.36 | 127.78 | 124.51 |
| 25 | A | 1120 | CLA | CHA-C4D-ND | 2.36 | 137.44 | 132.50 |
| 25 | 5 | 605 | CLA | CMD-C2D-C3D | -2.36 | 122.19 | 127.61 |
| 26 | 4 | 618 | CHL | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 25 | A | 1105 | CLA | CHA-C4D-ND | 2.36 | 137.43 | 132.50 |
| 25 | 3 | 601 | CLA | CHA-C4D-ND | 2.36 | 137.43 | 132.50 |
| 25 | B | 1225 | CLA | CHA-C4D-ND | 2.36 | 137.43 | 132.50 |
| 25 | 9 | 606 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 25 | A | 1111 | CLA | C1C-C2C-C3C | -2.36 | 104.48 | 106.96 |
| 26 | 1 | 609 | CHL | C1-O2A-CGA | 2.36 | 122.63 | 116.44 |
| 26 | 7 | 613 | CHL | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 25 | O | 1802 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 29 | J | 4001 | BCR | C37-C22-C21 | -2.36 | 119.62 | 122.92 |
| 25 | 7 | 608 | CLA | CHA-C4D-ND | 2.36 | 137.43 | 132.50 |
| 29 | 3 | 504 | BCR | C30-C25-C26 | -2.36 | 119.30 | 122.61 |
| 25 | 1 | 603 | CLA | CHA-C4D-ND | 2.36 | 137.43 | 132.50 |
| 25 | B | 1211 | CLA | CMD-C2D-C3D | -2.36 | 122.20 | 127.61 |
| 25 | A | 1125 | CLA | C1D-ND-C4D | -2.36 | 104.66 | 106.33 |
| 25 | 7 | 604 | CLA | C1D-ND-C4D | -2.36 | 104.66 | 106.33 |
| 26 | 1 | 613 | CHL | C4D-CHA-C1A | 2.35 | 124.11 | 121.25 |
| 26 | 4 | 618 | CHL | C4D-CHA-C1A | 2.35 | 124.11 | 121.25 |
| 25 | B | 1228 | CLA | CMB-C2B-C1B | -2.35 | 124.84 | 128.46 |
| 25 | 4 | 610 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 25 | B | 1202 | CLA | C1D-ND-C4D | -2.35 | 104.66 | 106.33 |
| 43 | 3 | 502 | LUT | C35-C15-C14 | -2.35 | 118.65 | 123.47 |
| 25 | A | 1124 | CLA | CMB-C2B-C3B | 2.35 | 129.08 | 124.68 |
| 32 | A | 5005 | SQD | O3-C3-C2 | -2.35 | 104.91 | 110.35 |
| 25 | F | 1302 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 25 | a | 615 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 26 | 3 | 603 | CHL | C1-O2A-CGA | 2.35 | 122.61 | 116.44 |
| 25 | 1 | 601 | CLA | CMA-C3A-C4A | 2.35 | 118.09 | 111.77 |
| 25 | 3 | 610 | CLA | CHA-C4D-ND | 2.35 | 137.42 | 132.50 |
| 25 | A | 1122 | CLA | C1D-ND-C4D | -2.35 | 104.67 | 106.33 |
| 25 | 2 | 605 | CLA | C1D-ND-C4D | -2.35 | 104.67 | 106.33 |
| 29 | K | 4001 | BCR | C34-C9-C10 | -2.35 | 119.63 | 122.92 |
| 25 | B | 1234 | CLA | CMA-C3A-C4A | 2.35 | 119.34 | 112.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 612 | CLA | O2A-CGA-CBA | 2.35 | 119.28 | 111.91 |
| 25 | 5 | 603 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 25 | B | 1227 | CLA | CMA-C3A-C4A | 2.35 | 118.09 | 111.77 |
| 25 | 4 | 611 | CLA | CHA-C4D-ND | 2.35 | 137.41 | 132.50 |
| 26 | 1 | 604 | CHL | C1B-CHB-C4A | -2.35 | 125.47 | 130.12 |
| 25 | K | 1401 | CLA | CHA-C4D-ND | 2.35 | 137.41 | 132.50 |
| 25 | L | 1501 | CLA | CHA-C4D-ND | 2.35 | 137.41 | 132.50 |
| 25 | 4 | 603 | CLA | O2D-CGD-O1D | -2.35 | 119.25 | 123.84 |
| 25 | B | 1209 | CLA | C1D-ND-C4D | -2.35 | 104.67 | 106.33 |
| 25 | 8 | 611 | CLA | CHA-C4D-ND | 2.35 | 137.41 | 132.50 |
| 50 | 2 | 501 | XAT | C40-C33-C34 | -2.35 | 119.64 | 122.92 |
| 25 | 8 | 620 | CLA | O2D-CGD-O1D | -2.35 | 119.25 | 123.84 |
| 29 | 5 | 504 | BCR | C27-C26-C25 | -2.35 | 119.33 | 122.73 |
| 25 | A | 1106 | CLA | O1D-CGD-CBD | -2.35 | 119.68 | 124.48 |
| 25 | A | 1110 | CLA | CHA-C4D-ND | 2.35 | 137.41 | 132.50 |
| 25 | A | 1125 | CLA | C3D-C2D-C1D | -2.34 | 102.63 | 105.83 |
| 25 | B | 1237 | CLA | CHA-C4D-ND | 2.34 | 137.40 | 132.50 |
| 25 | H | 1703 | CLA | C1D-ND-C4D | -2.34 | 104.67 | 106.33 |
| 26 | 1 | 611 | CHL | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 43 | 4 | 502 | LUT | C31-C30-C29 | -2.34 | 123.97 | 127.31 |
| 25 | B | 1224 | CLA | CMA-C3A-C4A | 2.34 | 118.07 | 111.77 |
| 43 | 3 | 502 | LUT | C30-C31-C32 | -2.34 | 115.91 | 123.22 |
| 29 | B | 4002 | BCR | C3-C4-C5 | -2.34 | 109.89 | 114.08 |
| 25 | a | 605 | CLA | C1D-ND-C4D | -2.34 | 104.67 | 106.33 |
| 25 | 4 | 611 | CLA | C1D-ND-C4D | -2.34 | 104.67 | 106.33 |
| 25 | B | 1023 | CLA | CAA-C2A-C3A | -2.34 | 106.36 | 112.78 |
| 25 | 3 | 607 | CLA | CMB-C2B-C3B | 2.34 | 129.06 | 124.68 |
| 26 | 8 | 603 | CHL | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 25 | 5 | 615 | CLA | O2D-CGD-O1D | -2.34 | 119.26 | 123.84 |
| 25 | 5 | 609 | CLA | O2A-CGA-CBA | 2.34 | 119.25 | 111.91 |
| 25 | 3 | 606 | CLA | CMD-C2D-C3D | -2.34 | 122.23 | 127.61 |
| 29 | 6 | 504 | BCR | C8-C7-C6 | -2.34 | 120.64 | 127.20 |
| 25 | A | 1118 | CLA | CHA-C4D-ND | 2.34 | 137.39 | 132.50 |
| 25 | A | 1101 | CLA | C1D-ND-C4D | -2.34 | 104.67 | 106.33 |
| 25 | A | 1132 | CLA | CAA-C2A-C3A | -2.34 | 106.38 | 112.78 |
| 25 | 3 | 616 | CLA | CHA-C4D-ND | 2.34 | 137.39 | 132.50 |
| 43 | 3 | 502 | LUT | C38-C25-C24 | -2.34 | 118.56 | 123.56 |
| 29 | K | 4001 | BCR | C33-C5-C4 | 2.34 | 118.10 | 113.62 |
| 25 | 4 | 605 | CLA | CMD-C2D-C3D | -2.34 | 122.24 | 127.61 |
| 36 | B | 5003 | DGD | O6D-C5D-C6D | 2.34 | 111.38 | 106.67 |
| 26 | 1 | 611 | CHL | C1-O2A-CGA | 2.34 | 122.57 | 116.44 |
| 25 | A | 1140 | CLA | O2A-CGA-CBA | 2.34 | 119.24 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1111 | CLA | CMD-C2D-C3D | -2.34 | 122.24 | 127.61 |
| 25 | A | 1109 | CLA | O2A-CGA-CBA | 2.33 | 119.23 | 111.91 |
| 25 | 3 | 616 | CLA | C1-O2A-CGA | 2.33 | 122.57 | 116.44 |
| 25 | 8 | 612 | CLA | CHA-C4D-ND | 2.33 | 137.38 | 132.50 |
| 25 | 5 | 607 | CLA | O2A-CGA-CBA | 2.33 | 119.23 | 111.91 |
| 25 | 7 | 606 | CLA | O2D-CGD-O1D | -2.33 | 119.27 | 123.84 |
| 29 | A | 4001 | BCR | C33-C5-C4 | 2.33 | 118.10 | 113.62 |
| 25 | A | 1128 | CLA | C2D-C1D-ND | 2.33 | 111.82 | 110.10 |
| 25 | A | 1120 | CLA | C1D-ND-C4D | -2.33 | 104.68 | 106.33 |
| 25 | B | 1217 | CLA | C1D-ND-C4D | -2.33 | 104.68 | 106.33 |
| 25 | B | 1208 | CLA | CAB-C3B-C4B | -2.33 | 124.88 | 128.46 |
| 25 | B | 1230 | CLA | CMA-C3A-C4A | 2.33 | 118.05 | 111.77 |
| 25 | a | 608 | CLA | CHA-C4D-ND | 2.33 | 137.38 | 132.50 |
| 26 | 5 | 611 | CHL | C4D-CHA-C1A | 2.33 | 124.09 | 121.25 |
| 43 | a | 501 | LUT | C38-C25-C24 | -2.33 | 118.57 | 123.56 |
| 25 | A | 1118 | CLA | C1D-ND-C4D | -2.33 | 104.68 | 106.33 |
| 25 | 9 | 604 | CLA | CMD-C2D-C3D | -2.33 | 122.25 | 127.61 |
| 25 | A | 1013 | CLA | CHA-C4D-ND | 2.33 | 137.38 | 132.50 |
| 25 | B | 1206 | CLA | CHA-C4D-ND | 2.33 | 137.38 | 132.50 |
| 25 | 3 | 613 | CLA | CMB-C2B-C3B | 2.33 | 129.04 | 124.68 |
| 26 | 5 | 618 | CHL | C1-O2A-CGA | 2.33 | 122.56 | 116.44 |
| 25 | G | 1603 | CLA | C1D-ND-C4D | -2.33 | 104.68 | 106.33 |
| 43 | 9 | 502 | LUT | C10-C11-C12 | -2.33 | 115.95 | 123.22 |
| 43 | 6 | 502 | LUT | C2-C3-C4 | -2.33 | 107.12 | 110.30 |
| 25 | 7 | 601 | CLA | O2D-CGD-O1D | -2.33 | 119.28 | 123.84 |
| 25 | B | 1215 | CLA | CHA-C4D-ND | 2.33 | 137.37 | 132.50 |
| 25 | A | 1106 | CLA | CMA-C3A-C4A | 2.33 | 118.03 | 111.77 |
| 43 | 9 | 501 | LUT | C35-C15-C14 | -2.33 | 118.71 | 123.47 |
| 25 | a | 611 | CLA | CMB-C2B-C3B | 2.33 | 129.03 | 124.68 |
| 26 | 5 | 611 | CHL | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 25 | 9 | 612 | CLA | O2A-CGA-CBA | 2.33 | 119.21 | 111.91 |
| 25 | 7 | 605 | CLA | CMD-C2D-C3D | -2.33 | 122.26 | 127.61 |
| 26 | 1 | 604 | CHL | CHB-C4A-NA | 2.33 | 127.73 | 124.51 |
| 30 | 1 | 801 | LHG | C5-O7-C7 | -2.33 | 112.06 | 117.79 |
| 26 | 2 | 610 | CHL | C1B-CHB-C4A | -2.32 | 125.51 | 130.12 |
| 25 | H | 1703 | CLA | C1C-C2C-C3C | -2.32 | 104.51 | 106.96 |
| 25 | 6 | 603 | CLA | CHA-C4D-ND | 2.32 | 137.36 | 132.50 |
| 25 | 5 | 602 | CLA | C1D-ND-C4D | -2.32 | 104.68 | 106.33 |
| 25 | A | 1103 | CLA | C1C-C2C-C3C | -2.32 | 104.51 | 106.96 |
| 26 | 1 | 611 | CHL | CHD-C4C-C3C | 2.32 | 128.25 | 124.84 |
| 42 | M | 4001 | ECH | C11-C12-C13 | -2.32 | 119.89 | 126.42 |
| 25 | 2 | 615 | CLA | CHA-C4D-ND | 2.32 | 137.36 | 132.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 2 | 613 | CHL | C4A-NA-C1A | 2.32 | 107.75 | 106.71 |
| 25 | B | 1204 | CLA | CHA-C4D-ND | 2.32 | 137.36 | 132.50 |
| 25 | A | 1012 | CLA | CHA-C1A-NA | -2.32 | 121.08 | 126.40 |
| 25 | 5 | 602 | CLA | CMA-C3A-C4A | 2.32 | 118.01 | 111.77 |
| 25 | 4 | 601 | CLA | CHA-C4D-ND | 2.32 | 137.35 | 132.50 |
| 25 | 5 | 609 | CLA | CMB-C2B-C3B | 2.32 | 129.02 | 124.68 |
| 43 | 2 | 507 | LUT | C38-C25-C24 | -2.32 | 118.59 | 123.56 |
| 25 | 7 | 605 | CLA | O2D-CGD-O1D | -2.32 | 118.82 | 124.09 |
| 29 | B | 4004 | BCR | C4-C5-C6 | -2.32 | 119.36 | 122.73 |
| 25 | 2 | 603 | CLA | O2D-CGD-O1D | -2.32 | 119.30 | 123.84 |
| 25 | A | 1118 | CLA | O2A-CGA-CBA | 2.32 | 119.19 | 111.91 |
| 30 | 6 | 802 | LHG | C6-C5-C4 | -2.32 | 106.30 | 111.79 |
| 25 | 8 | 602 | CLA | C1D-ND-C4D | -2.32 | 104.69 | 106.33 |
| 25 | A | 1110 | CLA | O2A-CGA-CBA | 2.32 | 119.18 | 111.91 |
| 25 | B | 1230 | CLA | CHA-C4D-ND | 2.32 | 137.35 | 132.50 |
| 25 | B | 1226 | CLA | O2A-CGA-CBA | 2.32 | 119.18 | 111.91 |
| 25 | 5 | 605 | CLA | C1D-ND-C4D | -2.32 | 104.69 | 106.33 |
| 25 | 9 | 604 | CLA | CMB-C2B-C1B | -2.32 | 124.90 | 128.46 |
| 25 | 4 | 601 | CLA | C1D-ND-C4D | -2.32 | 104.69 | 106.33 |
| 25 | 6 | 601 | CLA | C1D-ND-C4D | -2.32 | 104.69 | 106.33 |
| 25 | 1 | 606 | CLA | O2A-CGA-CBA | 2.32 | 119.17 | 111.91 |
| 25 | A | 1103 | CLA | CMB-C2B-C3B | 2.31 | 129.01 | 124.68 |
| 25 | A | 1113 | CLA | CMD-C2D-C3D | -2.31 | 122.29 | 127.61 |
| 25 | A | 1138 | CLA | CMA-C3A-C4A | 2.31 | 117.99 | 111.77 |
| 25 | 2 | 603 | CLA | CBA-CAA-C2A | 2.31 | 120.69 | 113.86 |
| 43 | a | 503 | LUT | C8-C7-C6 | -2.31 | 120.70 | 127.20 |
| 25 | B | 1208 | CLA | CMD-C2D-C3D | -2.31 | 122.29 | 127.61 |
| 29 | 8 | 503 | BCR | C35-C13-C12 | 2.31 | 121.72 | 118.08 |
| 29 | 3 | 503 | BCR | C38-C26-C25 | -2.31 | 121.93 | 124.53 |
| 25 | B | 1216 | CLA | CMD-C2D-C3D | -2.31 | 122.29 | 127.61 |
| 25 | 6 | 604 | CLA | CHA-C4D-ND | 2.31 | 137.34 | 132.50 |
| 25 | a | 612 | CLA | O2A-CGA-CBA | 2.31 | 119.17 | 111.91 |
| 25 | B | 1223 | CLA | C1C-C2C-C3C | -2.31 | 104.53 | 106.96 |
| 25 | 1 | 601 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 25 | B | 1216 | CLA | C2D-C1D-ND | 2.31 | 111.81 | 110.10 |
| 26 | 5 | 617 | CHL | CHB-C4A-NA | 2.31 | 127.71 | 124.51 |
| 25 | 8 | 602 | CLA | CMD-C2D-C3D | -2.31 | 122.30 | 127.61 |
| 26 | 1 | 604 | CHL | C1-O2A-CGA | 2.31 | 122.50 | 116.44 |
| 25 | A | 1137 | CLA | CMA-C3A-C4A | 2.31 | 117.98 | 111.77 |
| 25 | A | 1138 | CLA | CMD-C2D-C3D | -2.31 | 122.30 | 127.61 |
| 25 | 4 | 606 | CLA | CMB-C2B-C1B | -2.31 | 124.92 | 128.46 |
| 25 | A | 1141 | CLA | CMD-C2D-C3D | -2.31 | 122.30 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 612 | CLA | O2A-CGA-CBA | 2.31 | 119.15 | 111.91 |
| 25 | 2 | 601 | CLA | CHA-C4D-ND | 2.31 | 137.33 | 132.50 |
| 29 | 3 | 505 | BCR | C27-C26-C25 | -2.31 | 119.38 | 122.73 |
| 26 | 1 | 609 | CHL | C4A-NA-C1A | 2.31 | 107.74 | 106.71 |
| 25 | 6 | 604 | CLA | CMD-C2D-C3D | -2.31 | 122.31 | 127.61 |
| 25 | B | 1240 | CLA | O1D-CGD-CBD | -2.31 | 119.77 | 124.48 |
| 26 | 2 | 609 | CHL | CHD-C4C-C3C | 2.31 | 128.23 | 124.84 |
| 26 | 9 | 610 | CHL | CHB-C4A-NA | 2.31 | 127.70 | 124.51 |
| 25 | A | 1127 | CLA | C1D-ND-C4D | -2.31 | 104.70 | 106.33 |
| 25 | 2 | 603 | CLA | CHA-C1A-NA | -2.31 | 121.12 | 126.40 |
| 26 | 6 | 611 | CHL | CHB-C4A-NA | 2.30 | 127.70 | 124.51 |
| 25 | L | 1504 | CLA | O2D-CGD-O1D | -2.30 | 119.33 | 123.84 |
| 43 | 6 | 502 | LUT | C35-C15-C14 | -2.30 | 118.76 | 123.47 |
| 25 | A | 1108 | CLA | CHA-C4D-ND | 2.30 | 137.32 | 132.50 |
| 25 | 2 | 606 | CLA | CMD-C2D-C3D | -2.30 | 122.32 | 127.61 |
| 43 | 9 | 501 | LUT | C11-C10-C9 | -2.30 | 124.02 | 127.31 |
| 32 | 7 | 805 | SQD | O3-C3-C2 | -2.30 | 105.03 | 110.35 |
| 26 | 9 | 608 | CHL | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 25 | 3 | 610 | CLA | CMB-C2B-C3B | 2.30 | 128.99 | 124.68 |
| 25 | 8 | 606 | CLA | CMD-C2D-C3D | -2.30 | 122.32 | 127.61 |
| 25 | 4 | 602 | CLA | C1D-ND-C4D | -2.30 | 104.70 | 106.33 |
| 25 | a | 603 | CLA | CMD-C2D-C3D | -2.30 | 122.32 | 127.61 |
| 25 | A | 1122 | CLA | CHA-C4D-ND | 2.30 | 137.31 | 132.50 |
| 39 | F | 4001 | NEX | C11-C10-C9 | 2.30 | 130.59 | 127.31 |
| 25 | B | 1235 | CLA | CMB-C2B-C3B | 2.30 | 128.98 | 124.68 |
| 25 | 4 | 602 | CLA | CMA-C3A-C4A | 2.30 | 117.95 | 111.77 |
| 26 | 9 | 608 | CHL | CHB-C4A-NA | 2.30 | 127.69 | 124.51 |
| 26 | 8 | 601 | CHL | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 25 | B | 1234 | CLA | CAA-CBA-CGA | -2.30 | 106.54 | 113.25 |
| 25 | O | 1802 | CLA | O2A-CGA-CBA | 2.30 | 119.12 | 111.91 |
| 29 | 5 | 504 | BCR | C38-C26-C27 | 2.30 | 118.03 | 113.62 |
| 43 | 3 | 501 | LUT | C31-C30-C29 | -2.30 | 124.03 | 127.31 |
| 25 | A | 1124 | CLA | O2A-CGA-CBA | 2.30 | 119.11 | 111.91 |
| 29 | I | 4001 | BCR | C36-C18-C17 | -2.30 | 119.71 | 122.92 |
| 29 | I | 4001 | BCR | C12-C13-C14 | -2.29 | 115.42 | 118.94 |
| 26 | 3 | 603 | CHL | CHB-C4A-NA | 2.29 | 127.68 | 124.51 |
| 25 | B | 1220 | CLA | CHA-C4D-ND | 2.29 | 137.30 | 132.50 |
| 29 | A | 4002 | BCR | C38-C26-C27 | 2.29 | 118.02 | 113.62 |
| 43 | 2 | 502 | LUT | C35-C34-C33 | -2.29 | 124.04 | 127.31 |
| 50 | 9 | 507 | XAT | C11-C10-C9 | 2.29 | 130.58 | 127.31 |
| 26 | A | 1114 | CHL | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 36 | 8 | 802 | DGD | C2G-O2G-C1B | -2.29 | 112.15 | 117.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | L | 4001 | BCR | C28-C27-C26 | -2.29 | 109.98 | 114.08 |
| 25 | 7 | 602 | CLA | C1D-ND-C4D | -2.29 | 104.71 | 106.33 |
| 25 | A | 1137 | CLA | O2A-CGA-CBA | 2.29 | 119.10 | 111.91 |
| 25 | 9 | 605 | CLA | CHA-C1A-NA | -2.29 | 121.15 | 126.40 |
| 25 | A | 1124 | CLA | CHA-C4D-ND | 2.29 | 137.29 | 132.50 |
| 26 | 4 | 613 | CHL | C1-C2-C3 | -2.29 | 122.08 | 126.04 |
| 25 | 6 | 601 | CLA | CMD-C2D-C3D | -2.29 | 122.35 | 127.61 |
| 25 | 6 | 606 | CLA | CMD-C2D-C3D | -2.29 | 122.35 | 127.61 |
| 43 | 5 | 501 | LUT | C38-C25-C24 | -2.29 | 118.66 | 123.56 |
| 25 | A | 1112 | CLA | CHA-C1A-NA | -2.29 | 121.16 | 126.40 |
| 25 | B | 1218 | CLA | CMD-C2D-C3D | -2.29 | 122.35 | 127.61 |
| 26 | 5 | 613 | CHL | CMB-C2B-C1B | -2.29 | 124.95 | 128.46 |
| 26 | a | 609 | CHL | C4A-NA-C1A | 2.29 | 107.73 | 106.71 |
| 25 | 6 | 604 | CLA | C2C-C1C-NC | 2.29 | 112.12 | 109.97 |
| 26 | 3 | 611 | CHL | C1-O2A-CGA | 2.29 | 122.45 | 116.44 |
| 29 | A | 4004 | BCR | C33-C5-C4 | 2.29 | 118.01 | 113.62 |
| 25 | A | 1140 | CLA | C1D-ND-C4D | -2.29 | 104.71 | 106.33 |
| 26 | 6 | 619 | CHL | CHB-C4A-NA | 2.29 | 127.67 | 124.51 |
| 25 | 3 | 612 | CLA | O2A-CGA-CBA | 2.29 | 119.08 | 111.91 |
| 26 | 5 | 617 | CHL | C1B-CHB-C4A | -2.29 | 125.59 | 130.12 |
| 43 | 3 | 501 | LUT | C11-C10-C9 | -2.29 | 124.05 | 127.31 |
| 26 | 8 | 604 | CHL | CHB-C4A-NA | 2.29 | 127.67 | 124.51 |
| 35 | 1 | 804 | LMT | C3'-C4'-C5' | -2.29 | 105.68 | 110.93 |
| 32 | H | 5001 | SQD | O3-C3-C2 | -2.29 | 105.06 | 110.35 |
| 25 | J | 1901 | CLA | CMD-C2D-C3D | -2.29 | 122.36 | 127.61 |
| 29 | 3 | 505 | BCR | C23-C24-C25 | -2.29 | 120.78 | 127.20 |
| 25 | 5 | 601 | CLA | CMD-C2D-C3D | -2.28 | 122.36 | 127.61 |
| 32 | I | 5001 | SQD | O3-C3-C2 | -2.28 | 105.07 | 110.35 |
| 29 | J | 4001 | BCR | C34-C9-C10 | -2.28 | 119.72 | 122.92 |
| 25 | 6 | 601 | CLA | O1D-CGD-CBD | -2.28 | 119.81 | 124.48 |
| 25 | A | 1121 | CLA | O2A-CGA-CBA | 2.28 | 119.08 | 111.91 |
| 26 | a | 610 | CHL | C1-O2A-CGA | 2.28 | 123.36 | 116.73 |
| 29 | K | 4002 | BCR | C38-C26-C27 | 2.28 | 118.00 | 113.62 |
| 29 | 5 | 504 | BCR | C37-C22-C23 | 2.28 | 121.67 | 118.08 |
| 25 | H | 1702 | CLA | O1D-CGD-CBD | -2.28 | 119.81 | 124.48 |
| 35 | B | 5006 | LMT | C1'-O5'-C5' | -2.28 | 109.21 | 113.69 |
| 26 | 6 | 613 | CHL | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 25 | A | 1013 | CLA | O2A-CGA-CBA | 2.28 | 119.06 | 111.91 |
| 43 | 6 | 501 | LUT | C20-C13-C12 | 2.28 | 121.67 | 118.08 |
| 25 | L | 1501 | CLA | C1D-ND-C4D | -2.28 | 104.72 | 106.33 |
| 29 | L | 4001 | BCR | C38-C26-C27 | 2.28 | 117.99 | 113.62 |
| 25 | B | 1218 | CLA | CHA-C4D-ND | 2.28 | 137.26 | 132.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 601 | CLA | O2D-CGD-O1D | -2.28 | 119.39 | 123.84 |
| 25 | B | 1023 | CLA | CAC-C3C-C4C | 2.28 | 127.77 | 124.81 |
| 26 | 5 | 610 | CHL | C1-O2A-CGA | 2.28 | 122.42 | 116.44 |
| 26 | 5 | 618 | CHL | C1B-CHB-C4A | -2.28 | 125.61 | 130.12 |
| 25 | 1 | 615 | CLA | CMB-C2B-C1B | -2.28 | 124.97 | 128.46 |
| 29 | 3 | 503 | BCR | C34-C9-C10 | -2.28 | 119.73 | 122.92 |
| 25 | B | 1207 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | 6 | 615 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | 5 | 604 | CLA | CMB-C2B-C3B | 2.27 | 128.93 | 124.68 |
| 25 | 6 | 618 | CLA | CAA-C2A-C3A | -2.27 | 106.55 | 112.78 |
| 25 | A | 1121 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | B | 1208 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | A | 1121 | CLA | CAA-C2A-C3A | -2.27 | 106.55 | 112.78 |
| 29 | B | 4007 | BCR | C33-C5-C4 | 2.27 | 117.98 | 113.62 |
| 50 | 7 | 502 | XAT | O4-C5-C4 | -2.27 | 111.67 | 113.38 |
| 25 | B | 1222 | CLA | CHA-C4D-ND | 2.27 | 137.25 | 132.50 |
| 25 | G | 1602 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | 4 | 612 | CLA | CAA-C2A-C3A | -2.27 | 106.56 | 112.78 |
| 25 | B | 1225 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | 4 | 608 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | B | 1232 | CLA | O2D-CGD-O1D | -2.27 | 119.40 | 123.84 |
| 43 | 6 | 502 | LUT | C38-C25-C24 | -2.27 | 118.70 | 123.56 |
| 40 | J | 4002 | RRX | C2-C1-C6 | 2.27 | 113.97 | 110.48 |
| 43 | a | 503 | LUT | C38-C25-C24 | -2.27 | 118.70 | 123.56 |
| 29 | 5 | 503 | BCR | C34-C9-C10 | -2.27 | 119.75 | 122.92 |
| 43 | 8 | 501 | LUT | C38-C25-C24 | -2.27 | 118.71 | 123.56 |
| 25 | 4 | 604 | CLA | CMD-C2D-C3D | -2.27 | 122.40 | 127.61 |
| 25 | 8 | 605 | CLA | CMD-C2D-C3D | -2.27 | 122.40 | 127.61 |
| 25 | 1 | 602 | CLA | C1D-ND-C4D | -2.27 | 104.72 | 106.33 |
| 25 | A | 1112 | CLA | O2A-CGA-CBA | 2.27 | 119.02 | 111.91 |
| 25 | a | 601 | CLA | O2D-CGD-O1D | -2.27 | 119.41 | 123.84 |
| 25 | B | 1238 | CLA | CMD-C2D-C3D | -2.26 | 122.41 | 127.61 |
| 25 | 4 | 603 | CLA | CMD-C2D-C3D | -2.26 | 122.41 | 127.61 |
| 25 | L | 1502 | CLA | CHA-C4D-ND | 2.26 | 137.24 | 132.50 |
| 43 | 5 | 502 | LUT | C38-C25-C24 | -2.26 | 118.72 | 123.56 |
| 25 | A | 1110 | CLA | C1D-ND-C4D | -2.26 | 104.73 | 106.33 |
| 25 | 4 | 617 | CLA | CMD-C2D-C3D | -2.26 | 122.41 | 127.61 |
| 26 | 6 | 609 | CHL | CHD-C4C-C3C | 2.26 | 128.17 | 124.84 |
| 29 | A | 4002 | BCR | C27-C26-C25 | -2.26 | 119.44 | 122.73 |
| 25 | B | 1240 | CLA | CHA-C1A-NA | -2.26 | 121.22 | 126.40 |
| 29 | 3 | 505 | BCR | C34-C9-C10 | -2.26 | 119.75 | 122.92 |
| 25 | 3 | 607 | CLA | O2A-CGA-CBA | 2.26 | 119.01 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | a | 609 | CHL | CMB-C2B-C1B | -2.26 | 124.99 | 128.46 |
| 25 | G | 1602 | CLA | CMA-C3A-C4A | 2.26 | 117.85 | 111.77 |
| 25 | 8 | 612 | CLA | C1D-ND-C4D | -2.26 | 104.73 | 106.33 |
| 25 | A | 1133 | CLA | C1-O2A-CGA | 2.26 | 122.38 | 116.44 |
| 25 | O | 1802 | CLA | CMD-C2D-C3D | -2.26 | 122.41 | 127.61 |
| 25 | A | 1122 | CLA | O2D-CGD-O1D | -2.26 | 119.42 | 123.84 |
| 43 | a | 502 | LUT | C38-C25-C24 | -2.26 | 118.72 | 123.56 |
| 29 | B | 4007 | BCR | C35-C13-C12 | 2.26 | 121.64 | 118.08 |
| 25 | B | 1211 | CLA | CMB-C2B-C1B | -2.26 | 124.99 | 128.46 |
| 29 | L | 4003 | BCR | C33-C5-C4 | 2.26 | 117.96 | 113.62 |
| 25 | a | 615 | CLA | C1D-ND-C4D | -2.26 | 104.73 | 106.33 |
| 25 | 3 | 605 | CLA | CMD-C2D-C3D | -2.26 | 122.42 | 127.61 |
| 29 | B | 4003 | BCR | C19-C18-C17 | 2.26 | 122.41 | 118.94 |
| 25 | 8 | 607 | CLA | CMA-C3A-C4A | 2.26 | 117.84 | 111.77 |
| 25 | 4 | 617 | CLA | O2D-CGD-O1D | -2.26 | 119.42 | 123.84 |
| 26 | 3 | 611 | CHL | C1-C2-C3 | -2.26 | 122.14 | 126.04 |
| 25 | 8 | 615 | CLA | C3D-C2D-C1D | -2.26 | 102.75 | 105.83 |
| 25 | 5 | 606 | CLA | CMD-C2D-C3D | -2.26 | 122.42 | 127.61 |
| 25 | B | 1211 | CLA | CMA-C3A-C4A | 2.26 | 117.84 | 111.77 |
| 25 | 4 | 603 | CLA | C1D-ND-C4D | -2.26 | 104.73 | 106.33 |
| 43 | 8 | 502 | LUT | C11-C10-C9 | -2.26 | 124.09 | 127.31 |
| 25 | A | 1119 | CLA | CMD-C2D-C3D | -2.26 | 122.42 | 127.61 |
| 25 | B | 1221 | CLA | CMD-C2D-C3D | -2.26 | 122.42 | 127.61 |
| 25 | G | 1602 | CLA | CMD-C2D-C3D | -2.26 | 122.42 | 127.61 |
| 25 | 8 | 611 | CLA | O2D-CGD-O1D | -2.26 | 119.43 | 123.84 |
| 25 | B | 1227 | CLA | O2A-CGA-CBA | 2.26 | 118.99 | 111.91 |
| 26 | 6 | 613 | CHL | CMB-C2B-C1B | -2.26 | 125.00 | 128.46 |
| 25 | 3 | 605 | CLA | C1D-ND-C4D | -2.26 | 104.73 | 106.33 |
| 25 | 9 | 606 | CLA | CMD-C2D-C3D | -2.25 | 122.43 | 127.61 |
| 43 | 5 | 502 | LUT | C39-C29-C28 | 2.25 | 121.63 | 118.08 |
| 26 | 9 | 601 | CHL | CHD-C4C-C3C | 2.25 | 128.15 | 124.84 |
| 25 | L | 1504 | CLA | O2A-CGA-CBA | 2.25 | 118.98 | 111.91 |
| 26 | 6 | 613 | CHL | CHD-C4C-C3C | 2.25 | 128.15 | 124.84 |
| 25 | 7 | 610 | CLA | CAA-C2A-C3A | -2.25 | 106.61 | 112.78 |
| 25 | 9 | 606 | CLA | CMA-C3A-C4A | 2.25 | 117.83 | 111.77 |
| 25 | 4 | 616 | CLA | O2A-CGA-CBA | 2.25 | 118.98 | 111.91 |
| 43 | 9 | 502 | LUT | C31-C32-C33 | -2.25 | 120.09 | 126.42 |
| 40 | 3 | 506 | RRX | C38-C26-C27 | 2.25 | 118.53 | 114.36 |
| 26 | 1 | 613 | CHL | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 26 | 5 | 618 | CHL | CHB-C4A-NA | 2.25 | 127.62 | 124.51 |
| 35 | A | 5008 | LMT | C3'-C4'-C5' | -2.25 | 105.77 | 110.93 |
| 25 | A | 1132 | CLA | CMD-C2D-C3D | -2.25 | 122.44 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 608 | CLA | CMA-C3A-C4A | 2.25 | 117.82 | 111.77 |
| 26 | a | 613 | CHL | C4D-CHA-C1A | 2.25 | 123.99 | 121.25 |
| 26 | 4 | 618 | CHL | C1-C2-C3 | -2.25 | 122.15 | 126.04 |
| 25 | 3 | 601 | CLA | CMB-C2B-C3B | 2.25 | 128.89 | 124.68 |
| 25 | 8 | 608 | CLA | CMD-C2D-C3D | -2.25 | 122.44 | 127.61 |
| 25 | a | 601 | CLA | C1D-ND-C4D | -2.25 | 104.74 | 106.33 |
| 29 | 5 | 504 | BCR | C36-C18-C17 | -2.25 | 119.77 | 122.92 |
| 43 | 1 | 501 | LUT | C31-C30-C29 | -2.25 | 124.10 | 127.31 |
| 26 | a | 609 | CHL | CHD-C4C-C3C | 2.25 | 128.15 | 124.84 |
| 25 | 6 | 608 | CLA | CMA-C3A-C4A | 2.25 | 117.82 | 111.77 |
| 26 | 1 | 610 | CHL | C4A-NA-C1A | 2.25 | 107.72 | 106.71 |
| 25 | 4 | 611 | CLA | CMD-C2D-C3D | -2.25 | 122.44 | 127.61 |
| 25 | 4 | 612 | CLA | O1D-CGD-CBD | -2.25 | 119.88 | 124.48 |
| 26 | 9 | 601 | CHL | CMB-C2B-C1B | -2.25 | 125.01 | 128.46 |
| 25 | 4 | 602 | CLA | O2A-CGA-CBA | 2.25 | 118.96 | 111.91 |
| 25 | A | 1132 | CLA | O1D-CGD-CBD | -2.25 | 119.89 | 124.48 |
| 29 | L | 4003 | BCR | C23-C24-C25 | -2.25 | 120.89 | 127.20 |
| 25 | A | 1117 | CLA | CMD-C2D-C3D | -2.25 | 122.44 | 127.61 |
| 25 | B | 1217 | CLA | CMD-C2D-C3D | -2.25 | 122.45 | 127.61 |
| 25 | B | 1228 | CLA | CMD-C2D-C3D | -2.25 | 122.45 | 127.61 |
| 43 | 4 | 502 | LUT | C38-C25-C24 | -2.25 | 118.75 | 123.56 |
| 25 | B | 1203 | CLA | CMD-C2D-C3D | -2.25 | 122.45 | 127.61 |
| 25 | A | 1130 | CLA | CMD-C2D-C3D | -2.25 | 122.45 | 127.61 |
| 25 | B | 1207 | CLA | CMD-C2D-C3D | -2.24 | 122.45 | 127.61 |
| 43 | 4 | 501 | LUT | C11-C10-C9 | -2.24 | 124.11 | 127.31 |
| 25 | A | 1103 | CLA | C1-O2A-CGA | 2.24 | 122.33 | 116.44 |
| 25 | A | 1133 | CLA | C1D-ND-C4D | -2.24 | 104.74 | 106.33 |
| 25 | B | 1205 | CLA | C1D-ND-C4D | -2.24 | 104.74 | 106.33 |
| 25 | B | 1235 | CLA | C1D-ND-C4D | -2.24 | 104.74 | 106.33 |
| 25 | 3 | 601 | CLA | C1D-ND-C4D | -2.24 | 104.74 | 106.33 |
| 29 | J | 4001 | BCR | C38-C26-C27 | 2.24 | 117.93 | 113.62 |
| 25 | A | 1101 | CLA | CMD-C2D-C3D | -2.24 | 122.45 | 127.61 |
| 25 | 4 | 601 | CLA | O2D-CGD-O1D | -2.24 | 119.45 | 123.84 |
| 25 | A | 1129 | CLA | CMB-C2B-C3B | 2.24 | 128.87 | 124.68 |
| 25 | 2 | 605 | CLA | OBD-CAD-C3D | -2.24 | 123.12 | 128.52 |
| 25 | a | 611 | CLA | CMD-C2D-C3D | -2.24 | 122.46 | 127.61 |
| 25 | 4 | 611 | CLA | O2A-CGA-CBA | 2.24 | 118.94 | 111.91 |
| 43 | 1 | 503 | LUT | C18-C5-C4 | 2.24 | 118.51 | 114.36 |
| 25 | K | 1401 | CLA | C1D-ND-C4D | -2.24 | 104.74 | 106.33 |
| 25 | B | 1021 | CLA | O2A-CGA-CBA | 2.24 | 118.94 | 111.91 |
| 25 | 3 | 610 | CLA | CMD-C2D-C3D | -2.24 | 122.46 | 127.61 |
| 25 | B | 1206 | CLA | CMB-C2B-C3B | 2.24 | 128.87 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | G | 4001 | BCR | C33-C5-C4 | 2.24 | 117.92 | 113.62 |
| 25 | 6 | 604 | CLA | C1C-C2C-C3C | -2.24 | 104.60 | 106.96 |
| 25 | A | 1103 | CLA | CMD-C2D-C3D | -2.24 | 122.46 | 127.61 |
| 25 | 7 | 612 | CLA | CMB-C2B-C3B | 2.24 | 128.87 | 124.68 |
| 25 | 1 | 608 | CLA | CHA-C4D-ND | 2.24 | 137.18 | 132.50 |
| 25 | O | 1802 | CLA | C1D-ND-C4D | -2.24 | 104.74 | 106.33 |
| 25 | B | 1234 | CLA | CMD-C2D-C3D | -2.24 | 122.46 | 127.61 |
| 25 | L | 1503 | CLA | CMD-C2D-C3D | -2.24 | 122.46 | 127.61 |
| 25 | 1 | 607 | CLA | CMD-C2D-C3D | -2.24 | 122.46 | 127.61 |
| 29 | L | 4001 | BCR | C15-C14-C13 | -2.24 | 124.11 | 127.31 |
| 25 | a | 605 | CLA | O1D-CGD-CBD | -2.24 | 119.90 | 124.48 |
| 26 | 1 | 610 | CHL | CHD-C4C-C3C | 2.24 | 128.13 | 124.84 |
| 25 | A | 1105 | CLA | CMD-C2D-C3D | -2.24 | 122.47 | 127.61 |
| 25 | 2 | 601 | CLA | CMD-C2D-C3D | -2.24 | 122.47 | 127.61 |
| 50 | 9 | 504 | XAT | C19-C9-C10 | -2.24 | 119.79 | 122.92 |
| 29 | B | 4005 | BCR | C23-C22-C21 | -2.24 | 115.51 | 118.94 |
| 25 | H | 1703 | CLA | CMD-C2D-C3D | -2.24 | 122.47 | 127.61 |
| 26 | 6 | 619 | CHL | CMB-C2B-C1B | -2.24 | 125.03 | 128.46 |
| 25 | A | 1130 | CLA | C1D-ND-C4D | -2.24 | 104.75 | 106.33 |
| 25 | 4 | 606 | CLA | C1D-ND-C4D | -2.24 | 104.75 | 106.33 |
| 25 | a | 601 | CLA | CMB-C2B-C3B | 2.24 | 128.86 | 124.68 |
| 30 | F | 5002 | LHG | C5-O7-C7 | -2.24 | 112.29 | 117.79 |
| 25 | A | 1125 | CLA | C1C-C2C-C3C | -2.24 | 104.61 | 106.96 |
| 25 | 7 | 605 | CLA | OBD-CAD-C3D | -2.24 | 123.14 | 128.52 |
| 26 | 9 | 613 | CHL | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 25 | a | 605 | CLA | CMA-C3A-C4A | 2.23 | 117.78 | 111.77 |
| 25 | 6 | 601 | CLA | CMB-C2B-C3B | 2.23 | 128.85 | 124.68 |
| 25 | 6 | 606 | CLA | O1D-CGD-CBD | -2.23 | 119.92 | 124.48 |
| 25 | 9 | 609 | CLA | CMD-C2D-C3D | -2.23 | 122.48 | 127.61 |
| 29 | I | 4001 | BCR | C37-C22-C23 | 2.23 | 121.59 | 118.08 |
| 25 | 4 | 616 | CLA | CMD-C2D-C3D | -2.23 | 122.48 | 127.61 |
| 29 | A | 4003 | BCR | C38-C26-C27 | 2.23 | 117.90 | 113.62 |
| 25 | A | 1116 | CLA | CMD-C2D-C3D | -2.23 | 122.48 | 127.61 |
| 25 | 2 | 601 | CLA | C1D-ND-C4D | -2.23 | 104.75 | 106.33 |
| 26 | 5 | 611 | CHL | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 29 | 6 | 503 | BCR | C35-C13-C12 | 2.23 | 121.59 | 118.08 |
| 25 | 1 | 606 | CLA | O1D-CGD-CBD | -2.23 | 119.92 | 124.48 |
| 25 | B | 1236 | CLA | CMA-C3A-C4A | 2.23 | 117.77 | 111.77 |
| 39 | F | 4001 | NEX | C11-C12-C13 | 2.23 | 132.68 | 126.42 |
| 25 | A | 1136 | CLA | CMD-C2D-C3D | -2.23 | 122.48 | 127.61 |
| 25 | 8 | 620 | CLA | CMD-C2D-C3D | -2.23 | 122.48 | 127.61 |
| 25 | L | 1504 | CLA | CHA-C1A-NA | -2.23 | 121.29 | 126.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1225 | CLA | O2A-CGA-CBA | 2.23 | 118.91 | 111.91 |
| 43 | a | 502 | LUT | C31-C30-C29 | -2.23 | 124.13 | 127.31 |
| 26 | 3 | 604 | CHL | C4D-CHA-C1A | 2.23 | 123.96 | 121.25 |
| 26 | a | 604 | CHL | C1B-CHB-C4A | -2.23 | 125.70 | 130.12 |
| 32 | G | 5001 | SQD | O3-C3-C2 | -2.23 | 105.20 | 110.35 |
| 29 | L | 4003 | BCR | C8-C7-C6 | -2.23 | 120.94 | 127.20 |
| 25 | 2 | 607 | CLA | O2A-CGA-CBA | 2.23 | 118.90 | 111.91 |
| 25 | B | 1210 | CLA | CMD-C2D-C3D | -2.23 | 122.49 | 127.61 |
| 29 | L | 4001 | BCR | C33-C5-C4 | 2.23 | 117.89 | 113.62 |
| 25 | F | 1301 | CLA | CMD-C2D-C3D | -2.23 | 122.50 | 127.61 |
| 25 | a | 601 | CLA | CMD-C2D-C3D | -2.23 | 122.50 | 127.61 |
| 43 | 8 | 501 | LUT | C20-C13-C12 | 2.23 | 121.58 | 118.08 |
| 26 | 1 | 610 | CHL | CHB-C4A-NA | 2.22 | 127.59 | 124.51 |
| 25 | A | 1119 | CLA | C1D-ND-C4D | -2.22 | 104.75 | 106.33 |
| 25 | B | 1218 | CLA | C1D-ND-C4D | -2.22 | 104.75 | 106.33 |
| 25 | 2 | 604 | CLA | C1D-ND-C4D | -2.22 | 104.75 | 106.33 |
| 25 | 1 | 612 | CLA | O2A-CGA-CBA | 2.22 | 118.89 | 111.91 |
| 26 | 6 | 617 | CHL | C4D-CHA-C1A | 2.22 | 123.95 | 121.25 |
| 25 | 9 | 612 | CLA | CHA-C1A-NA | -2.22 | 121.31 | 126.40 |
| 25 | 5 | 601 | CLA | C6-C5-C3 | -2.22 | 107.62 | 113.45 |
| 25 | L | 1503 | CLA | CMB-C2B-C1B | -2.22 | 125.05 | 128.46 |
| 25 | 3 | 612 | CLA | CMD-C2D-C3D | -2.22 | 122.50 | 127.61 |
| 26 | 6 | 609 | CHL | CMB-C2B-C1B | -2.22 | 125.05 | 128.46 |
| 25 | 2 | 604 | CLA | O2A-CGA-CBA | 2.22 | 118.88 | 111.91 |
| 25 | A | 1102 | CLA | CMD-C2D-C3D | -2.22 | 122.50 | 127.61 |
| 25 | A | 1126 | CLA | CMD-C2D-C3D | -2.22 | 122.50 | 127.61 |
| 25 | B | 1218 | CLA | CMB-C2B-C3B | 2.22 | 128.84 | 124.68 |
| 29 | H | 4001 | BCR | C38-C26-C27 | 2.22 | 117.88 | 113.62 |
| 26 | 8 | 604 | CHL | C1-O2A-CGA | 2.22 | 122.27 | 116.44 |
| 50 | 9 | 504 | XAT | C32-C33-C34 | 2.22 | 122.35 | 118.94 |
| 26 | 8 | 610 | CHL | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 25 | L | 1501 | CLA | CMD-C2D-C3D | -2.22 | 122.51 | 127.61 |
| 25 | F | 1302 | CLA | C1D-ND-C4D | -2.22 | 104.76 | 106.33 |
| 25 | A | 1129 | CLA | CMD-C2D-C3D | -2.22 | 122.51 | 127.61 |
| 25 | B | 1201 | CLA | O2A-CGA-CBA | 2.22 | 118.87 | 111.91 |
| 25 | 4 | 617 | CLA | CHA-C1A-NA | -2.22 | 121.32 | 126.40 |
| 26 | 1 | 613 | CHL | CMB-C2B-C1B | -2.22 | 125.05 | 128.46 |
| 25 | A | 1135 | CLA | C1D-ND-C4D | -2.22 | 104.76 | 106.33 |
| 25 | 8 | 606 | CLA | C1D-ND-C4D | -2.22 | 104.76 | 106.33 |
| 25 | B | 1210 | CLA | C1C-C2C-C3C | -2.22 | 104.62 | 106.96 |
| 25 | 3 | 606 | CLA | CMB-C2B-C3B | 2.22 | 128.83 | 124.68 |
| 25 | A | 1128 | CLA | O2A-CGA-CBA | 2.22 | 118.86 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | O | 1803 | CLA | CMD-C2D-C3D | -2.22 | 122.51 | 127.61 |
| 26 | 6 | 613 | CHL | C4D-CHA-C1A | 2.22 | 123.95 | 121.25 |
| 26 | 1 | 613 | CHL | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 26 | 7 | 611 | CHL | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 25 | B | 1224 | CLA | CMB-C2B-C3B | 2.22 | 128.82 | 124.68 |
| 29 | B | 4003 | BCR | C8-C9-C10 | 2.22 | 122.34 | 118.94 |
| 43 | 2 | 507 | LUT | C19-C9-C10 | -2.22 | 119.82 | 122.92 |
| 25 | G | 1603 | CLA | CMD-C2D-C3D | -2.21 | 122.52 | 127.61 |
| 25 | L | 1504 | CLA | CMD-C2D-C3D | -2.21 | 122.52 | 127.61 |
| 25 | F | 1301 | CLA | C1D-ND-C4D | -2.21 | 104.76 | 106.33 |
| 25 | 2 | 601 | CLA | CMB-C2B-C3B | 2.21 | 128.82 | 124.68 |
| 26 | 2 | 610 | CHL | C1-O2A-CGA | 2.21 | 123.16 | 116.73 |
| 25 | 1 | 605 | CLA | CMB-C2B-C3B | 2.21 | 128.82 | 124.68 |
| 25 | 8 | 611 | CLA | CMB-C2B-C3B | 2.21 | 128.82 | 124.68 |
| 29 | 7 | 503 | BCR | C31-C1-C6 | -2.21 | 106.71 | 110.30 |
| 25 | B | 1201 | CLA | C1D-ND-C4D | -2.21 | 104.76 | 106.33 |
| 25 | A | 1129 | CLA | CHA-C1A-NA | -2.21 | 121.33 | 126.40 |
| 29 | K | 4001 | BCR | C2-C1-C6 | 2.21 | 113.89 | 110.48 |
| 50 | 2 | 501 | XAT | C38-C25-C26 | -2.21 | 118.56 | 122.26 |
| 25 | B | 1221 | CLA | O1D-CGD-CBD | -2.21 | 119.96 | 124.48 |
| 29 | K | 4002 | BCR | C33-C5-C4 | 2.21 | 117.86 | 113.62 |
| 25 | 2 | 612 | CLA | CMD-C2D-C3D | -2.21 | 122.53 | 127.61 |
| 25 | 3 | 602 | CLA | CMB-C2B-C1B | -2.21 | 125.07 | 128.46 |
| 25 | 2 | 602 | CLA | C1D-ND-C4D | -2.21 | 104.77 | 106.33 |
| 25 | 2 | 602 | CLA | O2A-CGA-CBA | 2.21 | 118.84 | 111.91 |
| 25 | 6 | 615 | CLA | O2A-CGA-CBA | 2.21 | 118.84 | 111.91 |
| 25 | 4 | 606 | CLA | CAA-C2A-C3A | -2.21 | 106.73 | 112.78 |
| 25 | A | 1134 | CLA | O1D-CGD-CBD | -2.21 | 119.97 | 124.48 |
| 25 | B | 1232 | CLA | CMD-C2D-C3D | -2.21 | 122.53 | 127.61 |
| 25 | 1 | 603 | CLA | CMD-C2D-C3D | -2.21 | 122.53 | 127.61 |
| 25 | 4 | 612 | CLA | CMA-C3A-C4A | 2.21 | 117.70 | 111.77 |
| 25 | 2 | 603 | CLA | CMD-C2D-C3D | -2.21 | 122.54 | 127.61 |
| 25 | B | 1203 | CLA | O2A-CGA-CBA | 2.21 | 118.83 | 111.91 |
| 26 | 2 | 609 | CHL | CHB-C4A-NA | 2.21 | 127.56 | 124.51 |
| 25 | 8 | 611 | CLA | CMD-C2D-C3D | -2.21 | 122.54 | 127.61 |
| 25 | B | 1221 | CLA | O2A-CGA-CBA | 2.21 | 118.83 | 111.91 |
| 25 | 1 | 608 | CLA | C1D-ND-C4D | -2.21 | 104.77 | 106.33 |
| 25 | 5 | 606 | CLA | CMB-C2B-C3B | 2.21 | 128.81 | 124.68 |
| 25 | 3 | 602 | CLA | CMD-C2D-C3D | -2.21 | 122.54 | 127.61 |
| 25 | 9 | 605 | CLA | CMD-C2D-C3D | -2.21 | 122.54 | 127.61 |
| 25 | 3 | 613 | CLA | CMA-C3A-C4A | 2.21 | 117.70 | 111.77 |
| 43 | 9 | 501 | LUT | C20-C13-C12 | 2.20 | 121.55 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 603 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 25 | A | 1140 | CLA | CMD-C2D-C3D | -2.20 | 122.54 | 127.61 |
| 25 | 7 | 604 | CLA | C6-C5-C3 | -2.20 | 107.68 | 113.45 |
| 25 | B | 1220 | CLA | CMD-C2D-C3D | -2.20 | 122.55 | 127.61 |
| 25 | H | 1701 | CLA | CMD-C2D-C3D | -2.20 | 122.55 | 127.61 |
| 25 | 4 | 610 | CLA | CMD-C2D-C3D | -2.20 | 122.55 | 127.61 |
| 25 | 4 | 604 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 29 | 5 | 503 | BCR | C35-C13-C12 | 2.20 | 121.55 | 118.08 |
| 26 | 7 | 615 | CHL | C1B-CHB-C4A | -2.20 | 125.76 | 130.12 |
| 25 | A | 1136 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 25 | 6 | 602 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 25 | O | 1803 | CLA | O2D-CGD-O1D | -2.20 | 119.53 | 123.84 |
| 25 | 9 | 605 | CLA | C3D-C2D-C1D | -2.20 | 102.83 | 105.83 |
| 25 | A | 1139 | CLA | CMD-C2D-C3D | -2.20 | 122.55 | 127.61 |
| 50 | 9 | 504 | XAT | C40-C33-C34 | -2.20 | 119.84 | 122.92 |
| 25 | A | 1013 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 25 | 3 | 602 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 25 | 8 | 611 | CLA | O2A-CGA-CBA | 2.20 | 118.81 | 111.91 |
| 25 | A | 1122 | CLA | CMD-C2D-C3D | -2.20 | 122.55 | 127.61 |
| 25 | A | 1108 | CLA | CMD-C2D-C3D | -2.20 | 122.55 | 127.61 |
| 25 | B | 1212 | CLA | CMB-C2B-C3B | 2.20 | 128.79 | 124.68 |
| 25 | 9 | 604 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 25 | B | 1212 | CLA | O1D-CGD-CBD | -2.20 | 119.98 | 124.48 |
| 36 | 8 | 802 | DGD | C3G-C2G-C1G | -2.20 | 106.59 | 111.79 |
| 25 | 6 | 618 | CLA | CMD-C2D-C3D | -2.20 | 122.56 | 127.61 |
| 25 | 9 | 602 | CLA | C1D-ND-C4D | -2.20 | 104.77 | 106.33 |
| 43 | 9 | 501 | LUT | C31-C30-C29 | -2.20 | 124.17 | 127.31 |
| 25 | O | 1801 | CLA | O2D-CGD-O1D | -2.20 | 119.10 | 124.09 |
| 25 | 3 | 605 | CLA | O2A-CGA-CBA | 2.20 | 118.80 | 111.91 |
| 26 | 6 | 609 | CHL | CHB-C4A-NA | 2.20 | 127.55 | 124.51 |
| 43 | 5 | 505 | LUT | C11-C12-C13 | -2.20 | 120.25 | 126.42 |
| 25 | 2 | 615 | CLA | C1D-ND-C4D | -2.19 | 104.78 | 106.33 |
| 25 | A | 1107 | CLA | CMD-C2D-C3D | -2.19 | 122.57 | 127.61 |
| 25 | K | 1403 | CLA | CMD-C2D-C3D | -2.19 | 122.57 | 127.61 |
| 26 | 1 | 610 | CHL | CMB-C2B-C1B | -2.19 | 125.09 | 128.46 |
| 25 | 1 | 602 | CLA | CMD-C2D-C3D | -2.19 | 122.57 | 127.61 |
| 25 | 7 | 610 | CLA | CMD-C2D-C3D | -2.19 | 122.57 | 127.61 |
| 25 | A | 1108 | CLA | O2D-CGD-O1D | -2.19 | 119.55 | 123.84 |
| 25 | B | 1205 | CLA | CMD-C2D-C3D | -2.19 | 122.57 | 127.61 |
| 26 | 6 | 619 | CHL | CHD-C4C-C3C | 2.19 | 128.06 | 124.84 |
| 25 | 4 | 601 | CLA | O1D-CGD-CBD | -2.19 | 120.00 | 124.48 |
| 29 | K | 4002 | BCR | C35-C13-C12 | 2.19 | 121.53 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1239 | CLA | CMD-C2D-C3D | -2.19 | 122.58 | 127.61 |
| 25 | B | 1219 | CLA | CMB-C2B-C1B | -2.19 | 125.10 | 128.46 |
| 25 | 6 | 603 | CLA | C1-O2A-CGA | 2.19 | 122.19 | 116.44 |
| 43 | 8 | 501 | LUT | C31-C30-C29 | -2.19 | 124.19 | 127.31 |
| 25 | B | 1222 | CLA | CMD-C2D-C3D | -2.19 | 122.58 | 127.61 |
| 25 | K | 1404 | CLA | CMD-C2D-C3D | -2.19 | 122.58 | 127.61 |
| 25 | B | 1214 | CLA | CMD-C2D-C3D | -2.19 | 122.58 | 127.61 |
| 25 | B | 1022 | CLA | O2A-CGA-CBA | 2.19 | 118.77 | 111.91 |
| 25 | A | 1126 | CLA | O1D-CGD-CBD | -2.19 | 120.01 | 124.48 |
| 29 | 6 | 504 | BCR | C4-C5-C6 | -2.19 | 119.56 | 122.73 |
| 25 | B | 1213 | CLA | CMD-C2D-C3D | -2.19 | 122.58 | 127.61 |
| 26 | a | 610 | CHL | CHB-C4A-NA | 2.19 | 127.53 | 124.51 |
| 29 | B | 4004 | BCR | C36-C18-C17 | -2.19 | 119.86 | 122.92 |
| 43 | 5 | 501 | LUT | C8-C7-C6 | -2.19 | 121.06 | 127.20 |
| 26 | 5 | 617 | CHL | C4A-NA-C1A | 2.18 | 107.69 | 106.71 |
| 25 | A | 1105 | CLA | O2A-CGA-CBA | 2.18 | 118.76 | 111.91 |
| 25 | B | 1227 | CLA | C1-O2A-CGA | 2.18 | 122.17 | 116.44 |
| 25 | A | 1106 | CLA | CMD-C2D-C3D | -2.18 | 122.59 | 127.61 |
| 26 | 1 | 613 | CHL | C1-O2A-CGA | 2.18 | 123.07 | 116.73 |
| 26 | 3 | 604 | CHL | CHB-C4A-NA | 2.18 | 127.53 | 124.51 |
| 25 | B | 1021 | CLA | O1D-CGD-CBD | -2.18 | 120.02 | 124.48 |
| 25 | B | 1237 | CLA | CMD-C2D-C3D | -2.18 | 122.59 | 127.61 |
| 29 | K | 4002 | BCR | C38-C26-C25 | -2.18 | 122.08 | 124.53 |
| 25 | 1 | 612 | CLA | CMD-C2D-C3D | -2.18 | 122.59 | 127.61 |
| 25 | 7 | 603 | CLA | CMD-C2D-C3D | -2.18 | 122.59 | 127.61 |
| 25 | 1 | 615 | CLA | CHA-C1A-NA | -2.18 | 121.40 | 126.40 |
| 26 | 8 | 603 | CHL | C1-O2A-CGA | 2.18 | 122.17 | 116.44 |
| 25 | 2 | 612 | CLA | O2A-CGA-CBA | 2.18 | 118.75 | 111.91 |
| 26 | 8 | 601 | CHL | CMB-C2B-C1B | -2.18 | 125.11 | 128.46 |
| 25 | B | 1206 | CLA | O2A-CGA-CBA | 2.18 | 118.75 | 111.91 |
| 26 | 3 | 608 | CHL | CHD-C4C-C3C | 2.18 | 128.05 | 124.84 |
| 25 | 5 | 606 | CLA | O2A-CGA-CBA | 2.18 | 118.75 | 111.91 |
| 25 | K | 1402 | CLA | CMD-C2D-C3D | -2.18 | 122.60 | 127.61 |
| 25 | B | 1226 | CLA | CAA-C2A-C3A | -2.18 | 106.81 | 112.78 |
| 25 | A | 1110 | CLA | CMD-C2D-C3D | -2.18 | 122.60 | 127.61 |
| 25 | a | 602 | CLA | CAA-C2A-C3A | -2.18 | 106.81 | 112.78 |
| 25 | A | 1134 | CLA | CMD-C2D-C3D | -2.18 | 122.60 | 127.61 |
| 25 | 9 | 609 | CLA | C1D-ND-C4D | -2.18 | 104.79 | 106.33 |
| 26 | 7 | 609 | CHL | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 43 | 5 | 505 | LUT | C19-C9-C10 | -2.18 | 119.87 | 122.92 |
| 25 | 7 | 602 | CLA | CMD-C2D-C3D | -2.18 | 122.60 | 127.61 |
| 29 | A | 4003 | BCR | C35-C13-C12 | 2.18 | 121.51 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1230 | CLA | CMB-C2B-C3B | 2.18 | 128.75 | 124.68 |
| 43 | 5 | 505 | LUT | C31-C32-C33 | -2.18 | 120.30 | 126.42 |
| 26 | 3 | 611 | CHL | CHB-C4A-NA | 2.18 | 127.52 | 124.51 |
| 25 | B | 1230 | CLA | O1D-CGD-CBD | -2.18 | 120.03 | 124.48 |
| 25 | 9 | 602 | CLA | CMB-C2B-C1B | -2.18 | 125.12 | 128.46 |
| 25 | H | 1701 | CLA | O2A-CGA-CBA | 2.18 | 118.73 | 111.91 |
| 25 | A | 1129 | CLA | O2A-CGA-CBA | 2.18 | 118.73 | 111.91 |
| 25 | a | 608 | CLA | CMD-C2D-C3D | -2.18 | 122.61 | 127.61 |
| 25 | 5 | 602 | CLA | C6-C5-C3 | -2.18 | 111.06 | 114.62 |
| 25 | B | 1215 | CLA | C1D-ND-C4D | -2.17 | 104.79 | 106.33 |
| 25 | B | 1211 | CLA | O1D-CGD-CBD | -2.17 | 120.03 | 124.48 |
| 26 | 9 | 613 | CHL | C1B-CHB-C4A | -2.17 | 125.81 | 130.12 |
| 25 | 8 | 608 | CLA | C1D-ND-C4D | -2.17 | 104.79 | 106.33 |
| 26 | 3 | 604 | CHL | C1B-CHB-C4A | -2.17 | 125.81 | 130.12 |
| 26 | 6 | 611 | CHL | C1B-CHB-C4A | -2.17 | 125.81 | 130.12 |
| 25 | A | 1108 | CLA | O2A-CGA-CBA | 2.17 | 118.72 | 111.91 |
| 25 | O | 1802 | CLA | O1D-CGD-CBD | -2.17 | 120.04 | 124.48 |
| 25 | A | 1107 | CLA | CHA-C1A-NA | -2.17 | 121.42 | 126.40 |
| 25 | 9 | 606 | CLA | C1D-ND-C4D | -2.17 | 104.79 | 106.33 |
| 25 | B | 1223 | CLA | CHA-C1A-NA | -2.17 | 121.42 | 126.40 |
| 25 | 3 | 607 | CLA | CMD-C2D-C3D | -2.17 | 122.62 | 127.61 |
| 25 | 1 | 601 | CLA | C1D-ND-C4D | -2.17 | 104.79 | 106.33 |
| 25 | B | 1022 | CLA | CHA-C1A-NA | -2.17 | 121.43 | 126.40 |
| 43 | a | 501 | LUT | C11-C12-C13 | -2.17 | 120.32 | 126.42 |
| 25 | L | 1502 | CLA | O2A-CGA-CBA | 2.17 | 118.72 | 111.91 |
| 25 | 3 | 612 | CLA | CHA-C1A-NA | -2.17 | 121.43 | 126.40 |
| 25 | A | 1134 | CLA | C1D-ND-C4D | -2.17 | 104.79 | 106.33 |
| 40 | 3 | 506 | RRX | C2-C1-C6 | 2.17 | 113.82 | 110.48 |
| 25 | 4 | 611 | CLA | CAA-C2A-C3A | -2.17 | 106.84 | 112.78 |
| 25 | 2 | 603 | CLA | CMB-C2B-C3B | 2.17 | 128.73 | 124.68 |
| 26 | 6 | 610 | CHL | CHD-C4C-C3C | 2.17 | 128.03 | 124.84 |
| 25 | H | 1702 | CLA | CMD-C2D-C3D | -2.17 | 122.63 | 127.61 |
| 25 | A | 1135 | CLA | CMD-C2D-C3D | -2.17 | 122.63 | 127.61 |
| 25 | 3 | 601 | CLA | CMA-C3A-C4A | 2.17 | 117.60 | 111.77 |
| 25 | B | 1214 | CLA | O2A-CGA-CBA | 2.17 | 118.71 | 111.91 |
| 29 | 7 | 503 | BCR | C38-C26-C27 | 2.17 | 117.78 | 113.62 |
| 26 | a | 609 | CHL | CMA-C3A-C4A | 2.17 | 117.59 | 111.77 |
| 25 | B | 1229 | CLA | CMD-C2D-C3D | -2.17 | 122.63 | 127.61 |
| 25 | 4 | 601 | CLA | CMD-C2D-C3D | -2.17 | 122.63 | 127.61 |
| 25 | B | 1223 | CLA | C1D-ND-C4D | -2.17 | 104.80 | 106.33 |
| 25 | B | 1235 | CLA | CMD-C2D-C3D | -2.16 | 122.63 | 127.61 |
| 25 | B | 1023 | CLA | CHA-C1A-NA | -2.16 | 121.44 | 126.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1120 | CLA | O1D-CGD-CBD | -2.16 | 120.06 | 124.48 |
| 25 | 6 | 603 | CLA | CMD-C2D-C3D | -2.16 | 122.64 | 127.61 |
| 29 | B | 4002 | BCR | C34-C9-C10 | -2.16 | 119.89 | 122.92 |
| 25 | B | 1227 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 25 | a | 607 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 25 | A | 1102 | CLA | O1D-CGD-CBD | -2.16 | 120.06 | 124.48 |
| 26 | 7 | 615 | CHL | C4D-CHA-C1A | 2.16 | 123.88 | 121.25 |
| 25 | 6 | 612 | CLA | O2A-CGA-CBA | 2.16 | 118.70 | 111.91 |
| 25 | B | 1211 | CLA | O2A-CGA-CBA | 2.16 | 118.69 | 111.91 |
| 25 | 7 | 603 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 25 | B | 1220 | CLA | O2D-CGD-O1D | -2.16 | 119.61 | 123.84 |
| 25 | A | 1117 | CLA | C1-O2A-CGA | 2.16 | 122.12 | 116.44 |
| 25 | 8 | 612 | CLA | CMD-C2D-C3D | -2.16 | 122.64 | 127.61 |
| 50 | 7 | 502 | XAT | C40-C33-C34 | -2.16 | 119.89 | 122.92 |
| 25 | B | 1023 | CLA | C1C-C2C-C3C | -2.16 | 104.68 | 106.96 |
| 25 | B | 1224 | CLA | CMD-C2D-C3D | -2.16 | 122.64 | 127.61 |
| 29 | B | 4003 | BCR | C4-C5-C6 | -2.16 | 119.59 | 122.73 |
| 26 | 9 | 601 | CHL | CHB-C4A-NA | 2.16 | 127.50 | 124.51 |
| 25 | a | 603 | CLA | CMB-C2B-C1B | -2.16 | 125.14 | 128.46 |
| 43 | 1 | 503 | LUT | C30-C31-C32 | -2.16 | 116.48 | 123.22 |
| 26 | 7 | 615 | CHL | CMB-C2B-C1B | -2.16 | 125.14 | 128.46 |
| 25 | 7 | 610 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 25 | K | 1402 | CLA | CHA-C1A-NA | -2.16 | 121.45 | 126.40 |
| 26 | a | 609 | CHL | C1B-CHB-C4A | -2.16 | 125.84 | 130.12 |
| 25 | A | 1129 | CLA | O1D-CGD-CBD | -2.16 | 120.07 | 124.48 |
| 25 | A | 1101 | CLA | CHA-C1A-NA | -2.16 | 121.46 | 126.40 |
| 25 | A | 1115 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 25 | B | 1238 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 26 | 9 | 608 | CHL | C1-O2A-CGA | 2.16 | 122.99 | 116.73 |
| 25 | 4 | 615 | CLA | CHA-C1A-NA | -2.16 | 121.46 | 126.40 |
| 29 | G | 4001 | BCR | C36-C18-C17 | -2.16 | 119.90 | 122.92 |
| 29 | B | 4002 | BCR | C29-C28-C27 | 2.16 | 116.19 | 111.38 |
| 25 | 6 | 604 | CLA | O1D-CGD-CBD | -2.15 | 120.08 | 124.48 |
| 25 | 2 | 621 | CLA | CMD-C2D-C3D | -2.15 | 122.66 | 127.61 |
| 25 | 7 | 602 | CLA | CHA-C1A-NA | -2.15 | 121.47 | 126.40 |
| 25 | 6 | 602 | CLA | O2A-CGA-CBA | 2.15 | 118.67 | 111.91 |
| 25 | A | 1139 | CLA | O2A-CGA-CBA | 2.15 | 118.67 | 111.91 |
| 25 | A | 1137 | CLA | C1-O2A-CGA | 2.15 | 122.09 | 116.44 |
| 26 | 7 | 617 | CHL | CMB-C2B-C1B | -2.15 | 125.16 | 128.46 |
| 25 | A | 1137 | CLA | CMD-C2D-C3D | -2.15 | 122.66 | 127.61 |
| 29 | H | 4001 | BCR | C19-C18-C17 | 2.15 | 122.24 | 118.94 |
| 25 | A | 1101 | CLA | O1D-CGD-CBD | -2.15 | 120.08 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 610 | CLA | C1D-ND-C4D | -2.15 | 104.81 | 106.33 |
| 25 | a | 607 | CLA | CMD-C2D-C3D | -2.15 | 122.67 | 127.61 |
| 25 | 4 | 605 | CLA | CHA-C1A-NA | -2.15 | 121.47 | 126.40 |
| 25 | a | 601 | CLA | CAA-C2A-C3A | -2.15 | 106.89 | 112.78 |
| 43 | 2 | 502 | LUT | C30-C31-C32 | -2.15 | 116.50 | 123.22 |
| 25 | L | 1502 | CLA | C1-O2A-CGA | 2.15 | 122.09 | 116.44 |
| 25 | 5 | 609 | CLA | CMD-C2D-C3D | -2.15 | 122.67 | 127.61 |
| 25 | 3 | 601 | CLA | C1-O2A-CGA | 2.15 | 122.08 | 116.44 |
| 25 | A | 1128 | CLA | O1D-CGD-CBD | -2.15 | 120.09 | 124.48 |
| 29 | O | 4001 | BCR | C35-C13-C12 | 2.15 | 121.46 | 118.08 |
| 25 | A | 1104 | CLA | CMD-C2D-C3D | -2.15 | 122.67 | 127.61 |
| 25 | A | 1123 | CLA | O1D-CGD-CBD | -2.15 | 120.09 | 124.48 |
| 25 | J | 1901 | CLA | CHA-C1A-NA | -2.15 | 121.48 | 126.40 |
| 43 | 5 | 501 | LUT | C39-C29-C28 | 2.15 | 121.46 | 118.08 |
| 25 | 1 | 606 | CLA | CMB-C2B-C1B | -2.15 | 125.16 | 128.46 |
| 25 | 7 | 605 | CLA | C1D-ND-C4D | -2.15 | 104.81 | 106.33 |
| 26 | 1 | 610 | CHL | CHC-C1C-NC | 2.15 | 127.46 | 124.20 |
| 25 | a | 602 | CLA | O2A-CGA-CBA | 2.15 | 118.64 | 111.91 |
| 29 | 4 | 503 | BCR | C34-C9-C10 | -2.14 | 119.92 | 122.92 |
| 25 | B | 1237 | CLA | C1D-ND-C4D | -2.14 | 104.81 | 106.33 |
| 25 | B | 1239 | CLA | C1D-ND-C4D | -2.14 | 104.81 | 106.33 |
| 25 | 6 | 618 | CLA | C1D-ND-C4D | -2.14 | 104.81 | 106.33 |
| 25 | A | 1126 | CLA | CMB-C2B-C3B | 2.14 | 128.69 | 124.68 |
| 25 | 8 | 620 | CLA | CHA-C1A-NA | -2.14 | 121.49 | 126.40 |
| 25 | 6 | 603 | CLA | C1D-ND-C4D | -2.14 | 104.81 | 106.33 |
| 26 | 8 | 610 | CHL | CMB-C2B-C1B | -2.14 | 125.17 | 128.46 |
| 25 | A | 1138 | CLA | C1D-ND-C4D | -2.14 | 104.81 | 106.33 |
| 29 | L | 4002 | BCR | C38-C26-C27 | 2.14 | 117.73 | 113.62 |
| 41 | 4 | 805 | SPH | C3-C4-C5 | -2.14 | 120.02 | 124.79 |
| 26 | 6 | 610 | CHL | CHB-C4A-NA | 2.14 | 127.47 | 124.51 |
| 29 | 3 | 503 | BCR | C38-C26-C27 | 2.14 | 117.73 | 113.62 |
| 25 | B | 1021 | CLA | CHA-C1A-NA | -2.14 | 121.50 | 126.40 |
| 26 | a | 613 | CHL | CHD-C4C-C3C | 2.14 | 127.99 | 124.84 |
| 25 | 2 | 601 | CLA | O2A-CGA-CBA | 2.14 | 118.62 | 111.91 |
| 25 | A | 1115 | CLA | C1-O2A-CGA | 2.14 | 122.06 | 116.44 |
| 50 | 9 | 507 | XAT | C25-C24-C23 | -2.14 | 108.52 | 112.75 |
| 25 | 4 | 601 | CLA | CHA-C1A-NA | -2.14 | 121.50 | 126.40 |
| 25 | A | 1106 | CLA | CAA-C2A-C1A | -2.14 | 104.97 | 111.97 |
| 25 | B | 1216 | CLA | C1-O2A-CGA | 2.14 | 122.05 | 116.44 |
| 25 | A | 1102 | CLA | CHA-C1A-NA | -2.14 | 121.50 | 126.40 |
| 25 | 7 | 608 | CLA | O2A-CGA-CBA | 2.14 | 118.62 | 111.91 |
| 25 | 7 | 606 | CLA | CHA-C1A-NA | -2.14 | 121.50 | 126.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1123 | CLA | O2A-CGA-CBA | 2.14 | 118.61 | 111.91 |
| 25 | 2 | 608 | CLA | CMD-C2D-C3D | -2.14 | 122.70 | 127.61 |
| 25 | A | 1129 | CLA | CMA-C3A-C4A | 2.14 | 117.52 | 111.77 |
| 42 | M | 4001 | ECH | C37-C22-C23 | -2.14 | 114.71 | 118.08 |
| 25 | 5 | 608 | CLA | CMA-C3A-C4A | 2.14 | 117.51 | 111.77 |
| 25 | O | 1801 | CLA | C1D-ND-C4D | -2.14 | 104.82 | 106.33 |
| 25 | 4 | 605 | CLA | C1D-ND-C4D | -2.14 | 104.82 | 106.33 |
| 25 | B | 1236 | CLA | C3D-C2D-C1D | -2.14 | 102.92 | 105.83 |
| 29 | A | 4004 | BCR | C30-C25-C26 | -2.14 | 119.61 | 122.61 |
| 26 | 8 | 610 | CHL | CHD-C4C-C3C | 2.13 | 127.98 | 124.84 |
| 25 | 1 | 615 | CLA | CMD-C2D-C3D | -2.13 | 122.70 | 127.61 |
| 25 | A | 1103 | CLA | C1D-ND-C4D | -2.13 | 104.82 | 106.33 |
| 25 | B | 1207 | CLA | O2A-CGA-CBA | 2.13 | 118.60 | 111.91 |
| 25 | A | 1113 | CLA | CMB-C2B-C1B | -2.13 | 125.19 | 128.46 |
| 25 | B | 1204 | CLA | CAA-C2A-C3A | -2.13 | 106.94 | 112.78 |
| 25 | F | 1301 | CLA | O2A-CGA-CBA | 2.13 | 118.60 | 111.91 |
| 29 | A | 4001 | BCR | C34-C9-C10 | -2.13 | 119.94 | 122.92 |
| 26 | 7 | 609 | CHL | CMB-C2B-C1B | -2.13 | 125.19 | 128.46 |
| 25 | B | 1238 | CLA | O2A-CGA-CBA | 2.13 | 118.60 | 111.91 |
| 43 | 6 | 501 | LUT | C39-C29-C28 | 2.13 | 121.44 | 118.08 |
| 25 | B | 1022 | CLA | CMD-C2D-C3D | -2.13 | 122.71 | 127.61 |
| 25 | A | 1123 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 25 | A | 1109 | CLA | CMB-C2B-C3B | 2.13 | 128.67 | 124.68 |
| 26 | 3 | 608 | CHL | CMB-C2B-C1B | -2.13 | 125.19 | 128.46 |
| 25 | a | 612 | CLA | CMD-C2D-C3D | -2.13 | 122.71 | 127.61 |
| 25 | B | 1224 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 25 | 8 | 618 | CLA | C1D-ND-C4D | -2.13 | 104.82 | 106.33 |
| 26 | 8 | 604 | CHL | C1B-CHB-C4A | -2.13 | 125.90 | 130.12 |
| 25 | 8 | 605 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 43 | 6 | 502 | LUT | C39-C29-C28 | 2.13 | 121.43 | 118.08 |
| 25 | F | 1301 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 25 | A | 1133 | CLA | O2A-CGA-CBA | 2.13 | 118.59 | 111.91 |
| 25 | L | 1501 | CLA | O2A-CGA-CBA | 2.13 | 118.59 | 111.91 |
| 25 | A | 1012 | CLA | CMA-C3A-C4A | 2.13 | 117.50 | 111.77 |
| 25 | 8 | 609 | CLA | C3D-C2D-C1D | -2.13 | 102.93 | 105.83 |
| 25 | B | 1210 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 26 | 8 | 610 | CHL | CHC-C1C-NC | 2.13 | 127.43 | 124.20 |
| 25 | 4 | 616 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 43 | 6 | 501 | LUT | C31-C30-C29 | -2.13 | 124.27 | 127.31 |
| 26 | 1 | 604 | CHL | CMB-C2B-C1B | -2.13 | 125.19 | 128.46 |
| 25 | 3 | 616 | CLA | C1D-ND-C4D | -2.13 | 104.82 | 106.33 |
| 25 | 5 | 606 | CLA | C1D-ND-C4D | -2.13 | 104.82 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 5 | 614 | CLA | C1D-ND-C4D | -2.13 | 104.82 | 106.33 |
| 26 | a | 610 | CHL | CMB-C2B-C1B | -2.13 | 125.19 | 128.46 |
| 25 | A | 1112 | CLA | CMD-C2D-C3D | -2.13 | 122.72 | 127.61 |
| 25 | B | 1227 | CLA | CMD-C2D-C3D | -2.13 | 122.72 | 127.61 |
| 25 | A | 1135 | CLA | CHA-C1A-NA | -2.13 | 121.53 | 126.40 |
| 25 | 5 | 607 | CLA | C1D-ND-C4D | -2.13 | 104.83 | 106.33 |
| 26 | 9 | 613 | CHL | CMB-C2B-C1B | -2.13 | 125.20 | 128.46 |
| 25 | A | 1126 | CLA | O2D-CGD-O1D | -2.13 | 119.68 | 123.84 |
| 25 | B | 1230 | CLA | CAA-CBA-CGA | -2.13 | 107.04 | 113.25 |
| 43 | 4 | 502 | LUT | C11-C10-C9 | -2.12 | 124.28 | 127.31 |
| 25 | 1 | 607 | CLA | C1D-ND-C4D | -2.12 | 104.83 | 106.33 |
| 25 | A | 1127 | CLA | C1C-C2C-C3C | -2.12 | 104.72 | 106.96 |
| 25 | 9 | 612 | CLA | CAA-C2A-C3A | -2.12 | 106.96 | 112.78 |
| 25 | G | 1602 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 25 | 9 | 612 | CLA | C1-C2-C3 | -2.12 | 122.37 | 126.04 |
| 25 | 9 | 605 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 25 | 4 | 610 | CLA | CHA-C1A-NA | -2.12 | 121.53 | 126.40 |
| 25 | 6 | 602 | CLA | CMD-C2D-C3D | -2.12 | 122.73 | 127.61 |
| 26 | 4 | 618 | CHL | CMB-C2B-C1B | -2.12 | 125.20 | 128.46 |
| 25 | B | 1221 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 26 | 8 | 604 | CHL | C4D-CHA-C1A | 2.12 | 123.83 | 121.25 |
| 43 | 5 | 505 | LUT | C20-C13-C14 | -2.12 | 119.95 | 122.92 |
| 25 | 6 | 607 | CLA | O2A-CGA-CBA | 2.12 | 118.57 | 111.91 |
| 25 | 5 | 615 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 25 | 6 | 607 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 26 | 6 | 617 | CHL | CMB-C2B-C1B | -2.12 | 125.20 | 128.46 |
| 29 | 3 | 504 | BCR | C2-C1-C6 | 2.12 | 113.75 | 110.48 |
| 25 | 4 | 602 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 29 | 5 | 503 | BCR | C37-C22-C23 | 2.12 | 121.42 | 118.08 |
| 25 | A | 1111 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 43 | 1 | 501 | LUT | C8-C7-C6 | -2.12 | 121.25 | 127.20 |
| 26 | 7 | 611 | CHL | CMB-C2B-C1B | -2.12 | 125.20 | 128.46 |
| 43 | 9 | 501 | LUT | C38-C25-C24 | -2.12 | 119.02 | 123.56 |
| 25 | A | 1139 | CLA | C1D-ND-C4D | -2.12 | 104.83 | 106.33 |
| 25 | 2 | 621 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 26 | 1 | 609 | CHL | CMB-C2B-C1B | -2.12 | 125.21 | 128.46 |
| 26 | a | 606 | CHL | CMB-C2B-C1B | -2.12 | 125.21 | 128.46 |
| 25 | A | 1131 | CLA | CMD-C2D-C3D | -2.12 | 122.74 | 127.61 |
| 25 | A | 1111 | CLA | C1-O2A-CGA | 2.12 | 122.00 | 116.44 |
| 25 | 2 | 602 | CLA | CHA-C1A-NA | -2.12 | 121.55 | 126.40 |
| 44 | 1 | 502 | AXT | O3-C3-C4 | 2.12 | 114.22 | 109.68 |
| 25 | 4 | 612 | CLA | O2A-CGA-CBA | 2.12 | 118.56 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | A | 1113 | CLA | O1D-CGD-CBD | -2.12 | 120.15 | 124.48 |
| 25 | 8 | 609 | CLA | C1-O2A-CGA | 2.12 | 122.00 | 116.44 |
| 25 | A | 1134 | CLA | CHA-C1A-NA | -2.12 | 121.55 | 126.40 |
| 43 | 4 | 502 | LUT | C31-C32-C33 | -2.12 | 120.47 | 126.42 |
| 29 | H | 4001 | BCR | C38-C26-C25 | -2.12 | 122.15 | 124.53 |
| 26 | 7 | 613 | CHL | CMB-C2B-C1B | -2.12 | 125.21 | 128.46 |
| 25 | B | 1021 | CLA | C1D-ND-C4D | -2.12 | 104.83 | 106.33 |
| 25 | B | 1202 | CLA | CMD-C2D-C3D | -2.12 | 122.75 | 127.61 |
| 26 | 3 | 604 | CHL | CMB-C2B-C1B | -2.12 | 125.21 | 128.46 |
| 26 | 5 | 610 | CHL | CHD-C4C-C3C | 2.12 | 127.95 | 124.84 |
| 26 | 4 | 609 | CHL | CMB-C2B-C1B | -2.11 | 125.21 | 128.46 |
| 25 | 3 | 606 | CLA | C1D-ND-C4D | -2.11 | 104.83 | 106.33 |
| 25 | 3 | 613 | CLA | C1D-ND-C4D | -2.11 | 104.83 | 106.33 |
| 25 | 5 | 612 | CLA | C1D-ND-C4D | -2.11 | 104.83 | 106.33 |
| 25 | A | 1111 | CLA | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | 5 | 617 | CHL | CHD-C4C-C3C | 2.11 | 127.95 | 124.84 |
| 50 | 9 | 507 | XAT | C40-C33-C34 | -2.11 | 119.96 | 122.92 |
| 25 | 9 | 609 | CLA | CHA-C1A-NA | -2.11 | 121.56 | 126.40 |
| 25 | A | 1115 | CLA | O1D-CGD-CBD | -2.11 | 120.16 | 124.48 |
| 25 | B | 1212 | CLA | C1-O2A-CGA | 2.11 | 121.99 | 116.44 |
| 25 | 2 | 603 | CLA | C2A-C1A-CHA | 2.11 | 127.55 | 123.86 |
| 50 | 2 | 501 | XAT | C39-C29-C30 | -2.11 | 119.96 | 122.92 |
| 25 | L | 1503 | CLA | CHA-C1A-NA | -2.11 | 121.56 | 126.40 |
| 25 | 6 | 602 | CLA | CHA-C1A-NA | -2.11 | 121.56 | 126.40 |
| 25 | B | 1212 | CLA | C1D-ND-C4D | -2.11 | 104.83 | 106.33 |
| 25 | L | 1502 | CLA | C3D-C2D-C1D | -2.11 | 102.95 | 105.83 |
| 26 | 7 | 613 | CHL | C4D-CHA-C1A | 2.11 | 123.82 | 121.25 |
| 25 | 3 | 613 | CLA | CMD-C2D-C3D | -2.11 | 122.76 | 127.61 |
| 25 | K | 1402 | CLA | O2A-CGA-CBA | 2.11 | 118.53 | 111.91 |
| 26 | 6 | 611 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | 4 | 618 | CHL | C1-O2A-CGA | 2.11 | 121.98 | 116.44 |
| 25 | 3 | 618 | CLA | CMD-C2D-C3D | -2.11 | 122.76 | 127.61 |
| 26 | 1 | 611 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | a | 613 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | 5 | 611 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | 5 | 617 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 25 | 3 | 605 | CLA | CHA-C1A-NA | -2.11 | 121.57 | 126.40 |
| 25 | 5 | 602 | CLA | CHA-C1A-NA | -2.11 | 121.57 | 126.40 |
| 26 | 2 | 613 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 25 | 6 | 606 | CLA | C1D-ND-C4D | -2.11 | 104.84 | 106.33 |
| 26 | 4 | 613 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 29 | A | 4003 | BCR | C31-C1-C6 | -2.11 | 106.88 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | A | 1114 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | 2 | 610 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 25 | A | 1104 | CLA | C1-O2A-CGA | 2.11 | 121.97 | 116.44 |
| 39 | F | 4001 | NEX | C20-C13-C14 | -2.11 | 119.97 | 122.92 |
| 26 | 6 | 610 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 26 | 8 | 613 | CHL | CMB-C2B-C1B | -2.11 | 125.22 | 128.46 |
| 43 | 3 | 501 | LUT | C8-C7-C6 | -2.11 | 121.28 | 127.20 |
| 25 | B | 1230 | CLA | CMD-C2D-C3D | -2.11 | 122.77 | 127.61 |
| 25 | 7 | 604 | CLA | CMB-C2B-C3B | 2.11 | 128.62 | 124.68 |
| 25 | 5 | 615 | CLA | C3D-C2D-C1D | -2.11 | 102.96 | 105.83 |
| 25 | B | 1212 | CLA | CMD-C2D-C3D | -2.11 | 122.77 | 127.61 |
| 25 | 3 | 601 | CLA | CMD-C2D-C3D | -2.11 | 122.77 | 127.61 |
| 25 | a | 608 | CLA | O2A-CGA-CBA | 2.11 | 118.52 | 111.91 |
| 26 | 3 | 603 | CHL | CMB-C2B-C1B | -2.11 | 125.23 | 128.46 |
| 26 | 9 | 608 | CHL | CMB-C2B-C1B | -2.11 | 125.23 | 128.46 |
| 25 | 1 | 603 | CLA | C1D-ND-C4D | -2.11 | 104.84 | 106.33 |
| 25 | B | 1229 | CLA | C3D-C2D-C1D | -2.11 | 102.96 | 105.83 |
| 26 | 9 | 610 | CHL | CMB-C2B-C1B | -2.10 | 125.23 | 128.46 |
| 25 | B | 1225 | CLA | CMD-C2D-C3D | -2.10 | 122.77 | 127.61 |
| 25 | 9 | 607 | CLA | O2A-CGA-CBA | 2.10 | 118.51 | 111.91 |
| 25 | 2 | 606 | CLA | CHA-C1A-NA | -2.10 | 121.58 | 126.40 |
| 43 | a | 503 | LUT | C40-C33-C34 | -2.10 | 119.98 | 122.92 |
| 25 | 6 | 612 | CLA | C1D-ND-C4D | -2.10 | 104.84 | 106.33 |
| 25 | 5 | 609 | CLA | CHA-C1A-NA | -2.10 | 121.58 | 126.40 |
| 26 | a | 606 | CHL | CHD-C4C-C3C | 2.10 | 127.93 | 124.84 |
| 25 | 1 | 605 | CLA | O1D-CGD-CBD | -2.10 | 120.18 | 124.48 |
| 40 | J | 4002 | RRX | C34-C9-C10 | -2.10 | 119.98 | 122.92 |
| 25 | 4 | 604 | CLA | CMB-C2B-C3B | 2.10 | 128.61 | 124.68 |
| 26 | 4 | 609 | CHL | C1B-CHB-C4A | -2.10 | 125.95 | 130.12 |
| 25 | A | 1123 | CLA | CMB-C2B-C3B | 2.10 | 128.61 | 124.68 |
| 26 | 4 | 613 | CHL | CHB-C4A-NA | 2.10 | 127.42 | 124.51 |
| 25 | B | 1211 | CLA | CAA-C2A-C3A | -2.10 | 107.02 | 112.78 |
| 29 | A | 4002 | BCR | C34-C9-C10 | -2.10 | 119.98 | 122.92 |
| 25 | 4 | 602 | CLA | CMD-C2D-C3D | -2.10 | 122.78 | 127.61 |
| 25 | 5 | 608 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 25 | 5 | 612 | CLA | CMD-C2D-C3D | -2.10 | 122.78 | 127.61 |
| 25 | 7 | 608 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 25 | 2 | 612 | CLA | C1D-ND-C4D | -2.10 | 104.84 | 106.33 |
| 29 | 3 | 503 | BCR | C29-C28-C27 | 2.10 | 116.07 | 111.38 |
| 25 | 5 | 601 | CLA | CMB-C2B-C3B | 2.10 | 128.61 | 124.68 |
| 25 | 6 | 605 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 25 | 9 | 607 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | 4 | 609 | CHL | C4A-NA-C1A | 2.10 | 107.65 | 106.71 |
| 25 | 3 | 610 | CLA | O1D-CGD-CBD | -2.10 | 120.19 | 124.48 |
| 25 | A | 1101 | CLA | C3D-C2D-C1D | -2.10 | 102.97 | 105.83 |
| 25 | 6 | 605 | CLA | C1D-ND-C4D | -2.10 | 104.84 | 106.33 |
| 25 | 6 | 615 | CLA | CAA-CBA-CGA | -2.10 | 107.12 | 113.25 |
| 29 | 6 | 503 | BCR | C38-C26-C27 | 2.10 | 117.65 | 113.62 |
| 26 | 3 | 603 | CHL | C1-C2-C3 | -2.10 | 122.41 | 126.04 |
| 25 | B | 1206 | CLA | CMB-C2B-C1B | -2.10 | 125.24 | 128.46 |
| 25 | 8 | 602 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 25 | G | 1602 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 30 | A | 5002 | LHG | C5-O7-C7 | -2.10 | 112.63 | 117.79 |
| 25 | 2 | 605 | CLA | CHA-C1A-NA | -2.10 | 121.59 | 126.40 |
| 26 | 5 | 610 | CHL | CMB-C2B-C1B | -2.10 | 125.24 | 128.46 |
| 29 | 4 | 503 | BCR | C38-C26-C27 | 2.10 | 117.64 | 113.62 |
| 25 | 9 | 602 | CLA | CHA-C1A-NA | -2.10 | 121.60 | 126.40 |
| 25 | 6 | 608 | CLA | C1D-ND-C4D | -2.10 | 104.85 | 106.33 |
| 25 | 2 | 621 | CLA | C6-C5-C3 | -2.10 | 107.96 | 113.45 |
| 43 | a | 502 | LUT | C20-C13-C12 | 2.10 | 121.38 | 118.08 |
| 25 | 8 | 620 | CLA | C3D-C2D-C1D | -2.09 | 102.97 | 105.83 |
| 26 | a | 613 | CHL | C1B-CHB-C4A | -2.09 | 125.97 | 130.12 |
| 26 | 8 | 603 | CHL | CMB-C2B-C1B | -2.09 | 125.25 | 128.46 |
| 25 | 3 | 602 | CLA | C3D-C2D-C1D | -2.09 | 102.97 | 105.83 |
| 25 | 3 | 607 | CLA | CHA-C1A-NA | -2.09 | 121.60 | 126.40 |
| 25 | B | 1229 | CLA | O1D-CGD-CBD | -2.09 | 120.20 | 124.48 |
| 29 | A | 4004 | BCR | C34-C9-C8 | 2.09 | 121.38 | 118.08 |
| 25 | a | 607 | CLA | CHA-C1A-NA | -2.09 | 121.61 | 126.40 |
| 26 | 8 | 604 | CHL | CMB-C2B-C1B | -2.09 | 125.25 | 128.46 |
| 25 | B | 1201 | CLA | CMD-C2D-C3D | -2.09 | 122.80 | 127.61 |
| 25 | 4 | 607 | CLA | CMD-C2D-C3D | -2.09 | 122.80 | 127.61 |
| 25 | F | 1302 | CLA | CMD-C2D-C3D | -2.09 | 122.80 | 127.61 |
| 25 | A | 1132 | CLA | CMA-C3A-C4A | 2.09 | 117.39 | 111.77 |
| 25 | A | 1101 | CLA | CAA-C2A-C3A | -2.09 | 107.05 | 112.78 |
| 25 | 5 | 607 | CLA | CAA-C2A-C3A | -2.09 | 107.05 | 112.78 |
| 25 | A | 1125 | CLA | CHA-C1A-NA | -2.09 | 121.61 | 126.40 |
| 25 | A | 1126 | CLA | C3D-C2D-C1D | -2.09 | 102.98 | 105.83 |
| 25 | A | 1127 | CLA | O2A-CGA-CBA | 2.09 | 118.47 | 111.91 |
| 26 | a | 604 | CHL | CMB-C2B-C1B | -2.09 | 125.25 | 128.46 |
| 25 | A | 1106 | CLA | C3D-C2D-C1D | -2.09 | 102.98 | 105.83 |
| 25 | A | 1124 | CLA | C1D-ND-C4D | -2.09 | 104.85 | 106.33 |
| 25 | J | 1901 | CLA | C1D-ND-C4D | -2.09 | 104.85 | 106.33 |
| 25 | 3 | 612 | CLA | C1D-ND-C4D | -2.09 | 104.85 | 106.33 |
| 26 | 7 | 611 | CHL | C4D-CHA-C1A | 2.09 | 123.79 | 121.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | O | 1803 | CLA | CHA-C1A-NA | -2.09 | 121.62 | 126.40 |
| 25 | B | 1208 | CLA | O1D-CGD-CBD | -2.09 | 120.21 | 124.48 |
| 26 | 9 | 603 | CHL | CMB-C2B-C1B | -2.09 | 125.25 | 128.46 |
| 25 | A | 1013 | CLA | CHA-C1A-NA | -2.09 | 121.62 | 126.40 |
| 25 | B | 1214 | CLA | CHA-C1A-NA | -2.09 | 121.62 | 126.40 |
| 25 | A | 1133 | CLA | CMD-C2D-C3D | -2.09 | 122.81 | 127.61 |
| 25 | 6 | 608 | CLA | CAA-C2A-C3A | -2.09 | 107.06 | 112.78 |
| 25 | B | 1228 | CLA | C1-O2A-CGA | 2.09 | 121.92 | 116.44 |
| 29 | A | 4005 | BCR | C37-C22-C23 | 2.09 | 121.36 | 118.08 |
| 29 | L | 4002 | BCR | C38-C26-C25 | -2.09 | 122.19 | 124.53 |
| 29 | B | 4002 | BCR | C28-C27-C26 | -2.09 | 110.35 | 114.08 |
| 29 | 7 | 503 | BCR | C3-C4-C5 | -2.09 | 110.35 | 114.08 |
| 25 | B | 1201 | CLA | CHA-C1A-NA | -2.09 | 121.62 | 126.40 |
| 25 | 4 | 606 | CLA | O1D-CGD-CBD | -2.08 | 120.22 | 124.48 |
| 25 | B | 1240 | CLA | CMB-C2B-C3B | 2.08 | 128.58 | 124.68 |
| 47 | 6 | 804 | PLM | C3-C2-C1 | -2.08 | 109.22 | 114.47 |
| 26 | 5 | 618 | CHL | CMB-C2B-C1B | -2.08 | 125.26 | 128.46 |
| 43 | a | 502 | LUT | C2-C3-C4 | -2.08 | 107.45 | 110.30 |
| 29 | L | 4001 | BCR | C19-C18-C17 | 2.08 | 122.14 | 118.94 |
| 25 | A | 1104 | CLA | C1D-ND-C4D | -2.08 | 104.86 | 106.33 |
| 25 | K | 1403 | CLA | CHA-C1A-NA | -2.08 | 121.63 | 126.40 |
| 25 | 9 | 607 | CLA | CMD-C2D-C3D | -2.08 | 122.82 | 127.61 |
| 25 | B | 1210 | CLA | C6-C5-C3 | -2.08 | 107.99 | 113.45 |
| 25 | 5 | 612 | CLA | CAA-C2A-C3A | -2.08 | 107.07 | 112.78 |
| 25 | a | 602 | CLA | CMD-C2D-C3D | -2.08 | 122.82 | 127.61 |
| 24 | A | 1011 | CL0 | C4D-C3D-CAD | 2.08 | 110.55 | 108.10 |
| 25 | a | 608 | CLA | C1D-ND-C4D | -2.08 | 104.86 | 106.33 |
| 26 | 2 | 609 | CHL | CMB-C2B-C1B | -2.08 | 125.27 | 128.46 |
| 25 | B | 1204 | CLA | C3D-C2D-C1D | -2.08 | 102.99 | 105.83 |
| 44 | 7 | 504 | AXT | C35-C15-C14 | 2.08 | 127.74 | 123.47 |
| 25 | 6 | 601 | CLA | O2D-CGD-O1D | -2.08 | 119.77 | 123.84 |
| 25 | O | 1803 | CLA | C1D-ND-C4D | -2.08 | 104.86 | 106.33 |
| 25 | 4 | 616 | CLA | C1D-ND-C4D | -2.08 | 104.86 | 106.33 |
| 36 | 8 | 803 | DGD | O2G-C1B-O1B | -2.08 | 118.67 | 123.70 |
| 25 | 2 | 607 | CLA | CMD-C2D-C3D | -2.08 | 122.83 | 127.61 |
| 25 | B | 1210 | CLA | CMA-C3A-C4A | 2.08 | 117.36 | 111.77 |
| 25 | 3 | 618 | CLA | CHA-C1A-NA | -2.08 | 121.63 | 126.40 |
| 30 | a | 801 | LHG | C5-O7-C7 | -2.08 | 112.67 | 117.79 |
| 25 | 7 | 605 | CLA | CMB-C2B-C1B | -2.08 | 125.27 | 128.46 |
| 25 | H | 1703 | CLA | O2A-CGA-CBA | 2.08 | 118.43 | 111.91 |
| 25 | A | 1118 | CLA | CMD-C2D-C3D | -2.08 | 122.83 | 127.61 |
| 25 | B | 1217 | CLA | C3D-C2D-C1D | -2.08 | 102.99 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | a | 609 | CHL | CHC-C1C-NC | 2.08 | 127.36 | 124.20 |
| 25 | 8 | 611 | CLA | C1D-ND-C4D | -2.08 | 104.86 | 106.33 |
| 43 | 9 | 502 | LUT | C39-C29-C28 | 2.08 | 121.35 | 118.08 |
| 25 | 3 | 602 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | A | 1013 | CLA | CAA-C2A-C3A | -2.08 | 107.09 | 112.78 |
| 25 | B | 1218 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | 1 | 602 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | 9 | 604 | CLA | O1D-CGD-CBD | -2.08 | 120.23 | 124.48 |
| 25 | O | 1802 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | a | 611 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | 4 | 610 | CLA | C3D-C2D-C1D | -2.08 | 103.00 | 105.83 |
| 25 | 6 | 612 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | 1 | 605 | CLA | CAA-C2A-C1A | -2.08 | 105.17 | 111.97 |
| 25 | 3 | 610 | CLA | O2A-CGA-CBA | 2.08 | 118.42 | 111.91 |
| 25 | F | 1302 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 25 | B | 1234 | CLA | C1C-C2C-C3C | -2.07 | 104.13 | 106.51 |
| 25 | A | 1134 | CLA | C3D-C2D-C1D | -2.07 | 103.00 | 105.83 |
| 25 | 2 | 612 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 29 | L | 4001 | BCR | C38-C26-C25 | -2.07 | 122.20 | 124.53 |
| 25 | A | 1113 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 25 | 5 | 601 | CLA | CMA-C3A-C4A | 2.07 | 117.35 | 111.77 |
| 25 | 1 | 607 | CLA | O2A-CGA-CBA | 2.07 | 118.41 | 111.91 |
| 32 | 7 | 805 | SQD | O5-C1-O6 | -2.07 | 105.06 | 109.97 |
| 25 | a | 612 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 25 | 6 | 606 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 29 | K | 4002 | BCR | C23-C24-C25 | -2.07 | 121.38 | 127.20 |
| 44 | 7 | 504 | AXT | C11-C12-C13 | -2.07 | 120.59 | 126.42 |
| 25 | A | 1137 | CLA | C6-C5-C3 | -2.07 | 108.02 | 113.45 |
| 25 | 8 | 606 | CLA | O2A-CGA-CBA | 2.07 | 118.41 | 111.91 |
| 43 | 2 | 507 | LUT | C40-C33-C34 | -2.07 | 120.02 | 122.92 |
| 26 | 9 | 610 | CHL | CHD-C4C-C3C | 2.07 | 127.89 | 124.84 |
| 25 | 9 | 612 | CLA | CMD-C2D-C3D | -2.07 | 122.85 | 127.61 |
| 25 | 4 | 611 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 25 | 7 | 612 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 26 | 6 | 617 | CHL | C4A-NA-C1A | 2.07 | 107.64 | 106.71 |
| 25 | K | 1401 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 25 | B | 1240 | CLA | CMD-C2D-C3D | -2.07 | 122.85 | 127.61 |
| 24 | A | 1011 | CL0 | C3C-C4C-NC | 2.07 | 112.89 | 110.57 |
| 25 | O | 1801 | CLA | CMB-C2B-C3B | 2.07 | 128.55 | 124.68 |
| 25 | a | 601 | CLA | C3D-C2D-C1D | -2.07 | 103.01 | 105.83 |
| 26 | 3 | 611 | CHL | CMB-C2B-C1B | -2.07 | 125.28 | 128.46 |
| 25 | 6 | 606 | CLA | CAA-CBA-CGA | -2.07 | 107.21 | 113.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | A | 4005 | BCR | C38-C26-C27 | 2.07 | 117.59 | 113.62 |
| 25 | 4 | 615 | CLA | CMD-C2D-C3D | -2.07 | 122.86 | 127.61 |
| 25 | 2 | 606 | CLA | C1D-ND-C4D | -2.07 | 104.87 | 106.33 |
| 26 | 5 | 613 | CHL | C1B-CHB-C4A | -2.07 | 126.02 | 130.12 |
| 26 | 6 | 609 | CHL | CHC-C1C-NC | 2.07 | 127.34 | 124.20 |
| 25 | B | 1229 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 25 | 2 | 605 | CLA | C3D-C2D-C1D | -2.07 | 103.01 | 105.83 |
| 25 | 4 | 612 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 26 | a | 610 | CHL | CHC-C1C-NC | 2.07 | 127.34 | 124.20 |
| 25 | 4 | 612 | CLA | CMB-C2B-C3B | 2.07 | 128.54 | 124.68 |
| 25 | B | 1237 | CLA | O2A-CGA-CBA | 2.07 | 118.39 | 111.91 |
| 25 | O | 1802 | CLA | C3D-C2D-C1D | -2.06 | 103.01 | 105.83 |
| 25 | A | 1131 | CLA | CHA-C1A-NA | -2.06 | 121.67 | 126.40 |
| 26 | 6 | 617 | CHL | C1B-CHB-C4A | -2.06 | 126.03 | 130.12 |
| 26 | 4 | 613 | CHL | C1-O2A-CGA | 2.06 | 121.86 | 116.44 |
| 29 | 7 | 503 | BCR | C12-C13-C14 | -2.06 | 115.77 | 118.94 |
| 25 | 2 | 615 | CLA | C3D-C2D-C1D | -2.06 | 103.02 | 105.83 |
| 25 | A | 1109 | CLA | CHA-C1A-NA | -2.06 | 121.67 | 126.40 |
| 25 | K | 1404 | CLA | CHA-C1A-NA | -2.06 | 121.67 | 126.40 |
| 25 | 3 | 606 | CLA | O2A-CGA-CBA | 2.06 | 118.38 | 111.91 |
| 25 | 5 | 609 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 25 | B | 1219 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 25 | 5 | 601 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 25 | A | 1104 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 25 | A | 1119 | CLA | O2A-CGA-CBA | 2.06 | 118.37 | 111.91 |
| 25 | 2 | 608 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 25 | A | 1135 | CLA | O2A-CGA-CBA | 2.06 | 118.37 | 111.91 |
| 25 | B | 1211 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 25 | 4 | 617 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 25 | A | 1121 | CLA | CMB-C2B-C3B | 2.06 | 128.53 | 124.68 |
| 25 | 3 | 616 | CLA | CMD-C2D-C3D | -2.06 | 122.88 | 127.61 |
| 25 | A | 1132 | CLA | O2A-CGA-CBA | 2.06 | 118.37 | 111.91 |
| 25 | G | 1601 | CLA | C1-O2A-CGA | 2.06 | 121.84 | 116.44 |
| 29 | 3 | 504 | BCR | C33-C5-C4 | 2.06 | 117.57 | 113.62 |
| 29 | L | 4003 | BCR | C37-C22-C21 | -2.06 | 120.04 | 122.92 |
| 29 | 5 | 504 | BCR | C34-C9-C10 | -2.06 | 120.04 | 122.92 |
| 25 | 3 | 618 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 26 | 3 | 608 | CHL | CHC-C1C-NC | 2.06 | 127.33 | 124.20 |
| 25 | B | 1212 | CLA | C3D-C2D-C1D | -2.06 | 103.02 | 105.83 |
| 25 | 7 | 603 | CLA | C3D-C2D-C1D | -2.06 | 103.02 | 105.83 |
| 26 | 8 | 613 | CHL | C4A-NA-C1A | 2.06 | 107.63 | 106.71 |
| 25 | 5 | 614 | CLA | CMD-C2D-C3D | -2.06 | 122.88 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 4 | 608 | CLA | C1-O2A-CGA | 2.06 | 121.84 | 116.44 |
| 25 | 2 | 615 | CLA | CHA-C1A-NA | -2.06 | 121.69 | 126.40 |
| 43 | 1 | 501 | LUT | C39-C29-C28 | 2.06 | 121.32 | 118.08 |
| 25 | 8 | 609 | CLA | CMD-C2D-C3D | -2.06 | 122.89 | 127.61 |
| 43 | 4 | 501 | LUT | C40-C33-C34 | -2.06 | 120.04 | 122.92 |
| 26 | 5 | 617 | CHL | C1-O2A-CGA | 2.06 | 122.88 | 116.11 |
| 25 | B | 1210 | CLA | O1D-CGD-CBD | -2.06 | 120.28 | 124.48 |
| 25 | B | 1227 | CLA | CMB-C2B-C3B | 2.05 | 128.52 | 124.68 |
| 25 | B | 1229 | CLA | CAA-C2A-C3A | -2.05 | 107.15 | 112.78 |
| 42 | M | 4001 | ECH | C28-C29-C30 | -2.05 | 109.89 | 113.18 |
| 25 | H | 1701 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 26 | a | 606 | CHL | CHC-C1C-NC | 2.05 | 127.32 | 124.20 |
| 25 | 6 | 607 | CLA | C1D-ND-C4D | -2.05 | 104.88 | 106.33 |
| 25 | a | 605 | CLA | CMB-C2B-C1B | -2.05 | 125.31 | 128.46 |
| 25 | 6 | 615 | CLA | C3D-C2D-C1D | -2.05 | 103.03 | 105.83 |
| 25 | B | 1222 | CLA | O2A-CGA-CBA | 2.05 | 118.35 | 111.91 |
| 25 | B | 1228 | CLA | C1D-ND-C4D | -2.05 | 104.88 | 106.33 |
| 25 | B | 1219 | CLA | CMD-C2D-C3D | -2.05 | 122.90 | 127.61 |
| 29 | 5 | 504 | BCR | C23-C22-C21 | -2.05 | 115.79 | 118.94 |
| 29 | B | 4001 | BCR | C37-C22-C23 | 2.05 | 121.31 | 118.08 |
| 25 | 2 | 605 | CLA | C1-O2A-CGA | 2.05 | 121.82 | 116.44 |
| 26 | 8 | 601 | CHL | C3B-C4B-NB | -2.05 | 106.56 | 109.21 |
| 25 | B | 1210 | CLA | CAC-C3C-C4C | 2.05 | 127.47 | 124.81 |
| 25 | 7 | 607 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 25 | 8 | 607 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 25 | G | 1603 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 25 | A | 1109 | CLA | C1D-ND-C4D | -2.05 | 104.88 | 106.33 |
| 25 | B | 1216 | CLA | O2A-CGA-CBA | 2.05 | 118.34 | 111.91 |
| 25 | 3 | 613 | CLA | CHA-C1A-NA | -2.05 | 121.71 | 126.40 |
| 25 | A | 1130 | CLA | CHA-C1A-NA | -2.05 | 121.71 | 126.40 |
| 25 | A | 1126 | CLA | CHA-C1A-NA | -2.05 | 121.71 | 126.40 |
| 25 | 8 | 615 | CLA | CHA-C1A-NA | -2.05 | 121.71 | 126.40 |
| 26 | 7 | 609 | CHL | C4D-CHA-C1A | 2.05 | 123.74 | 121.25 |
| 25 | B | 1206 | CLA | CHA-C1A-NA | -2.05 | 121.71 | 126.40 |
| 30 | 2 | 802 | LHG | O7-C7-O9 | -2.05 | 118.76 | 123.70 |
| 25 | 7 | 608 | CLA | CMD-C2D-C3D | -2.05 | 122.91 | 127.61 |
| 25 | B | 1226 | CLA | CHA-C1A-NA | -2.04 | 121.72 | 126.40 |
| 25 | 1 | 612 | CLA | CHA-C1A-NA | -2.04 | 121.72 | 126.40 |
| 25 | K | 1404 | CLA | C3D-C2D-C1D | -2.04 | 103.04 | 105.83 |
| 29 | J | 4001 | BCR | C33-C5-C4 | 2.04 | 117.54 | 113.62 |
| 25 | A | 1119 | CLA | CMB-C2B-C1B | -2.04 | 125.32 | 128.46 |
| 29 | 3 | 505 | BCR | C28-C27-C26 | -2.04 | 110.43 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | B | 1204 | CLA | CMD-C2D-C3D | -2.04 | 122.91 | 127.61 |
| 25 | 5 | 615 | CLA | CMD-C2D-C3D | -2.04 | 122.91 | 127.61 |
| 25 | 8 | 620 | CLA | CMB-C2B-C3B | 2.04 | 128.50 | 124.68 |
| 25 | A | 1120 | CLA | CAA-C2A-C3A | -2.04 | 107.18 | 112.78 |
| 29 | K | 4001 | BCR | C35-C13-C12 | 2.04 | 121.30 | 118.08 |
| 25 | 7 | 606 | CLA | C1D-ND-C4D | -2.04 | 104.88 | 106.33 |
| 25 | B | 1217 | CLA | O1D-CGD-CBD | -2.04 | 120.31 | 124.48 |
| 25 | B | 1232 | CLA | C1D-ND-C4D | -2.04 | 104.89 | 106.33 |
| 25 | B | 1202 | CLA | C3D-C2D-C1D | -2.04 | 103.05 | 105.83 |
| 25 | 5 | 601 | CLA | CAA-C2A-C3A | -2.04 | 107.19 | 112.78 |
| 25 | A | 1137 | CLA | C3D-C2D-C1D | -2.04 | 103.05 | 105.83 |
| 26 | 9 | 608 | CHL | CHD-C4C-C3C | 2.04 | 127.84 | 124.84 |
| 29 | K | 4001 | BCR | C31-C1-C6 | -2.04 | 106.99 | 110.30 |
| 25 | 4 | 607 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 26 | a | 604 | CHL | CHB-C4A-NA | 2.04 | 127.33 | 124.51 |
| 29 | B | 4007 | BCR | C38-C26-C27 | 2.04 | 117.53 | 113.62 |
| 25 | B | 1239 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 43 | 5 | 501 | LUT | C20-C13-C12 | 2.04 | 121.29 | 118.08 |
| 25 | 9 | 605 | CLA | OBD-CAD-C3D | -2.04 | 123.62 | 128.52 |
| 29 | L | 4001 | BCR | C27-C26-C25 | -2.04 | 119.77 | 122.73 |
| 25 | B | 1236 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 25 | 9 | 606 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 25 | 8 | 605 | CLA | CAA-C2A-C3A | -2.04 | 107.20 | 112.78 |
| 25 | B | 1236 | CLA | CMD-C2D-C3D | -2.04 | 122.93 | 127.61 |
| 25 | B | 1204 | CLA | C1-O2A-CGA | 2.04 | 121.78 | 116.44 |
| 29 | A | 4004 | BCR | C8-C7-C6 | -2.04 | 121.49 | 127.20 |
| 25 | 6 | 604 | CLA | CHA-C1A-NA | -2.03 | 121.74 | 126.40 |
| 26 | 7 | 613 | CHL | CHC-C1C-NC | 2.03 | 127.29 | 124.20 |
| 25 | B | 1227 | CLA | O1D-CGD-CBD | -2.03 | 120.32 | 124.48 |
| 29 | 5 | 504 | BCR | C36-C18-C19 | 2.03 | 121.28 | 118.08 |
| 43 | 6 | 501 | LUT | C38-C25-C24 | -2.03 | 119.21 | 123.56 |
| 26 | 7 | 615 | CHL | CHD-C4C-C3C | 2.03 | 127.83 | 124.84 |
| 25 | 5 | 603 | CLA | CMB-C2B-C3B | 2.03 | 128.48 | 124.68 |
| 25 | 5 | 606 | CLA | CHA-C1A-NA | -2.03 | 121.74 | 126.40 |
| 25 | a | 603 | CLA | C1D-ND-C4D | -2.03 | 104.89 | 106.33 |
| 25 | 1 | 608 | CLA | CMB-C2B-C3B | 2.03 | 128.48 | 124.68 |
| 43 | a | 503 | LUT | C19-C9-C8 | 2.03 | 121.28 | 118.08 |
| 25 | 5 | 608 | CLA | C1D-ND-C4D | -2.03 | 104.89 | 106.33 |
| 25 | A | 1120 | CLA | O2A-CGA-CBA | 2.03 | 118.28 | 111.91 |
| 25 | 5 | 607 | CLA | CMD-C2D-C3D | -2.03 | 122.94 | 127.61 |
| 25 | B | 1224 | CLA | C3D-C2D-C1D | -2.03 | 103.06 | 105.83 |
| 25 | 9 | 602 | CLA | CMD-C2D-C3D | -2.03 | 122.94 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 8 | 608 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 25 | 1 | 606 | CLA | C1D-ND-C4D | -2.03 | 104.89 | 106.33 |
| 35 | 2 | 804 | LMT | O5B-C5B-C4B | 2.03 | 113.38 | 109.69 |
| 25 | 4 | 604 | CLA | O1D-CGD-CBD | -2.03 | 120.33 | 124.48 |
| 25 | A | 1127 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 25 | A | 1137 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 25 | 5 | 614 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 25 | G | 1601 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 25 | 8 | 611 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 25 | 5 | 605 | CLA | OBD-CAD-C3D | -2.03 | 123.64 | 128.52 |
| 25 | A | 1121 | CLA | O1D-CGD-CBD | -2.03 | 120.33 | 124.48 |
| 25 | 3 | 610 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 30 | B | 5001 | LHG | C5-O7-C7 | -2.03 | 112.80 | 117.79 |
| 26 | 9 | 601 | CHL | CHC-C1C-NC | 2.03 | 127.28 | 124.20 |
| 25 | 2 | 606 | CLA | CMB-C2B-C1B | -2.03 | 125.35 | 128.46 |
| 25 | 4 | 607 | CLA | C1D-ND-C4D | -2.03 | 104.89 | 106.33 |
| 26 | 8 | 603 | CHL | C1B-CHB-C4A | -2.03 | 126.10 | 130.12 |
| 25 | B | 1023 | CLA | C1-O2A-CGA | 2.03 | 121.76 | 116.44 |
| 25 | 5 | 605 | CLA | CHA-C1A-NA | -2.03 | 121.76 | 126.40 |
| 25 | A | 1140 | CLA | CHA-C1A-NA | -2.03 | 121.76 | 126.40 |
| 25 | L | 1503 | CLA | O1D-CGD-CBD | -2.03 | 120.34 | 124.48 |
| 25 | 8 | 615 | CLA | CMD-C2D-C3D | -2.03 | 122.95 | 127.61 |
| 25 | B | 1222 | CLA | C3D-C2D-C1D | -2.03 | 103.07 | 105.83 |
| 25 | B | 1228 | CLA | C3D-C2D-C1D | -2.03 | 103.07 | 105.83 |
| 43 | 6 | 501 | LUT | C8-C7-C6 | -2.03 | 121.51 | 127.20 |
| 25 | 7 | 610 | CLA | CHA-C1A-NA | -2.03 | 121.76 | 126.40 |
| 29 | 5 | 504 | BCR | C15-C14-C13 | -2.02 | 124.42 | 127.31 |
| 25 | A | 1124 | CLA | C3D-C2D-C1D | -2.02 | 103.07 | 105.83 |
| 25 | 6 | 604 | CLA | C3D-C2D-C1D | -2.02 | 103.07 | 105.83 |
| 44 | 1 | 502 | AXT | C30-C31-C32 | 2.02 | 129.53 | 123.22 |
| 25 | 6 | 607 | CLA | CMD-C2D-C3D | -2.02 | 122.96 | 127.61 |
| 25 | 5 | 612 | CLA | CBC-CAC-C3C | -2.02 | 106.85 | 112.43 |
| 25 | a | 602 | CLA | CHA-C1A-NA | -2.02 | 121.76 | 126.40 |
| 25 | H | 1702 | CLA | C3D-C2D-C1D | -2.02 | 103.07 | 105.83 |
| 25 | 9 | 607 | CLA | C3D-C2D-C1D | -2.02 | 103.07 | 105.83 |
| 25 | 4 | 601 | CLA | CAA-C2A-C3A | -2.02 | 107.24 | 112.78 |
| 25 | B | 1022 | CLA | C6-C5-C3 | -2.02 | 108.15 | 113.45 |
| 26 | 7 | 617 | CHL | C4D-CHA-C1A | 2.02 | 123.71 | 121.25 |
| 43 | 3 | 501 | LUT | C20-C13-C12 | 2.02 | 121.26 | 118.08 |
| 25 | 6 | 604 | CLA | CMC-C2C-C1C | 2.02 | 128.12 | 125.04 |
| 25 | B | 1225 | CLA | CHA-C1A-NA | -2.02 | 121.77 | 126.40 |
| 41 | 6 | 806 | SPH | C3-C4-C5 | -2.02 | 120.28 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | 3 | 601 | CLA | O2A-CGA-CBA | 2.02 | 118.25 | 111.91 |
| 25 | A | 1132 | CLA | CHA-C1A-NA | -2.02 | 121.77 | 126.40 |
| 25 | 3 | 613 | CLA | O2A-CGA-CBA | 2.02 | 118.25 | 111.91 |
| 25 | 4 | 608 | CLA | CMD-C2D-C3D | -2.02 | 122.97 | 127.61 |
| 25 | 2 | 602 | CLA | C1-O2A-CGA | 2.02 | 121.74 | 116.44 |
| 25 | 5 | 601 | CLA | O1D-CGD-CBD | -2.02 | 120.35 | 124.48 |
| 25 | B | 1213 | CLA | C3D-C2D-C1D | -2.02 | 103.08 | 105.83 |
| 25 | 7 | 608 | CLA | C1D-ND-C4D | -2.02 | 104.90 | 106.33 |
| 25 | A | 1107 | CLA | O1D-CGD-CBD | -2.02 | 120.35 | 124.48 |
| 43 | 1 | 501 | LUT | C30-C31-C32 | -2.02 | 116.92 | 123.22 |
| 25 | 5 | 607 | CLA | CHA-C1A-NA | -2.02 | 121.78 | 126.40 |
| 25 | A | 1135 | CLA | C3D-C2D-C1D | -2.02 | 103.08 | 105.83 |
| 25 | B | 1235 | CLA | C3D-C2D-C1D | -2.02 | 103.08 | 105.83 |
| 25 | 4 | 617 | CLA | C3D-C2D-C1D | -2.02 | 103.08 | 105.83 |
| 25 | 2 | 607 | CLA | C3D-C2D-C1D | -2.02 | 103.08 | 105.83 |
| 25 | A | 1125 | CLA | CMD-C2D-C3D | -2.02 | 122.98 | 127.61 |
| 29 | B | 4004 | BCR | C3-C4-C5 | -2.02 | 110.48 | 114.08 |
| 25 | B | 1240 | CLA | C1D-ND-C4D | -2.02 | 104.90 | 106.33 |
| 25 | G | 1601 | CLA | C1D-ND-C4D | -2.02 | 104.90 | 106.33 |
| 25 | 2 | 603 | CLA | C1D-ND-C4D | -2.02 | 104.90 | 106.33 |
| 25 | 4 | 603 | CLA | O2A-CGA-CBA | 2.02 | 118.23 | 111.91 |
| 25 | 2 | 607 | CLA | CHA-C1A-NA | -2.02 | 121.78 | 126.40 |
| 25 | A | 1120 | CLA | C1-O2A-CGA | 2.01 | 121.73 | 116.44 |
| 25 | A | 1115 | CLA | O2A-CGA-CBA | 2.01 | 118.23 | 111.91 |
| 25 | B | 1211 | CLA | CHA-C1A-NA | -2.01 | 121.78 | 126.40 |
| 29 | B | 4006 | BCR | C34-C9-C10 | -2.01 | 120.10 | 122.92 |
| 25 | 5 | 602 | CLA | O2A-CGA-CBA | 2.01 | 118.23 | 111.91 |
| 25 | 1 | 608 | CLA | CMD-C2D-C3D | -2.01 | 122.98 | 127.61 |
| 25 | A | 1138 | CLA | O2D-CGD-O1D | -2.01 | 119.90 | 123.84 |
| 25 | 4 | 612 | CLA | CMD-C2D-C3D | -2.01 | 122.98 | 127.61 |
| 25 | 4 | 607 | CLA | C1-O2A-CGA | 2.01 | 121.72 | 116.44 |
| 25 | O | 1801 | CLA | CHA-C1A-NA | -2.01 | 121.89 | 126.41 |
| 25 | B | 1239 | CLA | C3D-C2D-C1D | -2.01 | 103.08 | 105.83 |
| 25 | A | 1111 | CLA | CMA-C3A-C4A | 2.01 | 117.18 | 111.77 |
| 26 | 4 | 613 | CHL | C1B-CHB-C4A | -2.01 | 126.13 | 130.12 |
| 25 | K | 1402 | CLA | C1D-ND-C4D | -2.01 | 104.91 | 106.33 |
| 25 | 9 | 604 | CLA | C1-O2A-CGA | 2.01 | 121.72 | 116.44 |
| 25 | A | 1140 | CLA | C3D-C2D-C1D | -2.01 | 103.09 | 105.83 |
| 25 | L | 1502 | CLA | CMB-C2B-C3B | 2.01 | 128.44 | 124.68 |
| 25 | O | 1803 | CLA | C3D-C2D-C1D | -2.01 | 103.09 | 105.83 |
| 25 | A | 1141 | CLA | C3D-C2D-C1D | -2.01 | 103.09 | 105.83 |
| 26 | 4 | 618 | CHL | CHD-C4C-C3C | 2.01 | 127.79 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | L | 1501 | CLA | CMB-C2B-C3B | 2.01 | 128.44 | 124.68 |
| 25 | 3 | 616 | CLA | C3D-C2D-C1D | -2.01 | 103.09 | 105.83 |
| 25 | B | 1216 | CLA | CMB-C2B-C1B | -2.01 | 125.38 | 128.46 |
| 25 | A | 1136 | CLA | C3D-C2D-C1D | -2.01 | 103.09 | 105.83 |
| 25 | 8 | 618 | CLA | CHA-C1A-NA | -2.01 | 121.80 | 126.40 |
| 25 | B | 1232 | CLA | CHA-C1A-NA | -2.01 | 121.80 | 126.40 |
| 25 | 7 | 605 | CLA | CHA-C1A-NA | -2.01 | 121.80 | 126.40 |
| 25 | A | 1104 | CLA | C3D-C2D-C1D | -2.01 | 103.09 | 105.83 |
| 25 | B | 1234 | CLA | OBD-CAD-C3D | -2.01 | 123.69 | 128.52 |
| 29 | B | 4006 | BCR | C37-C22-C23 | 2.01 | 121.24 | 118.08 |
| 25 | a | 615 | CLA | CHA-C1A-NA | -2.01 | 121.81 | 126.40 |
| 25 | B | 1203 | CLA | C3D-C2D-C1D | -2.00 | 103.09 | 105.83 |
| 29 | B | 4007 | BCR | C15-C14-C13 | -2.00 | 124.45 | 127.31 |
| 25 | 8 | 606 | CLA | CHA-C1A-NA | -2.00 | 121.81 | 126.40 |
| 26 | 6 | 609 | CHL | C1-C2-C3 | -2.00 | 122.58 | 126.04 |
| 29 | 5 | 503 | BCR | C3-C4-C5 | -2.00 | 110.50 | 114.08 |
| 25 | K | 1402 | CLA | CMB-C2B-C3B | 2.00 | 128.43 | 124.68 |
| 27 | B | 2002 | PQN | C2M-C2-C3 | -2.00 | 121.13 | 124.40 |
| 25 | K | 1403 | CLA | C3D-C2D-C1D | -2.00 | 103.10 | 105.83 |
| 26 | 6 | 611 | CHL | C4A-NA-C1A | 2.00 | 107.61 | 106.71 |
| 25 | K | 1403 | CLA | C1D-ND-C4D | -2.00 | 104.91 | 106.33 |
| 25 | B | 1216 | CLA | CHA-C1A-NA | -2.00 | 121.81 | 126.40 |
| 25 | B | 1221 | CLA | CMB-C2B-C1B | -2.00 | 125.39 | 128.46 |
| 25 | G | 1603 | CLA | C3D-C2D-C1D | -2.00 | 103.10 | 105.83 |
| 25 | 9 | 602 | CLA | C3D-C2D-C1D | -2.00 | 103.10 | 105.83 |
| 29 | A | 4001 | BCR | C31-C1-C6 | -2.00 | 107.05 | 110.30 |
| 25 | B | 1212 | CLA | O2A-CGA-CBA | 2.00 | 118.19 | 111.91 |
| 43 | 2 | 507 | LUT | C28-C29-C30 | 2.00 | 122.01 | 118.94 |
| 25 | A | 1122 | CLA | C3D-C2D-C1D | -2.00 | 103.10 | 105.83 |
| 25 | G | 1601 | CLA | CMD-C2D-C3D | -2.00 | 123.01 | 127.61 |
| 25 | 1 | 605 | CLA | CBC-CAC-C3C | -2.00 | 106.92 | 112.43 |
| 25 | 1 | 612 | CLA | C3D-C2D-C1D | -2.00 | 103.10 | 105.83 |

All (394) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 24 | A | 1011 | CL0 | NA |
| 24 | A | 1011 | CL0 | NC |
| 24 | A | 1011 | CL0 | ND |
| 25 | A | 1012 | CLA | ND |
| 25 | A | 1013 | CLA | ND |
| 25 | A | 1102 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 25 | A | 1103 | CLA | ND |
| 25 | A | 1104 | CLA | ND |
| 25 | A | 1105 | CLA | ND |
| 25 | A | 1106 | CLA | ND |
| 25 | A | 1107 | CLA | ND |
| 25 | A | 1108 | CLA | ND |
| 25 | A | 1109 | CLA | ND |
| 25 | A | 1110 | CLA | ND |
| 25 | A | 1111 | CLA | ND |
| 25 | A | 1112 | CLA | ND |
| 25 | A | 1113 | CLA | ND |
| 25 | A | 1115 | CLA | ND |
| 25 | A | 1116 | CLA | ND |
| 25 | A | 1117 | CLA | ND |
| 25 | A | 1118 | CLA | ND |
| 25 | A | 1119 | CLA | ND |
| 25 | A | 1120 | CLA | ND |
| 25 | A | 1121 | CLA | ND |
| 25 | A | 1122 | CLA | ND |
| 25 | A | 1123 | CLA | ND |
| 25 | A | 1124 | CLA | ND |
| 25 | A | 1125 | CLA | ND |
| 25 | A | 1126 | CLA | ND |
| 25 | A | 1127 | CLA | ND |
| 25 | A | 1128 | CLA | ND |
| 25 | A | 1129 | CLA | ND |
| 25 | A | 1130 | CLA | ND |
| 25 | A | 1131 | CLA | ND |
| 25 | A | 1132 | CLA | ND |
| 25 | A | 1133 | CLA | ND |
| 25 | A | 1134 | CLA | ND |
| 25 | A | 1135 | CLA | ND |
| 25 | A | 1136 | CLA | ND |
| 25 | A | 1137 | CLA | ND |
| 25 | A | 1138 | CLA | ND |
| 25 | A | 1139 | CLA | ND |
| 25 | A | 1140 | CLA | ND |
| 25 | A | 1101 | CLA | ND |
| 25 | A | 1141 | CLA | ND |
| 25 | B | 1237 | CLA | ND |
| 25 | B | 1021 | CLA | ND |
| 25 | B | 1022 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 25 | B | 1023 | CLA | ND |
| 25 | B | 1201 | CLA | ND |
| 25 | B | 1202 | CLA | ND |
| 25 | B | 1203 | CLA | ND |
| 25 | B | 1204 | CLA | ND |
| 25 | B | 1205 | CLA | ND |
| 25 | B | 1206 | CLA | ND |
| 25 | B | 1208 | CLA | ND |
| 25 | B | 1209 | CLA | ND |
| 25 | B | 1210 | CLA | ND |
| 25 | B | 1211 | CLA | ND |
| 25 | B | 1212 | CLA | ND |
| 25 | B | 1213 | CLA | ND |
| 25 | B | 1214 | CLA | ND |
| 25 | B | 1215 | CLA | ND |
| 25 | B | 1216 | CLA | ND |
| 25 | B | 1217 | CLA | ND |
| 25 | B | 1218 | CLA | ND |
| 25 | B | 1219 | CLA | ND |
| 25 | B | 1220 | CLA | ND |
| 25 | B | 1221 | CLA | ND |
| 25 | B | 1222 | CLA | ND |
| 25 | B | 1223 | CLA | ND |
| 25 | B | 1224 | CLA | ND |
| 25 | B | 1225 | CLA | ND |
| 25 | B | 1226 | CLA | ND |
| 25 | B | 1227 | CLA | ND |
| 25 | B | 1228 | CLA | ND |
| 25 | B | 1229 | CLA | ND |
| 25 | B | 1230 | CLA | ND |
| 25 | B | 1231 | CLA | ND |
| 25 | B | 1232 | CLA | ND |
| 25 | B | 1235 | CLA | ND |
| 25 | B | 1236 | CLA | ND |
| 25 | B | 1238 | CLA | ND |
| 25 | B | 1239 | CLA | ND |
| 25 | B | 1240 | CLA | ND |
| 25 | B | 1207 | CLA | ND |
| 25 | F | 1301 | CLA | ND |
| 25 | F | 1302 | CLA | ND |
| 25 | G | 1601 | CLA | ND |
| 25 | G | 1602 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 25 | G | 1603 | CLA | ND |
| 25 | H | 1701 | CLA | ND |
| 25 | H | 1702 | CLA | ND |
| 25 | H | 1703 | CLA | ND |
| 25 | J | 1901 | CLA | ND |
| 25 | K | 1401 | CLA | ND |
| 25 | K | 1402 | CLA | ND |
| 25 | K | 1403 | CLA | ND |
| 25 | K | 1404 | CLA | ND |
| 25 | L | 1501 | CLA | ND |
| 25 | L | 1502 | CLA | ND |
| 25 | L | 1503 | CLA | ND |
| 25 | L | 1504 | CLA | ND |
| 25 | O | 1801 | CLA | ND |
| 25 | O | 1802 | CLA | ND |
| 25 | O | 1803 | CLA | ND |
| 25 | 1 | 601 | CLA | ND |
| 25 | 1 | 602 | CLA | ND |
| 25 | 1 | 603 | CLA | ND |
| 25 | 1 | 605 | CLA | ND |
| 25 | 1 | 606 | CLA | ND |
| 25 | 1 | 607 | CLA | ND |
| 25 | 1 | 608 | CLA | ND |
| 25 | 1 | 612 | CLA | ND |
| 25 | 1 | 615 | CLA | ND |
| 25 | a | 601 | CLA | ND |
| 25 | a | 602 | CLA | ND |
| 25 | a | 603 | CLA | ND |
| 25 | a | 605 | CLA | ND |
| 25 | a | 607 | CLA | ND |
| 25 | a | 608 | CLA | ND |
| 25 | a | 611 | CLA | ND |
| 25 | a | 612 | CLA | ND |
| 25 | a | 615 | CLA | ND |
| 25 | 3 | 601 | CLA | ND |
| 25 | 3 | 602 | CLA | ND |
| 25 | 3 | 605 | CLA | ND |
| 25 | 3 | 606 | CLA | ND |
| 25 | 3 | 607 | CLA | ND |
| 25 | 3 | 610 | CLA | ND |
| 25 | 3 | 612 | CLA | ND |
| 25 | 3 | 613 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 25 | 3 | 618 | CLA | ND |
| 25 | 3 | 616 | CLA | ND |
| 25 | 4 | 601 | CLA | ND |
| 25 | 4 | 602 | CLA | ND |
| 25 | 4 | 603 | CLA | ND |
| 25 | 4 | 604 | CLA | ND |
| 25 | 4 | 605 | CLA | ND |
| 25 | 4 | 606 | CLA | ND |
| 25 | 4 | 607 | CLA | ND |
| 25 | 4 | 608 | CLA | ND |
| 25 | 4 | 610 | CLA | ND |
| 25 | 4 | 611 | CLA | ND |
| 25 | 4 | 612 | CLA | ND |
| 25 | 4 | 615 | CLA | ND |
| 25 | 4 | 616 | CLA | ND |
| 25 | 4 | 617 | CLA | ND |
| 25 | 5 | 601 | CLA | ND |
| 25 | 5 | 602 | CLA | ND |
| 25 | 5 | 603 | CLA | ND |
| 25 | 5 | 604 | CLA | ND |
| 25 | 5 | 605 | CLA | ND |
| 25 | 5 | 606 | CLA | ND |
| 25 | 5 | 607 | CLA | ND |
| 25 | 5 | 608 | CLA | ND |
| 25 | 5 | 609 | CLA | ND |
| 25 | 5 | 612 | CLA | ND |
| 25 | 5 | 614 | CLA | ND |
| 25 | 5 | 615 | CLA | ND |
| 25 | 6 | 608 | CLA | ND |
| 25 | 6 | 601 | CLA | ND |
| 25 | 6 | 602 | CLA | ND |
| 25 | 6 | 603 | CLA | ND |
| 25 | 6 | 604 | CLA | ND |
| 25 | 6 | 605 | CLA | ND |
| 25 | 6 | 606 | CLA | ND |
| 25 | 6 | 607 | CLA | ND |
| 25 | 6 | 612 | CLA | ND |
| 25 | 6 | 615 | CLA | ND |
| 25 | 6 | 618 | CLA | ND |
| 25 | 7 | 601 | CLA | ND |
| 25 | 7 | 602 | CLA | ND |
| 25 | 7 | 603 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 25 | 7 | 604 | CLA | ND |
| 25 | 7 | 605 | CLA | ND |
| 25 | 7 | 606 | CLA | ND |
| 25 | 7 | 607 | CLA | ND |
| 25 | 7 | 608 | CLA | ND |
| 25 | 7 | 610 | CLA | ND |
| 25 | 7 | 612 | CLA | ND |
| 25 | 8 | 602 | CLA | ND |
| 25 | 8 | 605 | CLA | ND |
| 25 | 8 | 606 | CLA | ND |
| 25 | 8 | 607 | CLA | ND |
| 25 | 8 | 608 | CLA | ND |
| 25 | 8 | 609 | CLA | ND |
| 25 | 8 | 611 | CLA | ND |
| 25 | 8 | 612 | CLA | ND |
| 25 | 8 | 615 | CLA | ND |
| 25 | 8 | 618 | CLA | ND |
| 25 | 8 | 620 | CLA | ND |
| 25 | 2 | 601 | CLA | ND |
| 25 | 2 | 602 | CLA | ND |
| 25 | 2 | 603 | CLA | ND |
| 25 | 2 | 604 | CLA | ND |
| 25 | 2 | 605 | CLA | ND |
| 25 | 2 | 606 | CLA | ND |
| 25 | 2 | 607 | CLA | ND |
| 25 | 2 | 608 | CLA | ND |
| 25 | 2 | 612 | CLA | ND |
| 25 | 2 | 615 | CLA | ND |
| 25 | 2 | 621 | CLA | ND |
| 25 | 9 | 602 | CLA | ND |
| 25 | 9 | 604 | CLA | ND |
| 25 | 9 | 605 | CLA | ND |
| 25 | 9 | 606 | CLA | ND |
| 25 | 9 | 607 | CLA | ND |
| 25 | 9 | 609 | CLA | ND |
| 25 | 9 | 612 | CLA | ND |
| 26 | A | 1114 | CHL | NA |
| 26 | A | 1114 | CHL | NC |
| 26 | A | 1114 | CHL | ND |
| 26 | A | 1114 | CHL | C8 |
| 26 | 1 | 604 | CHL | NA |
| 26 | 1 | 604 | CHL | NC |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 26 | 1 | 604 | CHL | ND |
| 26 | 1 | 604 | CHL | C8 |
| 26 | 1 | 610 | CHL | NA |
| 26 | 1 | 610 | CHL | NC |
| 26 | 1 | 610 | CHL | ND |
| 26 | 1 | 611 | CHL | NA |
| 26 | 1 | 611 | CHL | NC |
| 26 | 1 | 611 | CHL | ND |
| 26 | 1 | 611 | CHL | C8 |
| 26 | 1 | 613 | CHL | NA |
| 26 | 1 | 613 | CHL | NC |
| 26 | 1 | 613 | CHL | ND |
| 26 | 1 | 609 | CHL | NA |
| 26 | 1 | 609 | CHL | NC |
| 26 | 1 | 609 | CHL | ND |
| 26 | 1 | 609 | CHL | C8 |
| 26 | a | 604 | CHL | NA |
| 26 | a | 604 | CHL | NC |
| 26 | a | 604 | CHL | ND |
| 26 | a | 604 | CHL | C8 |
| 26 | a | 606 | CHL | NA |
| 26 | a | 606 | CHL | NC |
| 26 | a | 606 | CHL | ND |
| 26 | a | 606 | CHL | C8 |
| 26 | a | 609 | CHL | NA |
| 26 | a | 609 | CHL | NC |
| 26 | a | 609 | CHL | ND |
| 26 | a | 610 | CHL | NA |
| 26 | a | 610 | CHL | NC |
| 26 | a | 610 | CHL | ND |
| 26 | a | 613 | CHL | NA |
| 26 | a | 613 | CHL | NC |
| 26 | a | 613 | CHL | ND |
| 26 | 3 | 603 | CHL | NA |
| 26 | 3 | 603 | CHL | NC |
| 26 | 3 | 603 | CHL | ND |
| 26 | 3 | 603 | CHL | C8 |
| 26 | 3 | 604 | CHL | NA |
| 26 | 3 | 604 | CHL | NC |
| 26 | 3 | 604 | CHL | ND |
| 26 | 3 | 604 | CHL | C8 |
| 26 | 3 | 608 | CHL | NA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 26 | 3 | 608 | CHL | NC |
| 26 | 3 | 608 | CHL | ND |
| 26 | 3 | 611 | CHL | NA |
| 26 | 3 | 611 | CHL | NC |
| 26 | 3 | 611 | CHL | ND |
| 26 | 3 | 611 | CHL | C8 |
| 26 | 4 | 613 | CHL | NA |
| 26 | 4 | 613 | CHL | NC |
| 26 | 4 | 613 | CHL | ND |
| 26 | 4 | 618 | CHL | NA |
| 26 | 4 | 618 | CHL | NC |
| 26 | 4 | 618 | CHL | ND |
| 26 | 4 | 618 | CHL | C8 |
| 26 | 4 | 609 | CHL | NA |
| 26 | 4 | 609 | CHL | NC |
| 26 | 4 | 609 | CHL | ND |
| 26 | 4 | 609 | CHL | C8 |
| 26 | 5 | 610 | CHL | NA |
| 26 | 5 | 610 | CHL | NC |
| 26 | 5 | 610 | CHL | ND |
| 26 | 5 | 610 | CHL | C8 |
| 26 | 5 | 611 | CHL | NA |
| 26 | 5 | 611 | CHL | NC |
| 26 | 5 | 611 | CHL | ND |
| 26 | 5 | 613 | CHL | NA |
| 26 | 5 | 613 | CHL | NC |
| 26 | 5 | 613 | CHL | ND |
| 26 | 5 | 613 | CHL | C8 |
| 26 | 5 | 617 | CHL | NA |
| 26 | 5 | 617 | CHL | NC |
| 26 | 5 | 617 | CHL | ND |
| 26 | 5 | 618 | CHL | NA |
| 26 | 5 | 618 | CHL | NC |
| 26 | 5 | 618 | CHL | ND |
| 26 | 6 | 609 | CHL | NA |
| 26 | 6 | 609 | CHL | NC |
| 26 | 6 | 609 | CHL | ND |
| 26 | 6 | 609 | CHL | C8 |
| 26 | 6 | 610 | CHL | NA |
| 26 | 6 | 610 | CHL | NC |
| 26 | 6 | 610 | CHL | ND |
| 26 | 6 | 610 | CHL | C8 |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 26 | 6 | 611 | CHL | NA |
| 26 | 6 | 611 | CHL | NC |
| 26 | 6 | 611 | CHL | ND |
| 26 | 6 | 613 | CHL | NA |
| 26 | 6 | 613 | CHL | NC |
| 26 | 6 | 613 | CHL | ND |
| 26 | 6 | 617 | CHL | NA |
| 26 | 6 | 617 | CHL | NC |
| 26 | 6 | 617 | CHL | ND |
| 26 | 6 | 619 | CHL | C3A |
| 26 | 6 | 619 | CHL | ND |
| 26 | 6 | 619 | CHL | C8 |
| 26 | 6 | 619 | CHL | NA |
| 26 | 6 | 619 | CHL | NC |
| 26 | 7 | 609 | CHL | NA |
| 26 | 7 | 609 | CHL | NC |
| 26 | 7 | 609 | CHL | ND |
| 26 | 7 | 609 | CHL | C8 |
| 26 | 7 | 611 | CHL | NA |
| 26 | 7 | 611 | CHL | NC |
| 26 | 7 | 611 | CHL | ND |
| 26 | 7 | 611 | CHL | C8 |
| 26 | 7 | 613 | CHL | NA |
| 26 | 7 | 613 | CHL | NC |
| 26 | 7 | 613 | CHL | ND |
| 26 | 7 | 613 | CHL | C8 |
| 26 | 7 | 615 | CHL | NA |
| 26 | 7 | 615 | CHL | NC |
| 26 | 7 | 615 | CHL | ND |
| 26 | 7 | 617 | CHL | NA |
| 26 | 7 | 617 | CHL | NC |
| 26 | 7 | 617 | CHL | ND |
| 26 | 7 | 617 | CHL | C8 |
| 26 | 8 | 601 | CHL | NA |
| 26 | 8 | 601 | CHL | NC |
| 26 | 8 | 601 | CHL | ND |
| 26 | 8 | 601 | CHL | C8 |
| 26 | 8 | 603 | CHL | NA |
| 26 | 8 | 603 | CHL | NC |
| 26 | 8 | 603 | CHL | ND |
| 26 | 8 | 603 | CHL | C8 |
| 26 | 8 | 604 | CHL | NA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 26 | 8 | 604 | CHL | NC |
| 26 | 8 | 604 | CHL | ND |
| 26 | 8 | 604 | CHL | C8 |
| 26 | 8 | 610 | CHL | C3A |
| 26 | 8 | 610 | CHL | ND |
| 26 | 8 | 610 | CHL | C8 |
| 26 | 8 | 610 | CHL | NA |
| 26 | 8 | 610 | CHL | NC |
| 26 | 8 | 613 | CHL | NA |
| 26 | 8 | 613 | CHL | NC |
| 26 | 8 | 613 | CHL | ND |
| 26 | 2 | 609 | CHL | NA |
| 26 | 2 | 609 | CHL | NC |
| 26 | 2 | 609 | CHL | ND |
| 26 | 2 | 609 | CHL | C8 |
| 26 | 2 | 610 | CHL | NA |
| 26 | 2 | 610 | CHL | NC |
| 26 | 2 | 610 | CHL | C3A |
| 26 | 2 | 610 | CHL | ND |
| 26 | 2 | 613 | CHL | NA |
| 26 | 2 | 613 | CHL | NC |
| 26 | 2 | 613 | CHL | ND |
| 26 | 9 | 601 | CHL | NA |
| 26 | 9 | 601 | CHL | NC |
| 26 | 9 | 601 | CHL | ND |
| 26 | 9 | 601 | CHL | C8 |
| 26 | 9 | 603 | CHL | NA |
| 26 | 9 | 603 | CHL | NC |
| 26 | 9 | 603 | CHL | ND |
| 26 | 9 | 603 | CHL | C8 |
| 26 | 9 | 608 | CHL | NA |
| 26 | 9 | 608 | CHL | NC |
| 26 | 9 | 608 | CHL | ND |
| 26 | 9 | 610 | CHL | NA |
| 26 | 9 | 610 | CHL | NC |
| 26 | 9 | 610 | CHL | ND |
| 26 | 9 | 613 | CHL | NA |
| 26 | 9 | 613 | CHL | NC |
| 26 | 9 | 613 | CHL | ND |
| 39 | F | 4001 | NEX | C25 |
| 40 | J | 4002 | RRX | C28 |
| 40 | 3 | 506 | RRX | C28 |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 43 | 4 | 501 | LUT | C26 |
| 43 | 7 | 501 | LUT | C26 |
| 43 | 2 | 507 | LUT | C26 |
| 46 | a | 504 | QTB | C12 |
| 50 | 7 | 502 | XAT | C26 |
| 50 | 7 | 502 | XAT | C6 |
| 50 | 2 | 501 | XAT | C26 |
| 50 | 2 | 501 | XAT | C6 |
| 50 | 9 | 504 | XAT | C6 |
| 50 | 9 | 507 | XAT | C26 |

All (4852) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1102 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1102 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1103 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1103 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1103 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1103 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1106 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1108 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1108 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1108 | CLA | C4-C3-C5-C6 |
| 25 | A | 1109 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1109 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1111 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1111 | CLA | C2-C3-C5-C6 |
| 25 | A | 1111 | CLA | C4-C3-C5-C6 |
| 25 | A | 1111 | CLA | C11-C10-C8-C9 |
| 25 | A | 1113 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1115 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1115 | CLA | C4-C3-C5-C6 |
| 25 | A | 1116 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1116 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1116 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1117 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1117 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1118 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1118 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1118 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1118 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1119 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1119 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1119 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1121 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1122 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1122 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1122 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1123 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1125 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1125 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1125 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1125 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1125 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1126 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1126 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1126 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1126 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1126 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1127 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1128 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1128 | CLA | C6-C7-C8-C9 |
| 25 | A | 1129 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1130 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1130 | CLA | C2-C3-C5-C6 |
| 25 | A | 1130 | CLA | C4-C3-C5-C6 |
| 25 | A | 1131 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1131 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1131 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1132 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1132 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1133 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1136 | CLA | C2-C3-C5-C6 |
| 25 | A | 1136 | CLA | C4-C3-C5-C6 |
| 25 | A | 1137 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1137 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1137 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1138 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1138 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1139 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1139 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1139 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1140 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1140 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1140 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1101 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1101 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1101 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1141 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1141 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1141 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1141 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 1237 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1021 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1021 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1021 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1022 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1023 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1023 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1023 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1023 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1201 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1201 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1202 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1202 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1202 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1202 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 1203 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1203 | CLA | C6-C7-C8-C9 |
| 25 | B | 1204 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1204 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1205 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1206 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1208 | CLA | C2-C3-C5-C6 |
| 25 | B | 1208 | CLA | C4-C3-C5-C6 |
| 25 | B | 1210 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1210 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1214 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1214 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1215 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1215 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1216 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1216 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1216 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1217 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1217 | CLA | C4-C3-C5-C6 |
| 25 | B | 1218 | CLA | C2-C3-C5-C6 |
| 25 | B | 1218 | CLA | C4-C3-C5-C6 |
| 25 | B | 1220 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1220 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1220 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1220 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1220 | CLA | C2-C3-C5-C6 |
| 25 | B | 1220 | CLA | C4-C3-C5-C6 |
| 25 | B | 1222 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1222 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1223 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1224 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1224 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1224 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1224 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1225 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1225 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1228 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1228 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1228 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1228 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1230 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1231 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1232 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1232 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1234 | CLA | C6-C7-C8-C9 |
| 25 | B | 1235 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1235 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1235 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 1235 | CLA | C2-C3-C5-C6 |
| 25 | B | 1235 | CLA | C4-C3-C5-C6 |
| 25 | B | 1236 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1238 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1239 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1239 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1239 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1207 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1207 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1207 | CLA | C11-C10-C8-C9 |
| 25 | F | 1301 | CLA | CHA-CBD-CGD-O1D |
| 25 | F | 1301 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | F | 1301 | CLA | CBD-CGD-O2D-CED |
| 25 | F | 1302 | CLA | CBD-CGD-O2D-CED |
| 25 | G | 1601 | CLA | CBD-CGD-O2D-CED |
| 25 | G | 1602 | CLA | CBA-CGA-O2A-C1 |
| 25 | G | 1602 | CLA | O1A-CGA-O2A-C1 |
| 25 | G | 1602 | CLA | CHA-CBD-CGD-O1D |
| 25 | G | 1602 | CLA | CHA-CBD-CGD-O2D |
| 25 | G | 1602 | CLA | CBD-CGD-O2D-CED |
| 25 | G | 1603 | CLA | C1A-C2A-CAA-CBA |
| 25 | G | 1603 | CLA | C3A-C2A-CAA-CBA |
| 25 | G | 1603 | CLA | C2A-CAA-CBA-CGA |
| 25 | G | 1603 | CLA | CBD-CGD-O2D-CED |
| 25 | H | 1701 | CLA | CHA-CBD-CGD-O1D |
| 25 | H | 1701 | CLA | CHA-CBD-CGD-O2D |
| 25 | H | 1702 | CLA | CHA-CBD-CGD-O1D |
| 25 | H | 1702 | CLA | CHA-CBD-CGD-O2D |
| 25 | H | 1703 | CLA | C2-C3-C5-C6 |
| 25 | H | 1703 | CLA | C4-C3-C5-C6 |
| 25 | J | 1901 | CLA | C1A-C2A-CAA-CBA |
| 25 | J | 1901 | CLA | C3A-C2A-CAA-CBA |
| 25 | J | 1901 | CLA | CHA-CBD-CGD-O1D |
| 25 | J | 1901 | CLA | CHA-CBD-CGD-O2D |
| 25 | J | 1901 | CLA | CBD-CGD-O2D-CED |
| 25 | K | 1401 | CLA | CHA-CBD-CGD-O1D |
| 25 | K | 1401 | CLA | CHA-CBD-CGD-O2D |
| 25 | K | 1401 | CLA | CBD-CGD-O2D-CED |
| 25 | K | 1403 | CLA | CHA-CBD-CGD-O1D |
| 25 | K | 1403 | CLA | CHA-CBD-CGD-O2D |
| 25 | K | 1403 | CLA | CAD-CBD-CGD-O1D |
| 25 | K | 1403 | CLA | CAD-CBD-CGD-O2D |
| 25 | K | 1404 | CLA | CAD-CBD-CGD-O1D |
| 25 | L | 1501 | CLA | CHA-CBD-CGD-O1D |
| 25 | L | 1503 | CLA | C3A-C2A-CAA-CBA |
| 25 | 1 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 605 | CLA | C2-C1-O2A-CGA |
| 25 | 1 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 606 | CLA | C3A-C2A-CAA-CBA |
| 25 | 1 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 1 | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | 1 | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | 1 | 608 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 612 | CLA | C3A-C2A-CAA-CBA |
| 25 | 1 | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 1 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 1 | 615 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 615 | CLA | C3A-C2A-CAA-CBA |
| 25 | a | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 602 | CLA | C2-C1-O2A-CGA |
| 25 | a | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 608 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 608 | CLA | C3A-C2A-CAA-CBA |
| 25 | a | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | a | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | a | 611 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 611 | CLA | C3A-C2A-CAA-CBA |
| 25 | a | 611 | CLA | C2-C1-O2A-CGA |
| 25 | a | 611 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 612 | CLA | C3A-C2A-CAA-CBA |
| 25 | a | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 3 | 601 | CLA | C3A-C2A-CAA-CBA |
| 25 | 3 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 3 | 606 | CLA | C3A-C2A-CAA-CBA |
| 25 | 3 | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | 3 | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | 3 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | 3 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 3 | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | 3 | 612 | CLA | C1A-C2A-CAA-CBA |
| 25 | 3 | 612 | CLA | C3A-C2A-CAA-CBA |
| 25 | 3 | 612 | CLA | C2A-CAA-CBA-CGA |
| 25 | 3 | 613 | CLA | C6-C7-C8-C9 |
| 25 | 3 | 618 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 616 | CLA | C2-C3-C5-C6 |
| 25 | 3 | 616 | CLA | C4-C3-C5-C6 |
| 25 | 4 | 601 | CLA | C2-C3-C5-C6 |
| 25 | 4 | 601 | CLA | C4-C3-C5-C6 |
| 25 | 4 | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | 4 | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | 4 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 608 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 4 | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | 4 | 610 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 611 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 4 | 612 | CLA | C2-C3-C5-C6 |
| 25 | 4 | 612 | CLA | C4-C3-C5-C6 |
| 25 | 4 | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 603 | CLA | C4-C3-C5-C6 |
| 25 | 5 | 603 | CLA | C11-C10-C8-C7 |
| 25 | 5 | 604 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 604 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 5 | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 608 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 609 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 609 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 609 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 614 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 615 | CLA | C1A-C2A-CAA-CBA |
| 25 | 6 | 608 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | 6 | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | 6 | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 604 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 605 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 612 | CLA | C1A-C2A-CAA-CBA |
| 25 | 6 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 618 | CLA | CHA-CBD-CGD-O1D |
| 25 | 6 | 618 | CLA | CHA-CBD-CGD-O2D |
| 25 | 6 | 618 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 602 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 7 | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | 7 | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | 7 | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | 7 | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | 7 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 7 | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | 7 | 610 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 7 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 605 | CLA | C3A-C2A-CAA-CBA |
| 25 | 8 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 606 | CLA | C2-C3-C5-C6 |
| 25 | 8 | 606 | CLA | C4-C3-C5-C6 |
| 25 | 8 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 612 | CLA | C3A-C2A-CAA-CBA |
| 25 | 8 | 618 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 618 | CLA | C3A-C2A-CAA-CBA |
| 25 | 8 | 620 | CLA | C3A-C2A-CAA-CBA |
| 25 | 8 | 620 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 601 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 604 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 604 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 605 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 608 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 608 | CLA | C3A-C2A-CAA-CBA |
| 25 | 2 | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | 2 | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | 2 | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 2 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 2 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 615 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 615 | CLA | C3A-C2A-CAA-CBA |
| 25 | 2 | 621 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 621 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 2 | 621 | CLA | CHA-CBD-CGD-O1D |
| 25 | 2 | 621 | CLA | CHA-CBD-CGD-O2D |
| 25 | 9 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 9 | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | 9 | 609 | CLA | C1A-C2A-CAA-CBA |
| 25 | 9 | 609 | CLA | C3A-C2A-CAA-CBA |
| 25 | 9 | 609 | CLA | CBA-CGA-O2A-C1 |
| 25 | 9 | 609 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 612 | CLA | C1A-C2A-CAA-CBA |
| 26 | 1 | 604 | CHL | C3A-C2A-CAA-CBA |
| 26 | 1 | 604 | CHL | C11-C10-C8-C9 |
| 26 | 1 | 604 | CHL | C12-C13-C15-C16 |
| 26 | 1 | 609 | CHL | C1A-C2A-CAA-CBA |
| 26 | 1 | 609 | CHL | C3A-C2A-CAA-CBA |
| 26 | a | 604 | CHL | C3A-C2A-CAA-CBA |
| 26 | a | 604 | CHL | CHA-CBD-CGD-O2D |
| 26 | a | 606 | CHL | C3A-C2A-CAA-CBA |
| 26 | a | 609 | CHL | CHA-CBD-CGD-O1D |
| 26 | a | 609 | CHL | CHA-CBD-CGD-O2D |
| 26 | 3 | 604 | CHL | C2-C1-O2A-CGA |
| 26 | 4 | 618 | CHL | C2-C3-C5-C6 |
| 26 | 4 | 618 | CHL | C4-C3-C5-C6 |
| 26 | 4 | 609 | CHL | CHA-CBD-CGD-O1D |
| 26 | 4 | 609 | CHL | CHA-CBD-CGD-O2D |
| 26 | 5 | 610 | CHL | C1A-C2A-CAA-CBA |
| 26 | 5 | 610 | CHL | C3A-C2A-CAA-CBA |
| 26 | 5 | 613 | CHL | C2-C3-C5-C6 |
| 26 | 5 | 613 | CHL | C4-C3-C5-C6 |
| 26 | 5 | 618 | CHL | C1A-C2A-CAA-CBA |
| 26 | 6 | 609 | CHL | C14-C13-C15-C16 |
| 26 | 6 | 610 | CHL | CHA-CBD-CGD-O1D |
| 26 | 6 | 610 | CHL | CHA-CBD-CGD-O2D |
| 26 | 6 | 611 | CHL | C1A-C2A-CAA-CBA |
| 26 | 6 | 611 | CHL | C3A-C2A-CAA-CBA |
| 26 | 6 | 619 | CHL | C1A-C2A-CAA-CBA |
| 26 | 6 | 619 | CHL | CHA-CBD-CGD-O1D |
| 26 | 6 | 619 | CHL | CHA-CBD-CGD-O2D |
| 26 | 7 | 611 | CHL | C1A-C2A-CAA-CBA |
| 26 | 7 | 615 | CHL | C2A-CAA-CBA-CGA |
| 26 | 7 | 617 | CHL | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | 7 | 617 | CHL | CHA-CBD-CGD-O2D |
| 26 | 7 | 617 | CHL | CAD-CBD-CGD-O1D |
| 26 | 8 | 601 | CHL | C1A-C2A-CAA-CBA |
| 26 | 8 | 601 | CHL | C3A-C2A-CAA-CBA |
| 26 | 8 | 604 | CHL | C3A-C2A-CAA-CBA |
| 26 | 9 | 601 | CHL | C3A-C2A-CAA-CBA |
| 26 | 9 | 603 | CHL | C1A-C2A-CAA-CBA |
| 26 | 9 | 603 | CHL | C3A-C2A-CAA-CBA |
| 29 | A | 4001 | BCR | C11-C10-C9-C8 |
| 29 | A | 4001 | BCR | C11-C10-C9-C34 |
| 29 | A | 4001 | BCR | C10-C11-C12-C13 |
| 29 | A | 4001 | BCR | C11-C12-C13-C14 |
| 29 | A | 4001 | BCR | C11-C12-C13-C35 |
| 29 | A | 4002 | BCR | C7-C8-C9-C10 |
| 29 | A | 4002 | BCR | C7-C8-C9-C34 |
| 29 | A | 4002 | BCR | C11-C10-C9-C8 |
| 29 | A | 4002 | BCR | C11-C10-C9-C34 |
| 29 | A | 4002 | BCR | C10-C11-C12-C13 |
| 29 | A | 4002 | BCR | C13-C14-C15-C16 |
| 29 | A | 4002 | BCR | C36-C18-C19-C20 |
| 29 | A | 4003 | BCR | C11-C10-C9-C8 |
| 29 | A | 4003 | BCR | C11-C10-C9-C34 |
| 29 | A | 4003 | BCR | C9-C10-C11-C12 |
| 29 | A | 4003 | BCR | C10-C11-C12-C13 |
| 29 | A | 4003 | BCR | C17-C18-C19-C20 |
| 29 | A | 4003 | BCR | C36-C18-C19-C20 |
| 29 | A | 4003 | BCR | C23-C24-C25-C30 |
| 29 | A | 4004 | BCR | C7-C8-C9-C10 |
| 29 | A | 4004 | BCR | C7-C8-C9-C34 |
| 29 | A | 4004 | BCR | C11-C10-C9-C8 |
| 29 | A | 4004 | BCR | C11-C10-C9-C34 |
| 29 | A | 4004 | BCR | C10-C11-C12-C13 |
| 29 | A | 4005 | BCR | C11-C10-C9-C8 |
| 29 | A | 4005 | BCR | C11-C10-C9-C34 |
| 29 | A | 4005 | BCR | C17-C18-C19-C20 |
| 29 | A | 4005 | BCR | C36-C18-C19-C20 |
| 29 | A | 4005 | BCR | C21-C22-C23-C24 |
| 29 | A | 4005 | BCR | C37-C22-C23-C24 |
| 29 | B | 4001 | BCR | C7-C8-C9-C10 |
| 29 | B | 4001 | BCR | C7-C8-C9-C34 |
| 29 | B | 4001 | BCR | C17-C18-C19-C20 |
| 29 | B | 4001 | BCR | C36-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | B | 4001 | BCR | C21-C22-C23-C24 |
| 29 | B | 4001 | BCR | C37-C22-C23-C24 |
| 29 | B | 4002 | BCR | C1-C6-C7-C8 |
| 29 | B | 4002 | BCR | C5-C6-C7-C8 |
| 29 | B | 4002 | BCR | C7-C8-C9-C10 |
| 29 | B | 4002 | BCR | C7-C8-C9-C34 |
| 29 | B | 4002 | BCR | C11-C10-C9-C8 |
| 29 | B | 4002 | BCR | C11-C10-C9-C34 |
| 29 | B | 4002 | BCR | C10-C11-C12-C13 |
| 29 | B | 4002 | BCR | C17-C18-C19-C20 |
| 29 | B | 4002 | BCR | C36-C18-C19-C20 |
| 29 | B | 4002 | BCR | C21-C22-C23-C24 |
| 29 | B | 4002 | BCR | C37-C22-C23-C24 |
| 29 | B | 4002 | BCR | C23-C24-C25-C30 |
| 29 | B | 4004 | BCR | C23-C24-C25-C30 |
| 29 | B | 4005 | BCR | C7-C8-C9-C34 |
| 29 | B | 4005 | BCR | C11-C10-C9-C8 |
| 29 | B | 4005 | BCR | C11-C10-C9-C34 |
| 29 | B | 4005 | BCR | C10-C11-C12-C13 |
| 29 | B | 4005 | BCR | C17-C18-C19-C20 |
| 29 | B | 4005 | BCR | C36-C18-C19-C20 |
| 29 | B | 4007 | BCR | C11-C10-C9-C8 |
| 29 | B | 4007 | BCR | C11-C10-C9-C34 |
| 29 | B | 4007 | BCR | C10-C11-C12-C13 |
| 29 | B | 4006 | BCR | C11-C10-C9-C8 |
| 29 | B | 4006 | BCR | C11-C10-C9-C34 |
| 29 | B | 4006 | BCR | C9-C10-C11-C12 |
| 29 | B | 4006 | BCR | C10-C11-C12-C13 |
| 29 | B | 4006 | BCR | C17-C18-C19-C20 |
| 29 | B | 4006 | BCR | C36-C18-C19-C20 |
| 29 | G | 4001 | BCR | C11-C10-C9-C8 |
| 29 | G | 4001 | BCR | C11-C10-C9-C34 |
| 29 | G | 4001 | BCR | C10-C11-C12-C13 |
| 29 | G | 4001 | BCR | C13-C14-C15-C16 |
| 29 | G | 4001 | BCR | C21-C22-C23-C24 |
| 29 | G | 4001 | BCR | C37-C22-C23-C24 |
| 29 | H | 4001 | BCR | C11-C10-C9-C8 |
| 29 | H | 4001 | BCR | C11-C10-C9-C34 |
| 29 | J | 4001 | BCR | C11-C10-C9-C8 |
| 29 | J | 4001 | BCR | C11-C10-C9-C34 |
| 29 | J | 4001 | BCR | C10-C11-C12-C13 |
| 29 | J | 4001 | BCR | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | J | 4001 | BCR | C36-C18-C19-C20 |
| 29 | K | 4001 | BCR | C7-C8-C9-C34 |
| 29 | K | 4001 | BCR | C11-C10-C9-C8 |
| 29 | K | 4001 | BCR | C11-C10-C9-C34 |
| 29 | K | 4002 | BCR | C11-C10-C9-C8 |
| 29 | K | 4002 | BCR | C11-C10-C9-C34 |
| 29 | K | 4002 | BCR | C10-C11-C12-C13 |
| 29 | K | 4002 | BCR | C36-C18-C19-C20 |
| 29 | L | 4002 | BCR | C11-C10-C9-C8 |
| 29 | L | 4002 | BCR | C11-C10-C9-C34 |
| 29 | L | 4003 | BCR | C11-C10-C9-C8 |
| 29 | L | 4003 | BCR | C11-C10-C9-C34 |
| 29 | L | 4003 | BCR | C10-C11-C12-C13 |
| 29 | L | 4003 | BCR | C23-C24-C25-C30 |
| 29 | L | 4001 | BCR | C11-C10-C9-C8 |
| 29 | L | 4001 | BCR | C11-C10-C9-C34 |
| 29 | L | 4001 | BCR | C10-C11-C12-C13 |
| 29 | L | 4001 | BCR | C21-C22-C23-C24 |
| 29 | L | 4001 | BCR | C37-C22-C23-C24 |
| 29 | L | 4001 | BCR | C23-C24-C25-C26 |
| 29 | L | 4001 | BCR | C23-C24-C25-C30 |
| 29 | I | 4001 | BCR | C7-C8-C9-C10 |
| 29 | I | 4001 | BCR | C7-C8-C9-C34 |
| 29 | I | 4001 | BCR | C11-C10-C9-C8 |
| 29 | I | 4001 | BCR | C11-C10-C9-C34 |
| 29 | I | 4001 | BCR | C10-C11-C12-C13 |
| 29 | I | 4001 | BCR | C17-C18-C19-C20 |
| 29 | I | 4001 | BCR | C36-C18-C19-C20 |
| 29 | O | 4001 | BCR | C11-C10-C9-C8 |
| 29 | O | 4001 | BCR | C11-C10-C9-C34 |
| 29 | O | 4001 | BCR | C17-C18-C19-C20 |
| 29 | O | 4001 | BCR | C36-C18-C19-C20 |
| 29 | 3 | 503 | BCR | C5-C6-C7-C8 |
| 29 | 3 | 503 | BCR | C7-C8-C9-C10 |
| 29 | 3 | 503 | BCR | C7-C8-C9-C34 |
| 29 | 3 | 503 | BCR | C11-C10-C9-C8 |
| 29 | 3 | 503 | BCR | C11-C10-C9-C34 |
| 29 | 3 | 503 | BCR | C10-C11-C12-C13 |
| 29 | 3 | 503 | BCR | C23-C24-C25-C30 |
| 29 | 3 | 504 | BCR | C7-C8-C9-C10 |
| 29 | 3 | 504 | BCR | C7-C8-C9-C34 |
| 29 | 3 | 504 | BCR | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | 3 | 504 | BCR | C11-C10-C9-C34 |
| 29 | 3 | 504 | BCR | C10-C11-C12-C13 |
| 29 | 3 | 504 | BCR | C17-C18-C19-C20 |
| 29 | 3 | 504 | BCR | C36-C18-C19-C20 |
| 29 | 3 | 504 | BCR | C21-C22-C23-C24 |
| 29 | 3 | 504 | BCR | C37-C22-C23-C24 |
| 29 | 3 | 505 | BCR | C11-C10-C9-C8 |
| 29 | 3 | 505 | BCR | C11-C10-C9-C34 |
| 29 | 3 | 505 | BCR | C9-C10-C11-C12 |
| 29 | 3 | 505 | BCR | C10-C11-C12-C13 |
| 29 | 3 | 505 | BCR | C17-C18-C19-C20 |
| 29 | 3 | 505 | BCR | C36-C18-C19-C20 |
| 29 | 3 | 505 | BCR | C21-C22-C23-C24 |
| 29 | 3 | 505 | BCR | C37-C22-C23-C24 |
| 29 | 4 | 503 | BCR | C7-C8-C9-C10 |
| 29 | 4 | 503 | BCR | C7-C8-C9-C34 |
| 29 | 4 | 503 | BCR | C11-C10-C9-C8 |
| 29 | 4 | 503 | BCR | C11-C10-C9-C34 |
| 29 | 4 | 503 | BCR | C9-C10-C11-C12 |
| 29 | 4 | 503 | BCR | C10-C11-C12-C13 |
| 29 | 4 | 503 | BCR | C17-C18-C19-C20 |
| 29 | 4 | 503 | BCR | C36-C18-C19-C20 |
| 29 | 4 | 503 | BCR | C21-C22-C23-C24 |
| 29 | 4 | 503 | BCR | C37-C22-C23-C24 |
| 29 | 4 | 503 | BCR | C23-C24-C25-C26 |
| 29 | 4 | 503 | BCR | C23-C24-C25-C30 |
| 29 | 5 | 503 | BCR | C5-C6-C7-C8 |
| 29 | 5 | 503 | BCR | C11-C10-C9-C8 |
| 29 | 5 | 503 | BCR | C11-C10-C9-C34 |
| 29 | 5 | 503 | BCR | C10-C11-C12-C13 |
| 29 | 5 | 503 | BCR | C17-C18-C19-C20 |
| 29 | 5 | 503 | BCR | C36-C18-C19-C20 |
| 29 | 5 | 504 | BCR | C36-C18-C19-C20 |
| 29 | 5 | 504 | BCR | C21-C22-C23-C24 |
| 29 | 5 | 504 | BCR | C37-C22-C23-C24 |
| 29 | 6 | 503 | BCR | C11-C10-C9-C8 |
| 29 | 6 | 503 | BCR | C11-C10-C9-C34 |
| 29 | 6 | 503 | BCR | C10-C11-C12-C13 |
| 29 | 6 | 503 | BCR | C11-C12-C13-C14 |
| 29 | 6 | 503 | BCR | C11-C12-C13-C35 |
| 29 | 6 | 503 | BCR | C36-C18-C19-C20 |
| 29 | 6 | 503 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | 6 | 503 | BCR | C37-C22-C23-C24 |
| 29 | 6 | 503 | BCR | C23-C24-C25-C26 |
| 29 | 6 | 503 | BCR | C23-C24-C25-C30 |
| 29 | 6 | 504 | BCR | C10-C11-C12-C13 |
| 29 | 6 | 504 | BCR | C21-C22-C23-C24 |
| 29 | 7 | 503 | BCR | C7-C8-C9-C10 |
| 29 | 7 | 503 | BCR | C7-C8-C9-C34 |
| 29 | 7 | 503 | BCR | C11-C10-C9-C8 |
| 29 | 7 | 503 | BCR | C11-C10-C9-C34 |
| 29 | 7 | 503 | BCR | C10-C11-C12-C13 |
| 29 | 8 | 503 | BCR | C5-C6-C7-C8 |
| 29 | 8 | 503 | BCR | C7-C8-C9-C10 |
| 29 | 8 | 503 | BCR | C7-C8-C9-C34 |
| 29 | 8 | 503 | BCR | C11-C10-C9-C8 |
| 29 | 8 | 503 | BCR | C11-C10-C9-C34 |
| 29 | 8 | 503 | BCR | C10-C11-C12-C13 |
| 29 | 8 | 503 | BCR | C21-C22-C23-C24 |
| 29 | 8 | 503 | BCR | C37-C22-C23-C24 |
| 29 | 8 | 503 | BCR | C23-C24-C25-C26 |
| 29 | 8 | 503 | BCR | C23-C24-C25-C30 |
| 30 | A | 5001 | LHG | O1-C1-C2-C3 |
| 30 | A | 5001 | LHG | C3-O3-P-O4 |
| 30 | A | 5001 | LHG | C3-O3-P-O5 |
| 30 | A | 5001 | LHG | C3-O3-P-O6 |
| 30 | A | 5001 | LHG | C4-O6-P-O3 |
| 30 | A | 5001 | LHG | C4-O6-P-O4 |
| 30 | A | 5001 | LHG | C4-O6-P-O5 |
| 30 | A | 5001 | LHG | O6-C4-C5-O7 |
| 30 | A | 5001 | LHG | O9-C7-O7-C5 |
| 30 | A | 5002 | LHG | O1-C1-C2-C3 |
| 30 | A | 5002 | LHG | C4-O6-P-O4 |
| 30 | A | 5003 | LHG | C4-O6-P-O3 |
| 30 | A | 5003 | LHG | C4-O6-P-O4 |
| 30 | A | 5003 | LHG | C4-O6-P-O5 |
| 30 | B | 5001 | LHG | O1-C1-C2-O2 |
| 30 | B | 5001 | LHG | O1-C1-C2-C3 |
| 30 | B | 5001 | LHG | O2-C2-C3-O3 |
| 30 | B | 5001 | LHG | C3-O3-P-O4 |
| 30 | B | 5001 | LHG | C3-O3-P-O5 |
| 30 | B | 5001 | LHG | O7-C5-C6-O8 |
| 30 | B | 5002 | LHG | C4-O6-P-O3 |
| 30 | F | 5002 | LHG | C1-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | F | 5001 | LHG | O1-C1-C2-C3 |
| 30 | F | 5001 | LHG | C3-O3-P-O6 |
| 30 | F | 5001 | LHG | C4-O6-P-O4 |
| 30 | 1 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 1 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 1 | 801 | LHG | O2-C2-C3-O3 |
| 30 | 1 | 801 | LHG | C4-O6-P-O4 |
| 30 | 1 | 802 | LHG | O1-C1-C2-C3 |
| 30 | 1 | 802 | LHG | O2-C2-C3-O3 |
| 30 | 1 | 802 | LHG | C3-O3-P-O5 |
| 30 | 1 | 802 | LHG | C3-O3-P-O6 |
| 30 | 1 | 802 | LHG | C4-O6-P-O5 |
| 30 | 1 | 802 | LHG | O7-C5-C6-O8 |
| 30 | 1 | 802 | LHG | O9-C7-O7-C5 |
| 30 | a | 801 | LHG | O1-C1-C2-C3 |
| 30 | a | 801 | LHG | C4-O6-P-O4 |
| 30 | a | 801 | LHG | C4-O6-P-O5 |
| 30 | 3 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 3 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 3 | 801 | LHG | O2-C2-C3-O3 |
| 30 | 3 | 801 | LHG | C4-O6-P-O5 |
| 30 | 3 | 801 | LHG | O9-C7-O7-C5 |
| 30 | 4 | 802 | LHG | C3-O3-P-O4 |
| 30 | 4 | 802 | LHG | C3-O3-P-O5 |
| 30 | 4 | 802 | LHG | C8-C7-O7-C5 |
| 30 | 4 | 801 | LHG | C3-O3-P-O5 |
| 30 | 4 | 801 | LHG | C4-O6-P-O4 |
| 30 | 5 | 801 | LHG | C3-O3-P-O4 |
| 30 | 6 | 802 | LHG | O1-C1-C2-C3 |
| 30 | 6 | 802 | LHG | C1-C2-C3-O3 |
| 30 | 6 | 802 | LHG | C4-O6-P-O4 |
| 30 | 6 | 802 | LHG | C4-O6-P-O5 |
| 30 | 6 | 802 | LHG | C8-C7-O7-C5 |
| 30 | 6 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 6 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 7 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 7 | 801 | LHG | C4-O6-P-O4 |
| 30 | 7 | 801 | LHG | C4-O6-P-O5 |
| 30 | 7 | 801 | LHG | C8-C7-O7-C5 |
| 30 | 7 | 802 | LHG | C4-O6-P-O4 |
| 30 | 7 | 803 | LHG | C1-C2-C3-O3 |
| 30 | 7 | 803 | LHG | C3-O3-P-O4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 7 | 803 | LHG | C3-O3-P-O5 |
| 30 | 7 | 803 | LHG | C3-O3-P-O6 |
| 30 | 8 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 8 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 8 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 8 | 801 | LHG | C4-O6-P-O3 |
| 30 | 8 | 801 | LHG | C4-O6-P-O4 |
| 30 | 8 | 801 | LHG | C4-O6-P-O5 |
| 30 | 2 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 2 | 801 | LHG | C8-C7-O7-C5 |
| 30 | 2 | 802 | LHG | O1-C1-C2-C3 |
| 30 | 2 | 802 | LHG | C3-O3-P-O4 |
| 30 | 2 | 802 | LHG | O9-C7-O7-C5 |
| 30 | 9 | 802 | LHG | C1-C2-C3-O3 |
| 30 | 9 | 802 | LHG | C3-O3-P-O5 |
| 30 | 9 | 802 | LHG | C3-O3-P-O6 |
| 30 | 9 | 801 | LHG | O1-C1-C2-C3 |
| 32 | A | 5005 | SQD | C2-C1-O6-C44 |
| 32 | A | 5005 | SQD | O5-C1-O6-C44 |
| 32 | A | 5005 | SQD | C8-C7-O47-C45 |
| 32 | A | 5005 | SQD | O5-C5-C6-S |
| 32 | G | 5001 | SQD | C5-C6-S-O8 |
| 32 | G | 5001 | SQD | C5-C6-S-O9 |
| 32 | H | 5001 | SQD | C8-C7-O47-C45 |
| 32 | I | 5001 | SQD | C2-C1-O6-C44 |
| 32 | I | 5001 | SQD | C8-C7-O47-C45 |
| 32 | I | 5001 | SQD | C5-C6-S-O7 |
| 32 | I | 5001 | SQD | C5-C6-S-O8 |
| 32 | I | 5001 | SQD | C5-C6-S-O9 |
| 32 | 7 | 805 | SQD | C2-C1-O6-C44 |
| 32 | 7 | 805 | SQD | O5-C1-O6-C44 |
| 32 | 7 | 805 | SQD | O5-C5-C6-S |
| 33 | A | 5006 | PTY | C11-C8-O7-C6 |
| 33 | A | 5006 | PTY | C3-O11-P1-O13 |
| 33 | B | 5005 | PTY | N1-C2-C3-O11 |
| 33 | B | 5005 | PTY | C5-O14-P1-O13 |
| 33 | G | 5003 | PTY | N1-C2-C3-O11 |
| 33 | G | 5003 | PTY | C3-O11-P1-O12 |
| 33 | G | 5002 | PTY | N1-C2-C3-O11 |
| 33 | G | 5002 | PTY | O10-C8-O7-C6 |
| 33 | G | 5002 | PTY | C11-C8-O7-C6 |
| 33 | G | 5002 | PTY | C3-O11-P1-O12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | J | 5001 | PTY | O4-C1-C6-O7 |
| 33 | J | 5001 | PTY | C3-O11-P1-O12 |
| 33 | J | 5001 | PTY | C3-O11-P1-O13 |
| 33 | J | 5001 | PTY | C5-O14-P1-O13 |
| 33 | a | 803 | PTY | N1-C2-C3-O11 |
| 33 | a | 802 | PTY | C5-O14-P1-O11 |
| 33 | a | 802 | PTY | C5-O14-P1-O13 |
| 33 | 3 | 802 | PTY | N1-C2-C3-O11 |
| 33 | 3 | 802 | PTY | O10-C8-O7-C6 |
| 33 | 3 | 802 | PTY | C5-O14-P1-O11 |
| 33 | 3 | 802 | PTY | C5-O14-P1-O13 |
| 33 | 5 | 802 | PTY | C11-C8-O7-C6 |
| 33 | 5 | 802 | PTY | C5-O14-P1-O12 |
| 33 | 5 | 802 | PTY | C5-O14-P1-O13 |
| 33 | 7 | 804 | PTY | C5-C6-O7-C8 |
| 33 | 7 | 804 | PTY | C11-C8-O7-C6 |
| 33 | 9 | 803 | PTY | N1-C2-C3-O11 |
| 33 | 9 | 803 | PTY | C11-C8-O7-C6 |
| 33 | 9 | 803 | PTY | C5-O14-P1-O12 |
| 33 | 9 | 803 | PTY | C5-O14-P1-O13 |
| 34 | A | 5007 | 3PH | C1-O11-P-O14 |
| 34 | A | 5007 | 3PH | C1-O11-P-O12 |
| 34 | A | 5007 | 3PH | C22-C21-O21-C2 |
| 35 | A | 5008 | LMT | C2'-C1'-O1'-C1 |
| 35 | A | 5008 | LMT | O5'-C1'-O1'-C1 |
| 35 | B | 5006 | LMT | C2'-C1'-O1'-C1 |
| 35 | B | 5006 | LMT | O5'-C1'-O1'-C1 |
| 36 | 7 | 806 | DGD | C2A-C1A-O1G-C1G |
| 36 | 7 | 806 | DGD | O6E-C1E-O5D-C6D |
| 36 | 8 | 802 | DGD | O1B-C1B-O2G-C2G |
| 36 | 8 | 802 | DGD | C2D-C1D-O3G-C3G |
| 36 | 8 | 802 | DGD | O6D-C1D-O3G-C3G |
| 36 | 8 | 803 | DGD | O1B-C1B-O2G-C2G |
| 37 | B | 5004 | PCW | C32-C31-O2-C2 |
| 37 | B | 5004 | PCW | O31-C31-O2-C2 |
| 37 | K | 5002 | PCW | O2-C2-C3-O3 |
| 37 | K | 5002 | PCW | O4P-C4-C5-N |
| 37 | K | 5002 | PCW | C4-O4P-P-O2P |
| 37 | K | 5002 | PCW | C4-O4P-P-O3P |
| 37 | K | 5001 | PCW | O2-C2-C3-O3 |
| 37 | K | 5001 | PCW | C32-C31-O2-C2 |
| 37 | 6 | 803 | PCW | O2-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 6 | 803 | PCW | O4P-C4-C5-N |
| 37 | 6 | 803 | PCW | C4-O4P-P-O1P |
| 37 | 6 | 803 | PCW | C4-O4P-P-O2P |
| 38 | F | 5003 | LPX | C3-C4-C5-O6 |
| 38 | F | 5003 | LPX | O1-C3-C4-C5 |
| 38 | F | 5003 | LPX | C1-O2-P1-O1 |
| 39 | F | 4001 | NEX | C7-C8-C9-C10 |
| 39 | F | 4001 | NEX | C7-C8-C9-C19 |
| 39 | F | 4001 | NEX | C12-C13-C14-C15 |
| 39 | F | 4001 | NEX | C20-C13-C14-C15 |
| 39 | F | 4001 | NEX | C14-C15-C35-C34 |
| 39 | F | 4001 | NEX | C27-C28-C29-C30 |
| 39 | F | 4001 | NEX | C27-C28-C29-C39 |
| 40 | J | 4002 | RRX | C23-C24-C25-C30 |
| 40 | J | 4002 | RRX | C19-C20-C21-C22 |
| 40 | J | 4002 | RRX | C36-C18-C19-C20 |
| 40 | J | 4002 | RRX | C17-C18-C19-C20 |
| 40 | J | 4002 | RRX | C15-C16-C17-C18 |
| 40 | 3 | 506 | RRX | C7-C8-C9-C10 |
| 40 | 3 | 506 | RRX | C7-C8-C9-C34 |
| 40 | 3 | 506 | RRX | C5-C6-C7-C8 |
| 41 | J | 5002 | SPH | O1-C1-C2-N2 |
| 41 | J | 5002 | SPH | O1-C1-C2-C3 |
| 41 | J | 5002 | SPH | C2-C3-C4-C5 |
| 41 | J | 5002 | SPH | O3-C3-C4-C5 |
| 41 | 4 | 805 | SPH | C1-C2-C3-O3 |
| 41 | 4 | 805 | SPH | C1-C2-C3-C4 |
| 41 | 4 | 805 | SPH | N2-C2-C3-O3 |
| 41 | 4 | 805 | SPH | N2-C2-C3-C4 |
| 41 | 6 | 806 | SPH | O1-C1-C2-N2 |
| 41 | 6 | 806 | SPH | O1-C1-C2-C3 |
| 41 | 6 | 806 | SPH | C2-C3-C4-C5 |
| 41 | 6 | 806 | SPH | O3-C3-C4-C5 |
| 41 | 9 | 804 | SPH | O1-C1-C2-N2 |
| 41 | 9 | 804 | SPH | O1-C1-C2-C3 |
| 41 | 9 | 804 | SPH | C1-C2-C3-O3 |
| 41 | 9 | 804 | SPH | C1-C2-C3-C4 |
| 41 | 9 | 804 | SPH | N2-C2-C3-O3 |
| 41 | 9 | 804 | SPH | N2-C2-C3-C4 |
| 41 | 9 | 804 | SPH | C2-C3-C4-C5 |
| 41 | 9 | 804 | SPH | O3-C3-C4-C5 |
| 43 | 1 | 503 | LUT | C13-C14-C15-C35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | 1 | 503 | LUT | C21-C26-C27-C28 |
| 43 | 1 | 503 | LUT | C31-C32-C33-C34 |
| 43 | 1 | 503 | LUT | C31-C32-C33-C40 |
| 43 | a | 501 | LUT | C5-C6-C7-C8 |
| 43 | a | 503 | LUT | C21-C26-C27-C28 |
| 43 | a | 503 | LUT | C31-C32-C33-C40 |
| 43 | 4 | 501 | LUT | C21-C26-C27-C28 |
| 43 | 4 | 501 | LUT | C27-C28-C29-C30 |
| 43 | 4 | 501 | LUT | C27-C28-C29-C39 |
| 43 | 4 | 501 | LUT | C29-C30-C31-C32 |
| 43 | 5 | 505 | LUT | C21-C26-C27-C28 |
| 43 | 5 | 505 | LUT | C31-C32-C33-C34 |
| 43 | 5 | 505 | LUT | C31-C32-C33-C40 |
| 43 | 7 | 501 | LUT | C21-C26-C27-C28 |
| 43 | 7 | 501 | LUT | C27-C28-C29-C30 |
| 43 | 7 | 501 | LUT | C27-C28-C29-C39 |
| 43 | 2 | 502 | LUT | C31-C32-C33-C34 |
| 43 | 2 | 502 | LUT | C31-C32-C33-C40 |
| 43 | 2 | 507 | LUT | C7-C8-C9-C10 |
| 43 | 2 | 507 | LUT | C7-C8-C9-C19 |
| 43 | 2 | 507 | LUT | C11-C12-C13-C14 |
| 43 | 2 | 507 | LUT | C11-C12-C13-C20 |
| 44 | 1 | 502 | AXT | C9-C10-C11-C12 |
| 44 | 1 | 502 | AXT | C11-C12-C13-C20 |
| 44 | 1 | 502 | AXT | C31-C32-C33-C34 |
| 44 | 1 | 502 | AXT | C31-C32-C33-C40 |
| 44 | 7 | 504 | AXT | C7-C8-C9-C10 |
| 44 | 7 | 504 | AXT | C7-C8-C9-C19 |
| 44 | 7 | 504 | AXT | C25-C26-C27-C28 |
| 44 | 7 | 504 | AXT | C27-C28-C29-C30 |
| 46 | a | 504 | QTB | C09-C10-C11-C12 |
| 48 | 3 | 803 | DGA | CB2-CB1-OG2-CG2 |
| 48 | 3 | 803 | DGA | OG2-CG2-CG3-OXT |
| 48 | 5 | 803 | DGA | CA2-CA1-OG1-CG1 |
| 48 | 5 | 803 | DGA | CB2-CB1-OG2-CG2 |
| 48 | 5 | 803 | DGA | CG1-CG2-CG3-OXT |
| 48 | 5 | 803 | DGA | OG2-CG2-CG3-OXT |
| 48 | 8 | 804 | DGA | OG2-CG2-CG3-OXT |
| 48 | 2 | 803 | DGA | CG1-CG2-CG3-OXT |
| 48 | 2 | 803 | DGA | OG2-CG2-CG3-OXT |
| 50 | 9 | 504 | XAT | C12-C13-C14-C15 |
| 50 | 9 | 504 | XAT | C20-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 50 | 9 | 504 | XAT | C14-C15-C35-C34 |
| 50 | 9 | 504 | XAT | C27-C28-C29-C30 |
| 50 | 9 | 504 | XAT | C27-C28-C29-C39 |
| 50 | 9 | 504 | XAT | C32-C33-C34-C35 |
| 50 | 9 | 504 | XAT | C40-C33-C34-C35 |
| 50 | 9 | 504 | XAT | C33-C34-C35-C15 |
| 50 | 9 | 507 | XAT | C7-C8-C9-C10 |
| 50 | 9 | 507 | XAT | C7-C8-C9-C19 |
| 50 | 9 | 507 | XAT | C10-C11-C12-C13 |
| 52 | 8 | 805 | P5S | O-C-CA-N |
| 52 | 8 | 805 | P5S | O-C-CA-CB |
| 52 | 8 | 805 | P5S | OXT-C-CA-CB |
| 52 | 8 | 805 | P5S | C-CA-CB-OG |
| 52 | 8 | 805 | P5S | N-CA-CB-OG |
| 53 | 8 | 810 | LAP | O3-C14-C15-O4 |
| 53 | 8 | 810 | LAP | O6-C16-C17-N8 |
| 53 | 8 | 810 | LAP | C16-O6-P9-O4 |
| 53 | 8 | 810 | LAP | C16-O6-P9-O5 |
| 53 | 8 | 810 | LAP | C16-O6-P9-O7 |
| 25 | O | 1803 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 615 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1134 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1021 | CLA | O1D-CGD-O2D-CED |
| 25 | L | 1504 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 615 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 617 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 615 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1012 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1104 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1107 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1110 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1112 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1113 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1117 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1129 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1132 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1134 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1135 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1101 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1237 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1206 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1211 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1213 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1214 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1215 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1219 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1224 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1226 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1229 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1231 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1232 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1234 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1238 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1240 | CLA | CBD-CGD-O2D-CED |
| 25 | H | 1701 | CLA | CBD-CGD-O2D-CED |
| 25 | H | 1703 | CLA | CBD-CGD-O2D-CED |
| 25 | K | 1402 | CLA | CBD-CGD-O2D-CED |
| 25 | K | 1403 | CLA | CBD-CGD-O2D-CED |
| 25 | K | 1404 | CLA | CBD-CGD-O2D-CED |
| 25 | L | 1501 | CLA | CBD-CGD-O2D-CED |
| 25 | L | 1503 | CLA | CBD-CGD-O2D-CED |
| 25 | L | 1504 | CLA | CBD-CGD-O2D-CED |
| 25 | O | 1802 | CLA | CBD-CGD-O2D-CED |
| 25 | O | 1803 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 613 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 616 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 604 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 610 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 612 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 4 | 616 | CLA | CBD-CGD-O2D-CED |
| 25 | 4 | 617 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 609 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 608 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 611 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 618 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 603 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 608 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 621 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 604 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 606 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1101 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1201 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1218 | CLA | O1A-CGA-O2A-C1 |
| 25 | H | 1703 | CLA | O1A-CGA-O2A-C1 |
| 25 | a | 611 | CLA | O1A-CGA-O2A-C1 |
| 25 | 3 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 608 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 615 | CLA | O1A-CGA-O2A-C1 |
| 32 | A | 5005 | SQD | O10-C23-O48-C46 |
| 33 | 5 | 802 | PTY | O30-C30-O4-C1 |
| 36 | 7 | 806 | DGD | O1A-C1A-O1G-C1G |
| 48 | 5 | 803 | DGA | OA1-CA1-OG1-CG1 |
| 51 | 7 | 807 | 4RF | O42-C41-O40-C39 |
| 25 | 1 | 615 | CLA | O1A-CGA-O2A-C1 |
| 25 | a | 615 | CLA | O1A-CGA-O2A-C1 |
| 25 | 9 | 609 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1023 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1224 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1232 | CLA | O1D-CGD-O2D-CED |
| 25 | K | 1404 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 615 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 616 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 608 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 611 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 615 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 615 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 606 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1012 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1109 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1118 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1119 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1126 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1131 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1140 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1216 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1236 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1239 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1207 | CLA | O1D-CGD-O2D-CED |
| 25 | F | 1301 | CLA | O1D-CGD-O2D-CED |
| 25 | G | 1601 | CLA | O1D-CGD-O2D-CED |
| 25 | G | 1602 | CLA | O1D-CGD-O2D-CED |
| 25 | H | 1701 | CLA | O1D-CGD-O2D-CED |
| 25 | J | 1901 | CLA | O1D-CGD-O2D-CED |
| 25 | K | 1401 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 601 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 610 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 615 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 618 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 610 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 8 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 620 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 601 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 609 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1218 | CLA | CBA-CGA-O2A-C1 |
| 25 | 1 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 611 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 615 | CLA | CBA-CGA-O2A-C1 |
| 32 | A | 5005 | SQD | C24-C23-O48-C46 |
| 33 | 5 | 802 | PTY | C31-C30-O4-C1 |
| 51 | 7 | 807 | 4RF | C43-C41-O40-C39 |
| 25 | A | 1013 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1102 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1103 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1106 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1115 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1120 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1124 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1125 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1127 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1128 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1130 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1133 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1141 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1202 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1205 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1208 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1210 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1212 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1222 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1223 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1227 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1230 | CLA | CBD-CGD-O2D-CED |
| 25 | H | 1702 | CLA | CBD-CGD-O2D-CED |
| 25 | L | 1502 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 605 | CLA | CBD-CGD-O2D-CED |
| 25 | 3 | 601 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 4 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 6 | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 604 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 609 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 604 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 615 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1104 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1208 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1209 | CLA | O1A-CGA-O2A-C1 |
| 25 | 1 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 3 | 610 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 611 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 616 | CLA | O1A-CGA-O2A-C1 |
| 25 | 5 | 603 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 615 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 606 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 609 | CLA | O1A-CGA-O2A-C1 |
| 25 | 2 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 2 | 621 | CLA | O1A-CGA-O2A-C1 |
| 32 | G | 5001 | SQD | O10-C23-O48-C46 |
| 33 | a | 803 | PTY | O30-C30-O4-C1 |
| 33 | a | 802 | PTY | O30-C30-O4-C1 |
| 33 | 7 | 804 | PTY | O30-C30-O4-C1 |
| 33 | 9 | 803 | PTY | O30-C30-O4-C1 |
| 48 | 2 | 803 | DGA | OA1-CA1-OG1-CG1 |
| 25 | 8 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 615 | CLA | O1A-CGA-O2A-C1 |
| 25 | 2 | 606 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1022 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1203 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1228 | CLA | O1D-CGD-O2D-CED |
| 25 | F | 1302 | CLA | O1D-CGD-O2D-CED |
| 25 | G | 1603 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 611 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 612 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 7 | 603 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1116 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1121 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1139 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1206 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 618 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 611 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 614 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 608 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1201 | CLA | CBD-CGD-O2D-CED |
| 25 | 8 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1111 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1231 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 604 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 606 | CLA | O1D-CGD-O2D-CED |
| 30 | 4 | 802 | LHG | O9-C7-O7-C5 |
| 30 | 6 | 802 | LHG | O9-C7-O7-C5 |
| 30 | 7 | 801 | LHG | O9-C7-O7-C5 |
| 30 | 2 | 801 | LHG | O9-C7-O7-C5 |
| 32 | A | 5005 | SQD | O49-C7-O47-C45 |
| 32 | H | 5001 | SQD | O49-C7-O47-C45 |
| 32 | I | 5001 | SQD | O49-C7-O47-C45 |
| 33 | A | 5006 | PTY | O10-C8-O7-C6 |
| 33 | 5 | 802 | PTY | O10-C8-O7-C6 |
| 33 | 7 | 804 | PTY | O10-C8-O7-C6 |
| 33 | 9 | 803 | PTY | O10-C8-O7-C6 |
| 34 | A | 5007 | 3PH | O22-C21-O21-C2 |
| 37 | K | 5001 | PCW | O31-C31-O2-C2 |
| 48 | 5 | 803 | DGA | OB1-CB1-OG2-CG2 |
| 30 | F | 5002 | LHG | O10-C23-O8-C6 |
| 25 | 8 | 615 | CLA | CBA-CGA-O2A-C1 |
| 25 | K | 1401 | CLA | O1A-CGA-O2A-C1 |
| 30 | F | 5002 | LHG | C5-C6-O8-C23 |
| 25 | L | 1501 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1012 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1103 | CLA | C3-C5-C6-C7 |
| 25 | A | 1106 | CLA | C3-C5-C6-C7 |
| 25 | A | 1108 | CLA | C3-C5-C6-C7 |
| 25 | A | 1118 | CLA | C3-C5-C6-C7 |
| 25 | A | 1130 | CLA | C3-C5-C6-C7 |
| 25 | B | 1237 | CLA | C3-C5-C6-C7 |
| 25 | B | 1203 | CLA | C3-C5-C6-C7 |
| 25 | B | 1204 | CLA | C3-C5-C6-C7 |
| 25 | B | 1205 | CLA | C3-C5-C6-C7 |
| 25 | B | 1210 | CLA | C3-C5-C6-C7 |
| 25 | B | 1218 | CLA | C3-C5-C6-C7 |
| 25 | B | 1220 | CLA | C3-C5-C6-C7 |
| 25 | B | 1207 | CLA | C3-C5-C6-C7 |
| 25 | H | 1701 | CLA | C3-C5-C6-C7 |
| 25 | O | 1802 | CLA | C3-C5-C6-C7 |
| 25 | 1 | 606 | CLA | C3-C5-C6-C7 |
| 25 | a | 608 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 601 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 605 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 607 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 616 | CLA | C3-C5-C6-C7 |
| 25 | 4 | 612 | CLA | C3-C5-C6-C7 |
| 25 | 4 | 615 | CLA | C3-C5-C6-C7 |
| 25 | 6 | 608 | CLA | C3-C5-C6-C7 |
| 25 | 6 | 601 | CLA | C3-C5-C6-C7 |
| 25 | 2 | 601 | CLA | C3-C5-C6-C7 |
| 25 | 2 | 604 | CLA | C3-C5-C6-C7 |
| 25 | 2 | 607 | CLA | C3-C5-C6-C7 |
| 25 | A | 1118 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1101 | CLA | CBA-CGA-O2A-C1 |
| 25 | H | 1703 | CLA | CBA-CGA-O2A-C1 |
| 25 | 3 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 3 | 610 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 608 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 615 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 604 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 621 | CLA | CBA-CGA-O2A-C1 |
| 32 | G | 5001 | SQD | C24-C23-O48-C46 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | a | 803 | PTY | C31-C30-O4-C1 |
| 33 | 7 | 804 | PTY | C31-C30-O4-C1 |
| 33 | 9 | 803 | PTY | C31-C30-O4-C1 |
| 30 | A | 5001 | LHG | C8-C7-O7-C5 |
| 30 | 1 | 802 | LHG | C8-C7-O7-C5 |
| 30 | 3 | 801 | LHG | C8-C7-O7-C5 |
| 30 | 2 | 802 | LHG | C8-C7-O7-C5 |
| 33 | 3 | 802 | PTY | C11-C8-O7-C6 |
| 36 | 8 | 802 | DGD | C2B-C1B-O2G-C2G |
| 36 | 8 | 803 | DGD | C2B-C1B-O2G-C2G |
| 25 | A | 1104 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1107 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1112 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1237 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1214 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1229 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 601 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 613 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1105 | CLA | CBD-CGD-O2D-CED |
| 25 | 1 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | a | 608 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | 2 | 605 | CLA | O1A-CGA-O2A-C1 |
| 25 | K | 1401 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 602 | CLA | C3-C5-C6-C7 |
| 25 | B | 1213 | CLA | C4-C3-C5-C6 |
| 25 | 1 | 606 | CLA | C4-C3-C5-C6 |
| 25 | a | 607 | CLA | C4-C3-C5-C6 |
| 25 | 3 | 610 | CLA | C4-C3-C5-C6 |
| 25 | 6 | 615 | CLA | C4-C3-C5-C6 |
| 26 | 2 | 609 | CHL | C4-C3-C5-C6 |
| 25 | A | 1108 | CLA | C2-C3-C5-C6 |
| 25 | A | 1115 | CLA | C2-C3-C5-C6 |
| 25 | B | 1213 | CLA | C2-C3-C5-C6 |
| 25 | a | 607 | CLA | C2-C3-C5-C6 |
| 25 | 5 | 603 | CLA | C2-C3-C5-C6 |
| 25 | 6 | 615 | CLA | C2-C3-C5-C6 |
| 25 | A | 1106 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1111 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1113 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1118 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1119 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1125 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1135 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1140 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1237 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1204 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1209 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1216 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1225 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1227 | CLA | C2A-CAA-CBA-CGA |
| 25 | F | 1302 | CLA | C2A-CAA-CBA-CGA |
| 25 | a | 603 | CLA | C2A-CAA-CBA-CGA |
| 25 | 3 | 610 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 609 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 618 | CLA | C2A-CAA-CBA-CGA |
| 25 | 2 | 612 | CLA | C2A-CAA-CBA-CGA |
| 26 | 1 | 611 | CHL | C2A-CAA-CBA-CGA |
| 26 | 4 | 613 | CHL | C2A-CAA-CBA-CGA |
| 26 | 4 | 618 | CHL | C2A-CAA-CBA-CGA |
| 26 | 6 | 609 | CHL | C2A-CAA-CBA-CGA |
| 26 | 7 | 611 | CHL | C2A-CAA-CBA-CGA |
| 26 | 7 | 617 | CHL | C2A-CAA-CBA-CGA |
| 25 | a | 603 | CLA | O1A-CGA-O2A-C1 |
| 25 | 9 | 604 | CLA | O1A-CGA-O2A-C1 |
| 48 | 8 | 804 | DGA | OA1-CA1-OG1-CG1 |
| 25 | K | 1402 | CLA | O1D-CGD-O2D-CED |
| 25 | L | 1503 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 608 | CLA | O1D-CGD-O2D-CED |
| 36 | B | 5003 | DGD | C8A-C9A-CAA-CBA |
| 36 | B | 5003 | DGD | CBA-CCA-CDA-CEA |
| 36 | 7 | 806 | DGD | C8A-C9A-CAA-CBA |
| 36 | 8 | 802 | DGD | C8A-C9A-CAA-CBA |
| 25 | 6 | 605 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1112 | CLA | C3-C5-C6-C7 |
| 25 | A | 1121 | CLA | C3-C5-C6-C7 |
| 25 | A | 1122 | CLA | C3-C5-C6-C7 |
| 25 | A | 1131 | CLA | C3-C5-C6-C7 |
| 25 | B | 1211 | CLA | C3-C5-C6-C7 |
| 25 | B | 1212 | CLA | C3-C5-C6-C7 |
| 25 | F | 1302 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | H | 1703 | CLA | C3-C5-C6-C7 |
| 25 | a | 612 | CLA | C3-C5-C6-C7 |
| 25 | 7 | 610 | CLA | C3-C5-C6-C7 |
| 25 | 8 | 606 | CLA | C3-C5-C6-C7 |
| 25 | 2 | 605 | CLA | C3-C5-C6-C7 |
| 25 | 9 | 606 | CLA | C3-C5-C6-C7 |
| 25 | A | 1104 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1237 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1204 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1208 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1209 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1213 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1217 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1230 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1231 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1207 | CLA | CBA-CGA-O2A-C1 |
| 25 | F | 1302 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 606 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 611 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 616 | CLA | CBA-CGA-O2A-C1 |
| 25 | 5 | 603 | CLA | CBA-CGA-O2A-C1 |
| 25 | 5 | 607 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 603 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 606 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 609 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 618 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 612 | CLA | CBA-CGA-O2A-C1 |
| 25 | 9 | 604 | CLA | CBA-CGA-O2A-C1 |
| 30 | A | 5001 | LHG | C24-C23-O8-C6 |
| 30 | F | 5002 | LHG | C24-C23-O8-C6 |
| 33 | B | 5005 | PTY | C31-C30-O4-C1 |
| 33 | a | 802 | PTY | C31-C30-O4-C1 |
| 48 | 8 | 804 | DGA | CA2-CA1-OG1-CG1 |
| 48 | 2 | 803 | DGA | CA2-CA1-OG1-CG1 |
| 30 | 6 | 801 | LHG | C23-C24-C25-C26 |
| 25 | B | 1213 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1219 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 604 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1204 | CLA | CBD-CGD-O2D-CED |
| 25 | 5 | 604 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 8 | 612 | CLA | CBD-CGD-O2D-CED |
| 25 | 9 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1117 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1135 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1215 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1226 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 609 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 601 | CLA | O1D-CGD-O2D-CED |
| 30 | F | 5001 | LHG | O9-C7-O7-C5 |
| 48 | 3 | 803 | DGA | OB1-CB1-OG2-CG2 |
| 25 | A | 1102 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1118 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1237 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1207 | CLA | O1A-CGA-O2A-C1 |
| 25 | 7 | 606 | CLA | O1A-CGA-O2A-C1 |
| 25 | 7 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 618 | CLA | O1A-CGA-O2A-C1 |
| 30 | A | 5001 | LHG | O10-C23-O8-C6 |
| 33 | B | 5005 | PTY | O30-C30-O4-C1 |
| 52 | 8 | 805 | P5S | O18-C17-O19-C1 |
| 29 | B | 4005 | BCR | C9-C10-C11-C12 |
| 29 | B | 4007 | BCR | C9-C10-C11-C12 |
| 29 | G | 4001 | BCR | C9-C10-C11-C12 |
| 29 | O | 4001 | BCR | C13-C14-C15-C16 |
| 43 | 7 | 501 | LUT | C29-C30-C31-C32 |
| 25 | 4 | 601 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1110 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1132 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1238 | CLA | O1D-CGD-O2D-CED |
| 25 | H | 1703 | CLA | O1D-CGD-O2D-CED |
| 25 | K | 1403 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 618 | CLA | O1D-CGD-O2D-CED |
| 30 | A | 5003 | LHG | O2-C2-C3-O3 |
| 30 | F | 5002 | LHG | O2-C2-C3-O3 |
| 30 | a | 801 | LHG | O2-C2-C3-O3 |
| 30 | 6 | 801 | LHG | O2-C2-C3-O3 |
| 30 | 7 | 801 | LHG | O2-C2-C3-O3 |
| 30 | 8 | 801 | LHG | O2-C2-C3-O3 |
| 30 | 2 | 802 | LHG | O2-C2-C3-O3 |
| 30 | 9 | 801 | LHG | O2-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 38 | F | 5003 | LPX | O1-C3-C4-O5 |
| 25 | A | 1140 | CLA | C3-C5-C6-C7 |
| 25 | B | 1215 | CLA | C3-C5-C6-C7 |
| 25 | 5 | 603 | CLA | C3-C5-C6-C7 |
| 26 | 5 | 613 | CHL | C3-C5-C6-C7 |
| 26 | 6 | 619 | CHL | C3-C5-C6-C7 |
| 25 | A | 1111 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1113 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1117 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1120 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1126 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1139 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1215 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1236 | CLA | CBA-CGA-O2A-C1 |
| 25 | 3 | 616 | CLA | CBA-CGA-O2A-C1 |
| 25 | 5 | 604 | CLA | CBA-CGA-O2A-C1 |
| 25 | 5 | 612 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 608 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 601 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 604 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 606 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 605 | CLA | CBA-CGA-O2A-C1 |
| 25 | 9 | 605 | CLA | CBA-CGA-O2A-C1 |
| 52 | 8 | 805 | P5S | C20-C17-O19-C1 |
| 25 | A | 1111 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1204 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1213 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1217 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 601 | CLA | O1A-CGA-O2A-C1 |
| 25 | 7 | 604 | CLA | O1A-CGA-O2A-C1 |
| 25 | 9 | 605 | CLA | O1A-CGA-O2A-C1 |
| 36 | 8 | 802 | DGD | O1A-C1A-O1G-C1G |
| 35 | A | 5008 | LMT | O5B-C5B-C6B-O6B |
| 25 | A | 1113 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1129 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1240 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 621 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1123 | CLA | C8-C10-C11-C12 |
| 38 | F | 5003 | LPX | O5-C4-C5-O6 |
| 30 | F | 5001 | LHG | C8-C7-O7-C5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 8 | 801 | LHG | C8-C7-O7-C5 |
| 31 | A | 5004 | LMG | C11-C10-O7-C8 |
| 25 | 5 | 615 | CLA | CBA-CGA-O2A-C1 |
| 25 | 9 | 602 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1217 | CLA | CBD-CGD-O2D-CED |
| 36 | 8 | 803 | DGD | O6E-C5E-C6E-O5E |
| 25 | B | 1230 | CLA | O1A-CGA-O2A-C1 |
| 25 | 5 | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 5 | 612 | CLA | O1A-CGA-O2A-C1 |
| 25 | 7 | 603 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 608 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 612 | CLA | O1D-CGD-O2D-CED |
| 30 | 5 | 801 | LHG | C7-C8-C9-C10 |
| 25 | a | 607 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 1102 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 603 | CLA | CBA-CGA-O2A-C1 |
| 36 | 8 | 802 | DGD | C2A-C1A-O1G-C1G |
| 25 | B | 1234 | CLA | O1D-CGD-O2D-CED |
| 25 | O | 1802 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 616 | CLA | O1D-CGD-O2D-CED |
| 35 | 2 | 804 | LMT | O5'-C5'-C6'-O6' |
| 30 | 6 | 802 | LHG | C2-C3-O3-P |
| 25 | A | 1126 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1231 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1236 | CLA | O1A-CGA-O2A-C1 |
| 25 | F | 1302 | CLA | O1A-CGA-O2A-C1 |
| 25 | 3 | 616 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 606 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 604 | CLA | O1A-CGA-O2A-C1 |
| 25 | 2 | 612 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1121 | CLA | C4-C3-C5-C6 |
| 25 | A | 1133 | CLA | C4-C3-C5-C6 |
| 25 | B | 1215 | CLA | C4-C3-C5-C6 |
| 25 | O | 1802 | CLA | C4-C3-C5-C6 |
| 25 | 5 | 602 | CLA | C4-C3-C5-C6 |
| 26 | a | 606 | CHL | C4-C3-C5-C6 |
| 26 | 7 | 609 | CHL | C4-C3-C5-C6 |
| 25 | A | 1121 | CLA | C2-C3-C5-C6 |
| 25 | A | 1133 | CLA | C2-C3-C5-C6 |
| 25 | B | 1215 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | O | 1802 | CLA | C2-C3-C5-C6 |
| 25 | 3 | 610 | CLA | C2-C3-C5-C6 |
| 25 | 5 | 602 | CLA | C2-C3-C5-C6 |
| 26 | a | 606 | CHL | C2-C3-C5-C6 |
| 26 | 7 | 609 | CHL | C2-C3-C5-C6 |
| 25 | F | 1301 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 615 | CLA | C2A-CAA-CBA-CGA |
| 25 | 7 | 612 | CLA | C2A-CAA-CBA-CGA |
| 26 | a | 613 | CHL | C2A-CAA-CBA-CGA |
| 26 | 6 | 611 | CHL | C2A-CAA-CBA-CGA |
| 26 | 8 | 610 | CHL | C2A-CAA-CBA-CGA |
| 25 | B | 1211 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 606 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 601 | CLA | O1D-CGD-O2D-CED |
| 25 | 9 | 604 | CLA | O1D-CGD-O2D-CED |
| 35 | B | 5006 | LMT | O5'-C5'-C6'-O6' |
| 25 | A | 1113 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1117 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1120 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1139 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1215 | CLA | O1A-CGA-O2A-C1 |
| 25 | a | 607 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 608 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1115 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1123 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1219 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1221 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1228 | CLA | CBA-CGA-O2A-C1 |
| 25 | 9 | 606 | CLA | CBA-CGA-O2A-C1 |
| 36 | 8 | 803 | DGD | C2A-C1A-O1G-C1G |
| 25 | A | 1013 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1127 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1101 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1208 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1223 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 604 | CLA | O1D-CGD-O2D-CED |
| 25 | 7 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 604 | CLA | O1A-CGA-O2A-C1 |
| 35 | A | 5008 | LMT | C4B-C5B-C6B-O6B |
| 30 | B | 5002 | LHG | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1115 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1130 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1210 | CLA | O1D-CGD-O2D-CED |
| 25 | H | 1702 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 609 | CLA | O1D-CGD-O2D-CED |
| 32 | A | 5005 | SQD | C23-C24-C25-C26 |
| 30 | A | 5003 | LHG | C1-C2-C3-O3 |
| 30 | B | 5001 | LHG | C1-C2-C3-O3 |
| 30 | 1 | 802 | LHG | C1-C2-C3-O3 |
| 30 | 4 | 802 | LHG | C1-C2-C3-O3 |
| 30 | 5 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 7 | 801 | LHG | C1-C2-C3-O3 |
| 30 | 2 | 802 | LHG | C1-C2-C3-O3 |
| 30 | 9 | 801 | LHG | C1-C2-C3-O3 |
| 25 | B | 1219 | CLA | O1A-CGA-O2A-C1 |
| 53 | 8 | 810 | LAP | C16-C17-N8-C18 |
| 25 | A | 1109 | CLA | C3-C5-C6-C7 |
| 25 | B | 1022 | CLA | C3-C5-C6-C7 |
| 25 | A | 1102 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 604 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1106 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1108 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1112 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1124 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1125 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1131 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1133 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1134 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1136 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1140 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1023 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1202 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1210 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1220 | CLA | CBA-CGA-O2A-C1 |
| 25 | K | 1403 | CLA | CBA-CGA-O2A-C1 |
| 25 | L | 1501 | CLA | CBA-CGA-O2A-C1 |
| 25 | O | 1802 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 605 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 604 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 612 | CLA | CBA-CGA-O2A-C1 |
| 25 | 5 | 609 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 606 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 7 | 612 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 602 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 608 | CLA | CBA-CGA-O2A-C1 |
| 25 | 9 | 607 | CLA | CBA-CGA-O2A-C1 |
| 30 | 7 | 802 | LHG | C24-C23-O8-C6 |
| 48 | 3 | 803 | DGA | CA2-CA1-OG1-CG1 |
| 25 | A | 1103 | CLA | O1D-CGD-O2D-CED |
| 25 | 3 | 601 | CLA | O1D-CGD-O2D-CED |
| 29 | 4 | 503 | BCR | C19-C20-C21-C22 |
| 40 | 3 | 506 | RRX | C13-C14-C15-C16 |
| 50 | 9 | 507 | XAT | C13-C14-C15-C35 |
| 32 | G | 5001 | SQD | C7-C8-C9-C10 |
| 48 | 5 | 803 | DGA | CA1-CA2-CA3-CA4 |
| 25 | 1 | 608 | CLA | C5-C6-C7-C8 |
| 25 | 3 | 613 | CLA | C5-C6-C7-C8 |
| 36 | 8 | 803 | DGD | O1A-C1A-O1G-C1G |
| 35 | B | 5006 | LMT | C4'-C5'-C6'-O6' |
| 25 | A | 1124 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1125 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1109 | CLA | C10-C11-C12-C13 |
| 25 | B | 1202 | CLA | C10-C11-C12-C13 |
| 25 | B | 1239 | CLA | C15-C16-C17-C18 |
| 25 | 1 | 605 | CLA | C15-C16-C17-C18 |
| 25 | 3 | 607 | CLA | C13-C15-C16-C17 |
| 25 | 4 | 610 | CLA | C5-C6-C7-C8 |
| 25 | 5 | 604 | CLA | C15-C16-C17-C18 |
| 25 | 5 | 612 | CLA | C15-C16-C17-C18 |
| 30 | B | 5002 | LHG | O2-C2-C3-O3 |
| 30 | 4 | 802 | LHG | O2-C2-C3-O3 |
| 30 | 5 | 801 | LHG | O2-C2-C3-O3 |
| 30 | 7 | 803 | LHG | O2-C2-C3-O3 |
| 30 | 2 | 801 | LHG | O2-C2-C3-O3 |
| 33 | a | 803 | PTY | C30-C31-C32-C33 |
| 36 | 7 | 806 | DGD | C2D-C1D-O3G-C3G |
| 51 | 7 | 807 | 4RF | O18-C19-C20-O21 |
| 25 | A | 1129 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1108 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1125 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1136 | CLA | O1A-CGA-O2A-C1 |
| 25 | 7 | 612 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 608 | CLA | O1A-CGA-O2A-C1 |
| 25 | 9 | 606 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1128 | CLA | C4-C3-C5-C6 |
| 25 | 6 | 602 | CLA | C4-C3-C5-C6 |
| 35 | 2 | 804 | LMT | C4'-C5'-C6'-O6' |
| 25 | 1 | 606 | CLA | C2-C3-C5-C6 |
| 26 | 2 | 609 | CHL | C2-C3-C5-C6 |
| 25 | A | 1013 | CLA | C14-C13-C15-C16 |
| 25 | A | 1121 | CLA | C6-C7-C8-C9 |
| 25 | A | 1137 | CLA | C11-C10-C8-C9 |
| 25 | B | 1201 | CLA | C11-C10-C8-C9 |
| 25 | B | 1220 | CLA | C11-C10-C8-C9 |
| 25 | L | 1502 | CLA | C11-C10-C8-C9 |
| 25 | 1 | 605 | CLA | C6-C7-C8-C9 |
| 25 | 3 | 601 | CLA | C14-C13-C15-C16 |
| 25 | 3 | 605 | CLA | C6-C7-C8-C9 |
| 25 | 3 | 606 | CLA | C14-C13-C15-C16 |
| 25 | 3 | 613 | CLA | C11-C12-C13-C14 |
| 25 | 5 | 612 | CLA | C14-C13-C15-C16 |
| 25 | 7 | 601 | CLA | C11-C10-C8-C9 |
| 25 | 2 | 603 | CLA | C11-C10-C8-C9 |
| 25 | 9 | 605 | CLA | C6-C7-C8-C9 |
| 26 | 1 | 609 | CHL | C6-C7-C8-C9 |
| 26 | 3 | 604 | CHL | C6-C7-C8-C9 |
| 26 | 3 | 611 | CHL | C11-C10-C8-C9 |
| 26 | 5 | 610 | CHL | C11-C12-C13-C14 |
| 26 | 5 | 610 | CHL | C14-C13-C15-C16 |
| 26 | 7 | 609 | CHL | C11-C10-C8-C9 |
| 26 | 7 | 617 | CHL | C11-C12-C13-C14 |
| 26 | 8 | 603 | CHL | C11-C10-C8-C9 |
| 26 | 8 | 603 | CHL | C11-C12-C13-C14 |
| 25 | A | 1141 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1202 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1205 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1212 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1227 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1230 | CLA | O1D-CGD-O2D-CED |
| 25 | a | 605 | CLA | O1D-CGD-O2D-CED |
| 25 | 6 | 615 | CLA | O1D-CGD-O2D-CED |
| 30 | 8 | 801 | LHG | C24-C25-C26-C27 |
| 25 | 6 | 603 | CLA | C13-C15-C16-C17 |
| 25 | 9 | 612 | CLA | C8-C10-C11-C12 |
| 25 | B | 1213 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 603 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 7 | 610 | CLA | C2A-CAA-CBA-CGA |
| 26 | a | 606 | CHL | C2A-CAA-CBA-CGA |
| 29 | A | 4001 | BCR | C36-C18-C19-C20 |
| 29 | A | 4004 | BCR | C36-C18-C19-C20 |
| 29 | A | 4005 | BCR | C7-C8-C9-C34 |
| 29 | B | 4004 | BCR | C7-C8-C9-C34 |
| 29 | B | 4005 | BCR | C37-C22-C23-C24 |
| 29 | G | 4001 | BCR | C36-C18-C19-C20 |
| 29 | H | 4001 | BCR | C37-C22-C23-C24 |
| 29 | J | 4001 | BCR | C37-C22-C23-C24 |
| 29 | K | 4001 | BCR | C37-C22-C23-C24 |
| 40 | J | 4002 | RRX | C11-C12-C13-C35 |
| 40 | 3 | 506 | RRX | C11-C12-C13-C35 |
| 43 | 5 | 505 | LUT | C27-C28-C29-C39 |
| 44 | 7 | 504 | AXT | C11-C12-C13-C20 |
| 44 | 7 | 504 | AXT | C27-C28-C29-C39 |
| 29 | G | 4001 | BCR | C17-C18-C19-C20 |
| 29 | K | 4001 | BCR | C7-C8-C9-C10 |
| 29 | K | 4001 | BCR | C21-C22-C23-C24 |
| 29 | O | 4001 | BCR | C11-C12-C13-C14 |
| 40 | 3 | 506 | RRX | C11-C12-C13-C14 |
| 44 | 1 | 502 | AXT | C11-C12-C13-C14 |
| 44 | 7 | 504 | AXT | C11-C12-C13-C14 |
| 50 | 9 | 504 | XAT | C11-C12-C13-C14 |
| 25 | A | 1106 | CLA | O1D-CGD-O2D-CED |
| 32 | G | 5001 | SQD | C8-C7-O47-C45 |
| 30 | 2 | 802 | LHG | C23-C24-C25-C26 |
| 37 | 6 | 803 | PCW | C31-C32-C33-C34 |
| 48 | 8 | 804 | DGA | CB1-CB2-CB3-CB4 |
| 48 | 2 | 803 | DGA | CB1-CB2-CB3-CB4 |
| 25 | A | 1131 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1133 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1134 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1140 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1023 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1202 | CLA | O1A-CGA-O2A-C1 |
| 25 | a | 605 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 606 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 602 | CLA | O1A-CGA-O2A-C1 |
| 25 | 9 | 607 | CLA | O1A-CGA-O2A-C1 |
| 48 | 3 | 803 | DGA | OA1-CA1-OG1-CG1 |
| 25 | A | 1122 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1226 | CLA | C15-C16-C17-C18 |
| 25 | B | 1228 | CLA | C13-C15-C16-C17 |
| 25 | 1 | 607 | CLA | C5-C6-C7-C8 |
| 25 | 1 | 612 | CLA | C5-C6-C7-C8 |
| 25 | 1 | 612 | CLA | C8-C10-C11-C12 |
| 25 | 2 | 605 | CLA | C10-C11-C12-C13 |
| 25 | 9 | 605 | CLA | C10-C11-C12-C13 |
| 25 | A | 1133 | CLA | O1D-CGD-O2D-CED |
| 32 | A | 5005 | SQD | C27-C28-C29-C30 |
| 37 | B | 5004 | PCW | C12-C13-C14-C15 |
| 25 | 3 | 610 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 1226 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 610 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 610 | CLA | C8-C10-C11-C12 |
| 32 | I | 5001 | SQD | C24-C23-O48-C46 |
| 25 | A | 1013 | CLA | C8-C10-C11-C12 |
| 25 | A | 1111 | CLA | C15-C16-C17-C18 |
| 25 | A | 1125 | CLA | C8-C10-C11-C12 |
| 25 | A | 1128 | CLA | C10-C11-C12-C13 |
| 25 | A | 1128 | CLA | C15-C16-C17-C18 |
| 25 | B | 1237 | CLA | C15-C16-C17-C18 |
| 25 | B | 1206 | CLA | C15-C16-C17-C18 |
| 25 | B | 1209 | CLA | C13-C15-C16-C17 |
| 25 | B | 1215 | CLA | C5-C6-C7-C8 |
| 25 | B | 1216 | CLA | C10-C11-C12-C13 |
| 25 | B | 1216 | CLA | C13-C15-C16-C17 |
| 25 | B | 1228 | CLA | C15-C16-C17-C18 |
| 25 | K | 1402 | CLA | C5-C6-C7-C8 |
| 25 | L | 1502 | CLA | C8-C10-C11-C12 |
| 25 | 1 | 601 | CLA | C5-C6-C7-C8 |
| 25 | 1 | 607 | CLA | C8-C10-C11-C12 |
| 25 | 3 | 607 | CLA | C8-C10-C11-C12 |
| 25 | 3 | 607 | CLA | C10-C11-C12-C13 |
| 25 | 9 | 605 | CLA | C5-C6-C7-C8 |
| 27 | A | 2001 | PQN | C25-C26-C27-C28 |
| 27 | B | 2002 | PQN | C18-C20-C21-C22 |
| 30 | B | 5001 | LHG | C7-C8-C9-C10 |
| 30 | 9 | 801 | LHG | C23-C24-C25-C26 |
| 45 | 8 | 808 | OLA | C1-C2-C3-C4 |
| 45 | 8 | 809 | OLA | C1-C2-C3-C4 |
| 48 | 5 | 803 | DGA | CB1-CB2-CB3-CB4 |
| 25 | B | 1222 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 3 | 803 | DGA | CA2-CA3-CA4-CA5 |
| 25 | A | 1103 | CLA | C8-C10-C11-C12 |
| 25 | A | 1104 | CLA | C5-C6-C7-C8 |
| 25 | A | 1109 | CLA | C13-C15-C16-C17 |
| 25 | A | 1125 | CLA | C15-C16-C17-C18 |
| 25 | A | 1137 | CLA | C10-C11-C12-C13 |
| 25 | B | 1202 | CLA | C15-C16-C17-C18 |
| 25 | B | 1203 | CLA | C8-C10-C11-C12 |
| 25 | B | 1206 | CLA | C10-C11-C12-C13 |
| 25 | B | 1209 | CLA | C5-C6-C7-C8 |
| 25 | B | 1226 | CLA | C5-C6-C7-C8 |
| 25 | B | 1239 | CLA | C13-C15-C16-C17 |
| 25 | G | 1602 | CLA | C5-C6-C7-C8 |
| 25 | a | 601 | CLA | C10-C11-C12-C13 |
| 25 | a | 603 | CLA | C10-C11-C12-C13 |
| 25 | a | 612 | CLA | C5-C6-C7-C8 |
| 25 | 3 | 605 | CLA | C13-C15-C16-C17 |
| 25 | 3 | 606 | CLA | C15-C16-C17-C18 |
| 25 | 3 | 613 | CLA | C8-C10-C11-C12 |
| 25 | 4 | 612 | CLA | C10-C11-C12-C13 |
| 25 | 5 | 601 | CLA | C10-C11-C12-C13 |
| 25 | 6 | 604 | CLA | C15-C16-C17-C18 |
| 25 | 8 | 609 | CLA | C5-C6-C7-C8 |
| 26 | 2 | 609 | CHL | C10-C11-C12-C13 |
| 30 | F | 5001 | LHG | O1-C1-C2-O2 |
| 30 | 4 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 2 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 9 | 802 | LHG | O1-C1-C2-O2 |
| 30 | A | 5002 | LHG | C7-C8-C9-C10 |
| 30 | B | 5001 | LHG | C23-C24-C25-C26 |
| 30 | 1 | 801 | LHG | C7-C8-C9-C10 |
| 30 | 1 | 801 | LHG | C23-C24-C25-C26 |
| 30 | 1 | 802 | LHG | C23-C24-C25-C26 |
| 30 | 3 | 801 | LHG | C7-C8-C9-C10 |
| 30 | 6 | 802 | LHG | C23-C24-C25-C26 |
| 30 | 7 | 801 | LHG | C7-C8-C9-C10 |
| 30 | 7 | 803 | LHG | C7-C8-C9-C10 |
| 30 | 8 | 801 | LHG | C23-C24-C25-C26 |
| 33 | A | 5006 | PTY | C30-C31-C32-C33 |
| 33 | B | 5005 | PTY | C8-C11-C12-C13 |
| 33 | G | 5003 | PTY | C8-C11-C12-C13 |
| 33 | 7 | 804 | PTY | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | K | 5002 | PCW | C11-C12-C13-C14 |
| 37 | K | 5001 | PCW | C11-C12-C13-C14 |
| 37 | 6 | 803 | PCW | C11-C12-C13-C14 |
| 47 | 4 | 804 | PLM | C1-C2-C3-C4 |
| 48 | 3 | 803 | DGA | CA1-CA2-CA3-CA4 |
| 51 | 7 | 807 | 4RF | C41-C43-C44-C45 |
| 52 | 8 | 805 | P5S | C38-C39-C40-C41 |
| 30 | 2 | 802 | LHG | C32-C33-C34-C35 |
| 35 | 1 | 804 | LMT | C4B-C5B-C6B-O6B |
| 52 | 8 | 805 | P5S | OXT-C-CA-N |
| 25 | A | 1120 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1106 | CLA | C15-C16-C17-C18 |
| 25 | A | 1133 | CLA | C13-C15-C16-C17 |
| 25 | B | 1206 | CLA | C8-C10-C11-C12 |
| 25 | B | 1219 | CLA | C8-C10-C11-C12 |
| 25 | 1 | 612 | CLA | C10-C11-C12-C13 |
| 25 | a | 603 | CLA | C15-C16-C17-C18 |
| 25 | 4 | 603 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 610 | CLA | C8-C10-C11-C12 |
| 25 | 7 | 604 | CLA | C15-C16-C17-C18 |
| 25 | G | 1601 | CLA | CBA-CGA-O2A-C1 |
| 25 | L | 1502 | CLA | CBA-CGA-O2A-C1 |
| 30 | 2 | 802 | LHG | C24-C23-O8-C6 |
| 32 | H | 5001 | SQD | C16-C17-C18-C19 |
| 25 | 5 | 615 | CLA | O1A-CGA-O2A-C1 |
| 25 | L | 1502 | CLA | O1D-CGD-O2D-CED |
| 25 | 4 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | 2 | 615 | CLA | O1D-CGD-O2D-CED |
| 35 | 1 | 804 | LMT | O5B-C5B-C6B-O6B |
| 30 | 8 | 801 | LHG | O9-C7-O7-C5 |
| 31 | A | 5004 | LMG | O9-C10-O7-C8 |
| 32 | G | 5001 | SQD | O49-C7-O47-C45 |
| 25 | A | 1105 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1108 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1133 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1139 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1022 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1203 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1206 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1211 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1212 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1216 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1227 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1229 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1230 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1235 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1236 | CLA | C2-C1-O2A-CGA |
| 25 | F | 1301 | CLA | C2-C1-O2A-CGA |
| 25 | O | 1802 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 602 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 608 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 615 | CLA | C2-C1-O2A-CGA |
| 25 | 5 | 602 | CLA | C2-C1-O2A-CGA |
| 25 | 5 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 6 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 608 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 610 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 8 | 611 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 621 | CLA | C2-C1-O2A-CGA |
| 25 | 9 | 612 | CLA | C2-C1-O2A-CGA |
| 26 | 6 | 619 | CHL | C2-C1-O2A-CGA |
| 25 | A | 1115 | CLA | C10-C11-C12-C13 |
| 25 | A | 1121 | CLA | C8-C10-C11-C12 |
| 25 | B | 1201 | CLA | C15-C16-C17-C18 |
| 25 | B | 1206 | CLA | C5-C6-C7-C8 |
| 25 | B | 1216 | CLA | C8-C10-C11-C12 |
| 25 | 1 | 605 | CLA | C13-C15-C16-C17 |
| 25 | 4 | 615 | CLA | C5-C6-C7-C8 |
| 25 | 7 | 604 | CLA | C13-C15-C16-C17 |
| 25 | 7 | 612 | CLA | C8-C10-C11-C12 |
| 53 | 8 | 810 | LAP | C16-C17-N8-C19 |
| 30 | A | 5002 | LHG | C23-C24-C25-C26 |
| 30 | 7 | 801 | LHG | C23-C24-C25-C26 |
| 30 | 7 | 802 | LHG | C23-C24-C25-C26 |
| 30 | 7 | 803 | LHG | C23-C24-C25-C26 |
| 30 | 2 | 802 | LHG | C7-C8-C9-C10 |
| 32 | I | 5001 | SQD | C23-C24-C25-C26 |
| 36 | 8 | 803 | DGD | C1A-C2A-C3A-C4A |
| 51 | 7 | 807 | 4RF | C22-C24-C25-C26 |
| 25 | 6 | 602 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1012 | CLA | C5-C6-C7-C8 |
| 25 | B | 1204 | CLA | C15-C16-C17-C18 |
| 25 | B | 1205 | CLA | C10-C11-C12-C13 |
| 25 | B | 1224 | CLA | C8-C10-C11-C12 |
| 25 | B | 1234 | CLA | C15-C16-C17-C18 |
| 25 | 1 | 603 | CLA | C15-C16-C17-C18 |
| 25 | 5 | 601 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 1021 | CLA | C12-C13-C15-C16 |
| 25 | B | 1206 | CLA | C12-C13-C15-C16 |
| 25 | B | 1214 | CLA | C6-C7-C8-C10 |
| 25 | 2 | 604 | CLA | C6-C7-C8-C10 |
| 26 | 4 | 609 | CHL | C12-C13-C15-C16 |
| 26 | 7 | 617 | CHL | C11-C12-C13-C15 |
| 26 | 9 | 601 | CHL | C12-C13-C15-C16 |
| 27 | B | 2002 | PQN | C21-C22-C23-C25 |
| 25 | K | 1403 | CLA | O1A-CGA-O2A-C1 |
| 25 | L | 1501 | CLA | O1A-CGA-O2A-C1 |
| 25 | O | 1802 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 612 | CLA | O1A-CGA-O2A-C1 |
| 30 | 7 | 802 | LHG | O10-C23-O8-C6 |
| 32 | A | 5005 | SQD | C15-C16-C17-C18 |
| 29 | I | 4001 | BCR | C9-C10-C11-C12 |
| 29 | I | 4001 | BCR | C15-C16-C17-C18 |
| 29 | 5 | 503 | BCR | C9-C10-C11-C12 |
| 29 | 5 | 503 | BCR | C13-C14-C15-C16 |
| 29 | 5 | 503 | BCR | C15-C16-C17-C18 |
| 40 | 3 | 506 | RRX | C9-C10-C11-C12 |
| 43 | 2 | 507 | LUT | C9-C10-C11-C12 |
| 30 | B | 5002 | LHG | C23-C24-C25-C26 |
| 25 | A | 1110 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1232 | CLA | C2A-CAA-CBA-CGA |
| 25 | G | 1602 | CLA | C2A-CAA-CBA-CGA |
| 25 | H | 1703 | CLA | C2A-CAA-CBA-CGA |
| 25 | O | 1802 | CLA | C2A-CAA-CBA-CGA |
| 25 | 2 | 615 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1128 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1113 | CLA | C5-C6-C7-C8 |
| 25 | A | 1123 | CLA | C15-C16-C17-C18 |
| 25 | A | 1126 | CLA | C10-C11-C12-C13 |
| 25 | B | 1021 | CLA | C10-C11-C12-C13 |
| 25 | B | 1224 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | O | 1802 | CLA | C5-C6-C7-C8 |
| 25 | 2 | 605 | CLA | C8-C10-C11-C12 |
| 26 | A | 1114 | CHL | C5-C6-C7-C8 |
| 27 | B | 2002 | PQN | C25-C26-C27-C28 |
| 25 | A | 1124 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1220 | CLA | O1A-CGA-O2A-C1 |
| 25 | 4 | 604 | CLA | O1A-CGA-O2A-C1 |
| 36 | 8 | 803 | DGD | O6E-C1E-O5D-C6D |
| 25 | A | 1103 | CLA | C5-C6-C7-C8 |
| 25 | G | 1602 | CLA | C8-C10-C11-C12 |
| 25 | 3 | 616 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 610 | CLA | C10-C11-C12-C13 |
| 25 | 7 | 610 | CLA | C5-C6-C7-C8 |
| 30 | 6 | 801 | LHG | C7-C8-C9-C10 |
| 30 | 9 | 802 | LHG | C23-C24-C25-C26 |
| 33 | 5 | 802 | PTY | C8-C11-C12-C13 |
| 29 | A | 4005 | BCR | C10-C11-C12-C13 |
| 29 | H | 4001 | BCR | C10-C11-C12-C13 |
| 29 | K | 4001 | BCR | C10-C11-C12-C13 |
| 29 | O | 4001 | BCR | C10-C11-C12-C13 |
| 50 | 9 | 504 | XAT | C10-C11-C12-C13 |
| 25 | a | 608 | CLA | O1D-CGD-O2D-CED |
| 30 | A | 5001 | LHG | O2-C2-C3-O3 |
| 30 | A | 5002 | LHG | O2-C2-C3-O3 |
| 30 | F | 5001 | LHG | O2-C2-C3-O3 |
| 30 | 6 | 802 | LHG | O2-C2-C3-O3 |
| 30 | 9 | 802 | LHG | O2-C2-C3-O3 |
| 25 | 9 | 602 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1111 | CLA | C3-C5-C6-C7 |
| 25 | A | 1012 | CLA | C13-C15-C16-C17 |
| 25 | A | 1136 | CLA | C15-C16-C17-C18 |
| 25 | B | 1203 | CLA | C5-C6-C7-C8 |
| 25 | B | 1214 | CLA | C5-C6-C7-C8 |
| 25 | L | 1502 | CLA | C5-C6-C7-C8 |
| 25 | 3 | 606 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 610 | CLA | C15-C16-C17-C18 |
| 25 | 4 | 612 | CLA | C8-C10-C11-C12 |
| 25 | 5 | 612 | CLA | C5-C6-C7-C8 |
| 25 | 8 | 609 | CLA | C10-C11-C12-C13 |
| 25 | 2 | 607 | CLA | C8-C10-C11-C12 |
| 25 | 9 | 612 | CLA | C13-C15-C16-C17 |
| 25 | A | 1013 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 9 | 612 | CLA | CBA-CGA-O2A-C1 |
| 30 | 2 | 801 | LHG | C25-C26-C27-C28 |
| 35 | B | 5006 | LMT | C3'-C4'-O1B-C1B |
| 25 | B | 1201 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1106 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1112 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1115 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1123 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1221 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1228 | CLA | O1A-CGA-O2A-C1 |
| 25 | 5 | 609 | CLA | O1A-CGA-O2A-C1 |
| 32 | I | 5001 | SQD | O10-C23-O48-C46 |
| 25 | 3 | 618 | CLA | CBA-CGA-O2A-C1 |
| 25 | 4 | 605 | CLA | CBA-CGA-O2A-C1 |
| 30 | F | 5001 | LHG | C23-C24-C25-C26 |
| 25 | A | 1013 | CLA | C13-C15-C16-C17 |
| 25 | A | 1112 | CLA | C5-C6-C7-C8 |
| 25 | A | 1126 | CLA | C8-C10-C11-C12 |
| 25 | A | 1105 | CLA | O1D-CGD-O2D-CED |
| 25 | 1 | 607 | CLA | O1D-CGD-O2D-CED |
| 25 | 8 | 612 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1129 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1210 | CLA | O1A-CGA-O2A-C1 |
| 30 | A | 5002 | LHG | C8-C7-O7-C5 |
| 30 | B | 5002 | LHG | C8-C7-O7-C5 |
| 30 | 1 | 801 | LHG | C8-C7-O7-C5 |
| 30 | 7 | 803 | LHG | C8-C7-O7-C5 |
| 36 | B | 5003 | DGD | C6A-C7A-C8A-C9A |
| 25 | A | 1101 | CLA | C15-C16-C17-C18 |
| 25 | B | 1229 | CLA | C13-C15-C16-C17 |
| 25 | B | 1235 | CLA | C8-C10-C11-C12 |
| 25 | B | 1239 | CLA | C5-C6-C7-C8 |
| 25 | H | 1703 | CLA | C5-C6-C7-C8 |
| 25 | 1 | 608 | CLA | C10-C11-C12-C13 |
| 25 | 3 | 605 | CLA | C5-C6-C7-C8 |
| 25 | 7 | 601 | CLA | C10-C11-C12-C13 |
| 25 | 7 | 612 | CLA | C5-C6-C7-C8 |
| 25 | 9 | 612 | CLA | C15-C16-C17-C18 |
| 30 | A | 5002 | LHG | C3-O3-P-O6 |
| 30 | A | 5002 | LHG | C4-O6-P-O3 |
| 30 | B | 5001 | LHG | C3-O3-P-O6 |
| 30 | F | 5001 | LHG | C4-O6-P-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 1 | 801 | LHG | C4-O6-P-O3 |
| 30 | a | 801 | LHG | C4-O6-P-O3 |
| 30 | 3 | 801 | LHG | C3-O3-P-O6 |
| 30 | 3 | 801 | LHG | C4-O6-P-O3 |
| 30 | 4 | 802 | LHG | C3-O3-P-O6 |
| 30 | 4 | 801 | LHG | C4-O6-P-O3 |
| 30 | 5 | 801 | LHG | C3-O3-P-O6 |
| 30 | 6 | 802 | LHG | C3-O3-P-O6 |
| 30 | 6 | 802 | LHG | C4-O6-P-O3 |
| 30 | 6 | 801 | LHG | C3-O3-P-O6 |
| 30 | 6 | 801 | LHG | C4-O6-P-O3 |
| 30 | 7 | 801 | LHG | C4-O6-P-O3 |
| 30 | 7 | 802 | LHG | C4-O6-P-O3 |
| 30 | 7 | 803 | LHG | C4-O6-P-O3 |
| 30 | 8 | 801 | LHG | C3-O3-P-O6 |
| 30 | 9 | 802 | LHG | C4-O6-P-O3 |
| 33 | A | 5006 | PTY | C3-O11-P1-O14 |
| 33 | B | 5005 | PTY | C5-O14-P1-O11 |
| 33 | G | 5003 | PTY | C3-O11-P1-O14 |
| 33 | G | 5002 | PTY | C3-O11-P1-O14 |
| 33 | J | 5001 | PTY | C3-O11-P1-O14 |
| 33 | J | 5001 | PTY | C5-O14-P1-O11 |
| 33 | a | 803 | PTY | C5-O14-P1-O11 |
| 33 | 3 | 802 | PTY | C3-O11-P1-O14 |
| 33 | 5 | 802 | PTY | C5-O14-P1-O11 |
| 33 | 7 | 804 | PTY | C3-O11-P1-O14 |
| 33 | 9 | 803 | PTY | C5-O14-P1-O11 |
| 37 | B | 5004 | PCW | C1-O3P-P-O4P |
| 37 | 6 | 803 | PCW | C4-O4P-P-O3P |
| 53 | 8 | 810 | LAP | C15-O4-P9-O6 |
| 48 | 2 | 803 | DGA | CA5-CA6-CA7-CA8 |
| 25 | A | 1110 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1211 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1226 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1231 | CLA | C5-C6-C7-C8 |
| 25 | 6 | 607 | CLA | C5-C6-C7-C8 |
| 26 | 5 | 610 | CHL | C5-C6-C7-C8 |
| 25 | G | 1601 | CLA | O1A-CGA-O2A-C1 |
| 25 | 5 | 604 | CLA | O1D-CGD-O2D-CED |
| 25 | 5 | 607 | CLA | O1D-CGD-O2D-CED |
| 30 | A | 5001 | LHG | C1-C2-C3-O3 |
| 30 | F | 5001 | LHG | C1-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | a | 801 | LHG | C1-C2-C3-O3 |
| 30 | A | 5002 | LHG | O9-C7-O7-C5 |
| 30 | B | 5002 | LHG | O9-C7-O7-C5 |
| 30 | 7 | 803 | LHG | O9-C7-O7-C5 |
| 30 | 4 | 802 | LHG | C12-C13-C14-C15 |
| 25 | A | 1121 | CLA | C10-C11-C12-C13 |
| 25 | B | 1201 | CLA | C5-C6-C7-C8 |
| 25 | B | 1201 | CLA | C13-C15-C16-C17 |
| 25 | B | 1210 | CLA | C15-C16-C17-C18 |
| 25 | 4 | 615 | CLA | C8-C10-C11-C12 |
| 25 | A | 1104 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1139 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1208 | CLA | C2A-CAA-CBA-CGA |
| 25 | 3 | 616 | CLA | C2A-CAA-CBA-CGA |
| 25 | 7 | 604 | CLA | C2A-CAA-CBA-CGA |
| 25 | 2 | 605 | CLA | C2A-CAA-CBA-CGA |
| 26 | 9 | 601 | CHL | C2A-CAA-CBA-CGA |
| 25 | A | 1111 | CLA | C16-C17-C18-C20 |
| 25 | B | 1234 | CLA | C16-C17-C18-C20 |
| 25 | F | 1302 | CLA | C6-C7-C8-C10 |
| 25 | 4 | 607 | CLA | C6-C7-C8-C9 |
| 25 | 6 | 607 | CLA | C6-C7-C8-C10 |
| 25 | A | 1013 | CLA | C3-C5-C6-C7 |
| 25 | 8 | 605 | CLA | C3-C5-C6-C7 |
| 25 | A | 1116 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1234 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 602 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 602 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 603 | CLA | CBA-CGA-O2A-C1 |
| 37 | K | 5001 | PCW | C12-C11-O3-C3 |
| 35 | A | 5008 | LMT | O1'-C1-C2-C3 |
| 48 | 3 | 803 | DGA | CA4-CA5-CA6-CA7 |
| 30 | F | 5002 | LHG | C23-C24-C25-C26 |
| 25 | B | 1214 | CLA | C8-C10-C11-C12 |
| 35 | B | 5006 | LMT | C5'-C4'-O1B-C1B |
| 29 | B | 4007 | BCR | C13-C14-C15-C16 |
| 29 | J | 4001 | BCR | C9-C10-C11-C12 |
| 29 | L | 4001 | BCR | C9-C10-C11-C12 |
| 29 | 3 | 503 | BCR | C13-C14-C15-C16 |
| 41 | 9 | 804 | SPH | C5-C6-C7-C8 |
| 30 | 2 | 801 | LHG | C23-C24-C25-C26 |
| 30 | F | 5002 | LHG | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 3 | 801 | LHG | C9-C10-C11-C12 |
| 25 | B | 1204 | CLA | O1D-CGD-O2D-CED |
| 30 | 4 | 801 | LHG | C8-C7-O7-C5 |
| 29 | B | 4004 | BCR | C11-C10-C9-C34 |
| 29 | 5 | 504 | BCR | C11-C10-C9-C34 |
| 29 | 6 | 504 | BCR | C11-C10-C9-C34 |
| 39 | F | 4001 | NEX | C11-C10-C9-C19 |
| 39 | F | 4001 | NEX | C40-C33-C34-C35 |
| 25 | 4 | 610 | CLA | C3-C5-C6-C7 |
| 25 | 7 | 608 | CLA | C3-C5-C6-C7 |
| 30 | A | 5001 | LHG | C33-C34-C35-C36 |
| 30 | A | 5003 | LHG | C14-C15-C16-C17 |
| 30 | B | 5001 | LHG | C13-C14-C15-C16 |
| 30 | 1 | 801 | LHG | C30-C31-C32-C33 |
| 30 | 1 | 802 | LHG | C25-C26-C27-C28 |
| 30 | 1 | 802 | LHG | C34-C35-C36-C37 |
| 30 | 5 | 801 | LHG | C13-C14-C15-C16 |
| 30 | 5 | 801 | LHG | C31-C32-C33-C34 |
| 30 | 2 | 801 | LHG | C11-C12-C13-C14 |
| 30 | 9 | 802 | LHG | C11-C12-C13-C14 |
| 36 | B | 5003 | DGD | C3A-C4A-C5A-C6A |
| 36 | 8 | 802 | DGD | C7A-C8A-C9A-CAA |
| 48 | 8 | 804 | DGA | CA3-CA4-CA5-CA6 |
| 48 | 8 | 804 | DGA | CBB-CCB-CDB-CEB |
| 53 | 8 | 810 | LAP | C3-C4-C5-C6 |
| 25 | 4 | 601 | CLA | O1D-CGD-O2D-CED |
| 24 | A | 1011 | CL0 | C16-C17-C18-C19 |
| 25 | A | 1107 | CLA | C6-C7-C8-C9 |
| 25 | B | 1235 | CLA | C16-C17-C18-C19 |
| 25 | B | 1238 | CLA | C16-C17-C18-C19 |
| 25 | 1 | 612 | CLA | C16-C17-C18-C19 |
| 25 | 4 | 615 | CLA | C11-C12-C13-C15 |
| 25 | 5 | 601 | CLA | C11-C12-C13-C15 |
| 25 | A | 1128 | CLA | CBA-CGA-O2A-C1 |
| 30 | 2 | 801 | LHG | C24-C23-O8-C6 |
| 30 | A | 5002 | LHG | C34-C35-C36-C37 |
| 30 | F | 5001 | LHG | C11-C12-C13-C14 |
| 30 | 1 | 802 | LHG | C11-C12-C13-C14 |
| 30 | 6 | 802 | LHG | C24-C25-C26-C27 |
| 30 | 2 | 802 | LHG | C13-C14-C15-C16 |
| 36 | 8 | 802 | DGD | C9A-CAA-CBA-CCA |
| 41 | 4 | 805 | SPH | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 45 | a | 805 | OLA | C14-C15-C16-C17 |
| 47 | 6 | 804 | PLM | C4-C5-C6-C7 |
| 30 | 1 | 801 | LHG | O9-C7-O7-C5 |
| 30 | B | 5002 | LHG | C7-C8-C9-C10 |
| 30 | 4 | 801 | LHG | C23-C24-C25-C26 |
| 30 | A | 5002 | LHG | C30-C31-C32-C33 |
| 30 | B | 5001 | LHG | C11-C12-C13-C14 |
| 30 | B | 5001 | LHG | C31-C32-C33-C34 |
| 30 | 6 | 801 | LHG | C12-C13-C14-C15 |
| 30 | 9 | 802 | LHG | C34-C35-C36-C37 |
| 33 | a | 803 | PTY | C6-C5-O14-P1 |
| 33 | a | 802 | PTY | C6-C5-O14-P1 |
| 25 | L | 1502 | CLA | O1A-CGA-O2A-C1 |
| 30 | A | 5001 | LHG | C11-C12-C13-C14 |
| 30 | 1 | 802 | LHG | C10-C11-C12-C13 |
| 30 | 6 | 801 | LHG | C30-C31-C32-C33 |
| 33 | 9 | 803 | PTY | C34-C35-C36-C37 |
| 45 | 1 | 803 | OLA | C3-C4-C5-C6 |
| 45 | 1 | 803 | OLA | C13-C14-C15-C16 |
| 47 | 8 | 807 | PLM | C6-C7-C8-C9 |
| 25 | 6 | 615 | CLA | C8-C10-C11-C12 |
| 25 | 8 | 606 | CLA | C5-C6-C7-C8 |
| 30 | 3 | 801 | LHG | C31-C32-C33-C34 |
| 30 | 8 | 801 | LHG | C11-C12-C13-C14 |
| 37 | K | 5002 | PCW | C14-C15-C16-C17 |
| 25 | A | 1132 | CLA | C3-C5-C6-C7 |
| 36 | 8 | 803 | DGD | C1B-C2B-C3B-C4B |
| 29 | B | 4004 | BCR | C11-C10-C9-C8 |
| 29 | 6 | 504 | BCR | C11-C10-C9-C8 |
| 36 | 8 | 802 | DGD | C2E-C1E-O5D-C6D |
| 36 | 8 | 803 | DGD | C2D-C1D-O3G-C3G |
| 36 | 8 | 803 | DGD | C2E-C1E-O5D-C6D |
| 39 | F | 4001 | NEX | C11-C10-C9-C8 |
| 39 | F | 4001 | NEX | C32-C33-C34-C35 |
| 30 | A | 5002 | LHG | C9-C10-C11-C12 |
| 30 | F | 5001 | LHG | C26-C27-C28-C29 |
| 30 | 1 | 801 | LHG | C26-C27-C28-C29 |
| 30 | a | 801 | LHG | C26-C27-C28-C29 |
| 30 | 3 | 801 | LHG | C13-C14-C15-C16 |
| 30 | 4 | 801 | LHG | C17-C18-C19-C20 |
| 30 | 7 | 802 | LHG | C25-C26-C27-C28 |
| 30 | 2 | 801 | LHG | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 36 | 8 | 803 | DGD | C2B-C3B-C4B-C5B |
| 37 | K | 5002 | PCW | C12-C13-C14-C15 |
| 48 | 2 | 803 | DGA | CB7-CB8-CB9-CAB |
| 25 | A | 1103 | CLA | C10-C11-C12-C13 |
| 25 | A | 1132 | CLA | C15-C16-C17-C18 |
| 25 | a | 605 | CLA | C5-C6-C7-C8 |
| 25 | A | 1117 | CLA | C16-C17-C18-C20 |
| 25 | A | 1128 | CLA | C16-C17-C18-C20 |
| 25 | B | 1234 | CLA | C16-C17-C18-C19 |
| 25 | 8 | 605 | CLA | C6-C7-C8-C9 |
| 25 | 2 | 605 | CLA | C11-C12-C13-C15 |
| 27 | A | 2001 | PQN | C26-C27-C28-C30 |
| 25 | B | 1201 | CLA | C4-C3-C5-C6 |
| 25 | B | 1225 | CLA | C4-C3-C5-C6 |
| 25 | B | 1229 | CLA | C4-C3-C5-C6 |
| 25 | 5 | 612 | CLA | C4-C3-C5-C6 |
| 26 | 3 | 611 | CHL | C4-C3-C5-C6 |
| 30 | A | 5001 | LHG | C13-C14-C15-C16 |
| 30 | A | 5001 | LHG | C30-C31-C32-C33 |
| 30 | A | 5003 | LHG | C28-C29-C30-C31 |
| 30 | B | 5001 | LHG | C34-C35-C36-C37 |
| 30 | 6 | 802 | LHG | C28-C29-C30-C31 |
| 37 | K | 5001 | PCW | C32-C33-C34-C35 |
| 45 | a | 805 | OLA | C12-C13-C14-C15 |
| 45 | 8 | 809 | OLA | C14-C15-C16-C17 |
| 25 | A | 1112 | CLA | C2-C3-C5-C6 |
| 25 | B | 1201 | CLA | C2-C3-C5-C6 |
| 25 | B | 1229 | CLA | C2-C3-C5-C6 |
| 25 | A | 1115 | CLA | C11-C10-C8-C9 |
| 25 | A | 1138 | CLA | C11-C10-C8-C9 |
| 25 | B | 1224 | CLA | C6-C7-C8-C9 |
| 25 | 3 | 607 | CLA | C14-C13-C15-C16 |
| 25 | 7 | 610 | CLA | C11-C10-C8-C9 |
| 25 | 2 | 605 | CLA | C11-C10-C8-C9 |
| 26 | A | 1114 | CHL | C11-C12-C13-C14 |
| 26 | 4 | 609 | CHL | C14-C13-C15-C16 |
| 27 | A | 2001 | PQN | C19-C18-C20-C21 |
| 36 | B | 5003 | DGD | C2G-C1G-O1G-C1A |
| 30 | A | 5001 | LHG | C7-C8-C9-C10 |
| 30 | A | 5003 | LHG | C17-C18-C19-C20 |
| 33 | B | 5005 | PTY | C18-C19-C20-C21 |
| 37 | 6 | 803 | PCW | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 9 | 804 | SPH | C10-C11-C12-C13 |
| 47 | a | 804 | PLM | C4-C5-C6-C7 |
| 47 | 8 | 806 | PLM | C2-C3-C4-C5 |
| 25 | B | 1214 | CLA | C2A-CAA-CBA-CGA |
| 25 | 9 | 604 | CLA | C2A-CAA-CBA-CGA |
| 26 | 9 | 608 | CHL | C2A-CAA-CBA-CGA |
| 25 | B | 1211 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1234 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 602 | CLA | O1A-CGA-O2A-C1 |
| 30 | 2 | 802 | LHG | O10-C23-O8-C6 |
| 29 | B | 4006 | BCR | C11-C12-C13-C35 |
| 29 | O | 4001 | BCR | C11-C12-C13-C35 |
| 29 | 6 | 504 | BCR | C37-C22-C23-C24 |
| 43 | a | 501 | LUT | C7-C8-C9-C19 |
| 43 | 5 | 505 | LUT | C7-C8-C9-C19 |
| 43 | 2 | 507 | LUT | C31-C32-C33-C40 |
| 44 | 1 | 502 | AXT | C7-C8-C9-C19 |
| 44 | 1 | 502 | AXT | C27-C28-C29-C39 |
| 48 | 2 | 803 | DGA | CAB-CBB-CCB-CDB |
| 30 | A | 5003 | LHG | O1-C1-C2-C3 |
| 30 | B | 5002 | LHG | O1-C1-C2-C3 |
| 30 | F | 5002 | LHG | O1-C1-C2-C3 |
| 30 | 1 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 4 | 802 | LHG | O1-C1-C2-C3 |
| 30 | 4 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 5 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 6 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 7 | 802 | LHG | O1-C1-C2-C3 |
| 30 | 7 | 803 | LHG | O1-C1-C2-C3 |
| 30 | 2 | 801 | LHG | O1-C1-C2-C3 |
| 30 | 9 | 802 | LHG | O1-C1-C2-C3 |
| 29 | B | 4006 | BCR | C11-C12-C13-C14 |
| 29 | 6 | 503 | BCR | C17-C18-C19-C20 |
| 40 | J | 4002 | RRX | C11-C12-C13-C14 |
| 43 | a | 501 | LUT | C7-C8-C9-C10 |
| 43 | 2 | 507 | LUT | C31-C32-C33-C34 |
| 44 | 1 | 502 | AXT | C7-C8-C9-C10 |
| 44 | 1 | 502 | AXT | C27-C28-C29-C30 |
| 30 | 4 | 801 | LHG | O9-C7-O7-C5 |
| 30 | 9 | 802 | LHG | C8-C7-O7-C5 |
| 33 | G | 5003 | PTY | C11-C8-O7-C6 |
| 26 | 7 | 613 | CHL | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | F | 5001 | LHG | C13-C14-C15-C16 |
| 30 | 1 | 802 | LHG | C28-C29-C30-C31 |
| 30 | 4 | 802 | LHG | C11-C12-C13-C14 |
| 30 | 4 | 801 | LHG | C28-C29-C30-C31 |
| 30 | 7 | 802 | LHG | C28-C29-C30-C31 |
| 36 | B | 5003 | DGD | C2B-C3B-C4B-C5B |
| 37 | K | 5001 | PCW | C33-C34-C35-C36 |
| 38 | F | 5003 | LPX | C7-C8-C9-C10 |
| 45 | 8 | 809 | OLA | C12-C13-C14-C15 |
| 25 | A | 1122 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 5004 | PCW | C40-C41-C42-C43 |
| 30 | F | 5001 | LHG | C7-C8-C9-C10 |
| 30 | A | 5003 | LHG | C13-C14-C15-C16 |
| 30 | A | 5003 | LHG | C16-C17-C18-C19 |
| 30 | B | 5001 | LHG | C30-C31-C32-C33 |
| 30 | B | 5002 | LHG | C13-C14-C15-C16 |
| 30 | F | 5002 | LHG | C26-C27-C28-C29 |
| 30 | F | 5001 | LHG | C28-C29-C30-C31 |
| 30 | 6 | 801 | LHG | C28-C29-C30-C31 |
| 30 | 8 | 801 | LHG | C26-C27-C28-C29 |
| 30 | 2 | 801 | LHG | C31-C32-C33-C34 |
| 30 | 2 | 802 | LHG | C11-C12-C13-C14 |
| 33 | a | 802 | PTY | C33-C34-C35-C36 |
| 33 | 3 | 802 | PTY | C16-C17-C18-C19 |
| 36 | B | 5003 | DGD | C9A-CAA-CBA-CCA |
| 48 | 8 | 804 | DGA | CA2-CA3-CA4-CA5 |
| 51 | 7 | 807 | 4RF | C12-C13-C14-C15 |
| 53 | 8 | 810 | LAP | C16-C17-N8-C20 |
| 25 | A | 1107 | CLA | C6-C7-C8-C10 |
| 25 | B | 1211 | CLA | C6-C7-C8-C10 |
| 25 | B | 1213 | CLA | C6-C7-C8-C10 |
| 25 | a | 608 | CLA | C6-C7-C8-C9 |
| 25 | 4 | 607 | CLA | C6-C7-C8-C10 |
| 25 | 4 | 615 | CLA | C11-C12-C13-C14 |
| 25 | 5 | 601 | CLA | C11-C12-C13-C14 |
| 25 | 7 | 606 | CLA | C6-C7-C8-C9 |
| 25 | 7 | 606 | CLA | C6-C7-C8-C10 |
| 25 | 8 | 605 | CLA | C6-C7-C8-C10 |
| 35 | 1 | 804 | LMT | O5'-C1'-O1'-C1 |
| 36 | 8 | 802 | DGD | O6E-C1E-O5D-C6D |
| 36 | 8 | 803 | DGD | O6D-C1D-O3G-C3G |
| 25 | B | 1213 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 3 | 606 | CLA | C13-C15-C16-C17 |
| 26 | 6 | 619 | CHL | C5-C6-C7-C8 |
| 30 | B | 5001 | LHG | C14-C15-C16-C17 |
| 30 | a | 801 | LHG | C11-C10-C9-C8 |
| 30 | 2 | 802 | LHG | C12-C13-C14-C15 |
| 33 | B | 5005 | PTY | C13-C14-C15-C16 |
| 33 | a | 803 | PTY | C35-C36-C37-C38 |
| 41 | 6 | 806 | SPH | C11-C12-C13-C14 |
| 47 | 8 | 807 | PLM | CB-CC-CD-CE |
| 48 | 2 | 803 | DGA | CB9-CAB-CBB-CCB |
| 52 | 8 | 805 | P5S | C42-C43-C44-C45 |
| 33 | a | 802 | PTY | N1-C2-C3-O11 |
| 30 | B | 5001 | LHG | C28-C29-C30-C31 |
| 30 | 1 | 802 | LHG | C12-C13-C14-C15 |
| 30 | 3 | 801 | LHG | C11-C12-C13-C14 |
| 30 | 5 | 801 | LHG | C24-C25-C26-C27 |
| 30 | 7 | 801 | LHG | C11-C12-C13-C14 |
| 33 | a | 803 | PTY | C15-C16-C17-C18 |
| 35 | 1 | 804 | LMT | C5-C6-C7-C8 |
| 47 | 4 | 804 | PLM | C4-C5-C6-C7 |
| 30 | A | 5001 | LHG | C23-C24-C25-C26 |
| 25 | 5 | 612 | CLA | C10-C11-C12-C13 |
| 25 | A | 1013 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1110 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1226 | CLA | O1A-CGA-O2A-C1 |
| 30 | B | 5002 | LHG | C11-C12-C13-C14 |
| 30 | 9 | 802 | LHG | C13-C14-C15-C16 |
| 52 | 8 | 805 | P5S | C40-C41-C42-C43 |
| 25 | A | 1121 | CLA | CBA-CGA-O2A-C1 |
| 30 | 4 | 802 | LHG | C13-C14-C15-C16 |
| 32 | A | 5005 | SQD | C26-C27-C28-C29 |
| 35 | 1 | 804 | LMT | C6-C7-C8-C9 |
| 41 | J | 5002 | SPH | C11-C12-C13-C14 |
| 51 | 7 | 807 | 4RF | C43-C44-C45-C46 |
| 25 | A | 1104 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1109 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1126 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1130 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1133 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1135 | CLA | C3A-C2A-CAA-CBA |
| 25 | A | 1101 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1223 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1207 | CLA | C3A-C2A-CAA-CBA |
| 25 | H | 1701 | CLA | C3A-C2A-CAA-CBA |
| 25 | L | 1504 | CLA | C3A-C2A-CAA-CBA |
| 25 | 1 | 602 | CLA | C3A-C2A-CAA-CBA |
| 25 | a | 602 | CLA | C3A-C2A-CAA-CBA |
| 25 | 4 | 610 | CLA | C3A-C2A-CAA-CBA |
| 25 | 5 | 606 | CLA | C3A-C2A-CAA-CBA |
| 25 | 5 | 615 | CLA | C3A-C2A-CAA-CBA |
| 25 | 8 | 615 | CLA | C3A-C2A-CAA-CBA |
| 25 | 2 | 603 | CLA | C3A-C2A-CAA-CBA |
| 25 | 9 | 612 | CLA | C3A-C2A-CAA-CBA |
| 26 | 4 | 613 | CHL | C3A-C2A-CAA-CBA |
| 26 | 6 | 619 | CHL | C3A-C2A-CAA-CBA |
| 25 | a | 603 | CLA | C5-C6-C7-C8 |
| 30 | F | 5002 | LHG | C28-C29-C30-C31 |
| 30 | 6 | 801 | LHG | C13-C14-C15-C16 |
| 32 | A | 5005 | SQD | C30-C31-C32-C33 |
| 33 | B | 5005 | PTY | C23-C24-C25-C26 |
| 33 | G | 5003 | PTY | C13-C14-C15-C16 |
| 33 | J | 5001 | PTY | C32-C33-C34-C35 |
| 36 | 8 | 803 | DGD | C4E-C5E-C6E-O5E |
| 25 | a | 602 | CLA | O1A-CGA-O2A-C1 |
| 25 | 2 | 603 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1211 | CLA | C6-C7-C8-C9 |
| 25 | B | 1213 | CLA | C6-C7-C8-C9 |
| 25 | B | 1235 | CLA | C16-C17-C18-C20 |
| 25 | F | 1302 | CLA | C6-C7-C8-C9 |
| 25 | a | 608 | CLA | C6-C7-C8-C10 |
| 30 | A | 5001 | LHG | C28-C29-C30-C31 |
| 30 | A | 5001 | LHG | C31-C32-C33-C34 |
| 48 | 8 | 804 | DGA | CB3-CB4-CB5-CB6 |
| 33 | 5 | 802 | PTY | O4-C1-C6-C5 |
| 30 | 1 | 801 | LHG | C11-C10-C9-C8 |
| 25 | B | 1216 | CLA | C3-C5-C6-C7 |
| 26 | A | 1114 | CHL | C3-C5-C6-C7 |
| 30 | 6 | 801 | LHG | C11-C12-C13-C14 |
| 30 | 2 | 801 | LHG | C33-C34-C35-C36 |
| 48 | 5 | 803 | DGA | CA4-CA5-CA6-CA7 |
| 25 | A | 1101 | CLA | C13-C15-C16-C17 |
| 25 | A | 1112 | CLA | C4-C3-C5-C6 |
| 25 | F | 1301 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1103 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1225 | CLA | C2-C3-C5-C6 |
| 25 | B | 1234 | CLA | C2-C3-C5-C6 |
| 26 | 3 | 611 | CHL | C2-C3-C5-C6 |
| 30 | a | 801 | LHG | C8-C7-O7-C5 |
| 30 | 6 | 801 | LHG | C8-C7-O7-C5 |
| 37 | 6 | 803 | PCW | C32-C31-O2-C2 |
| 30 | 3 | 801 | LHG | C17-C18-C19-C20 |
| 48 | 2 | 803 | DGA | CB5-CB6-CB7-CB8 |
| 25 | B | 1023 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1217 | CLA | C2A-CAA-CBA-CGA |
| 25 | 7 | 608 | CLA | C2A-CAA-CBA-CGA |
| 30 | A | 5001 | LHG | O1-C1-C2-O2 |
| 30 | B | 5002 | LHG | O1-C1-C2-O2 |
| 30 | F | 5002 | LHG | O1-C1-C2-O2 |
| 30 | a | 801 | LHG | O1-C1-C2-O2 |
| 30 | 4 | 802 | LHG | O1-C1-C2-O2 |
| 30 | 7 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 7 | 802 | LHG | O1-C1-C2-O2 |
| 30 | 7 | 803 | LHG | O1-C1-C2-O2 |
| 30 | B | 5002 | LHG | C26-C27-C28-C29 |
| 30 | 4 | 802 | LHG | C11-C10-C9-C8 |
| 30 | 5 | 801 | LHG | C29-C30-C31-C32 |
| 30 | 7 | 802 | LHG | C26-C27-C28-C29 |
| 30 | 9 | 802 | LHG | C28-C29-C30-C31 |
| 33 | a | 802 | PTY | C11-C12-C13-C14 |
| 41 | 6 | 806 | SPH | C10-C11-C12-C13 |
| 48 | 8 | 804 | DGA | CB5-CB6-CB7-CB8 |
| 48 | 2 | 803 | DGA | CB2-CB3-CB4-CB5 |
| 51 | 7 | 807 | 4RF | C29-C30-C31-C32 |
| 30 | 4 | 802 | LHG | C23-C24-C25-C26 |
| 45 | 8 | 809 | OLA | C6-C7-C8-C9 |
| 25 | A | 1116 | CLA | O1A-CGA-O2A-C1 |
| 37 | K | 5001 | PCW | O11-C11-O3-C3 |
| 25 | A | 1128 | CLA | C16-C17-C18-C19 |
| 25 | 1 | 605 | CLA | C16-C17-C18-C19 |
| 25 | 1 | 612 | CLA | C16-C17-C18-C20 |
| 30 | 1 | 802 | LHG | C16-C17-C18-C19 |
| 30 | 2 | 802 | LHG | C30-C31-C32-C33 |
| 25 | A | 1125 | CLA | C13-C15-C16-C17 |
| 30 | 2 | 802 | LHG | C27-C28-C29-C30 |
| 25 | A | 1125 | CLA | C3-C5-C6-C7 |
| 25 | 6 | 603 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 7 | 801 | LHG | C28-C29-C30-C31 |
| 30 | 2 | 802 | LHG | C31-C32-C33-C34 |
| 30 | 9 | 802 | LHG | C33-C34-C35-C36 |
| 33 | a | 803 | PTY | C14-C15-C16-C17 |
| 33 | 3 | 802 | PTY | C12-C13-C14-C15 |
| 48 | 8 | 804 | DGA | CB6-CB7-CB8-CB9 |
| 25 | A | 1128 | CLA | O1A-CGA-O2A-C1 |
| 25 | 9 | 612 | CLA | O1A-CGA-O2A-C1 |
| 51 | 7 | 807 | 4RF | C13-C14-C15-C16 |
| 25 | A | 1119 | CLA | C13-C15-C16-C17 |
| 30 | B | 5001 | LHG | C33-C34-C35-C36 |
| 30 | 9 | 801 | LHG | C11-C10-C9-C8 |
| 34 | A | 5007 | 3PH | C24-C25-C26-C27 |
| 45 | a | 805 | OLA | C11-C12-C13-C14 |
| 30 | a | 801 | LHG | O9-C7-O7-C5 |
| 30 | 6 | 801 | LHG | O9-C7-O7-C5 |
| 33 | G | 5003 | PTY | O10-C8-O7-C6 |
| 37 | 6 | 803 | PCW | O31-C31-O2-C2 |
| 25 | A | 1103 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1112 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1118 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1119 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1124 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1140 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1101 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1201 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1208 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1219 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1220 | CLA | C2-C1-O2A-CGA |
| 25 | G | 1601 | CLA | C2-C1-O2A-CGA |
| 25 | H | 1701 | CLA | C2-C1-O2A-CGA |
| 25 | K | 1403 | CLA | C2-C1-O2A-CGA |
| 25 | L | 1501 | CLA | C2-C1-O2A-CGA |
| 25 | L | 1504 | CLA | C2-C1-O2A-CGA |
| 25 | 1 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | a | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 3 | 613 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 611 | CLA | C2-C1-O2A-CGA |
| 25 | 4 | 616 | CLA | C2-C1-O2A-CGA |
| 25 | 5 | 609 | CLA | C2-C1-O2A-CGA |
| 25 | 6 | 602 | CLA | C2-C1-O2A-CGA |
| 25 | 8 | 609 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 2 | 615 | CLA | C2-C1-O2A-CGA |
| 33 | 5 | 802 | PTY | C32-C33-C34-C35 |
| 48 | 8 | 804 | DGA | CA8-CA9-CAA-CBA |
| 25 | B | 1207 | CLA | C10-C11-C12-C13 |
| 25 | a | 601 | CLA | C5-C6-C7-C8 |
| 30 | 2 | 801 | LHG | O10-C23-O8-C6 |
| 25 | A | 1110 | CLA | C5-C6-C7-C8 |
| 25 | B | 1221 | CLA | C16-C17-C18-C19 |
| 25 | 5 | 612 | CLA | C16-C17-C18-C19 |
| 32 | H | 5001 | SQD | C7-C8-C9-C10 |
| 48 | 3 | 803 | DGA | CB1-CB2-CB3-CB4 |
| 29 | A | 4001 | BCR | C23-C24-C25-C26 |
| 29 | A | 4001 | BCR | C23-C24-C25-C30 |
| 29 | A | 4004 | BCR | C1-C6-C7-C8 |
| 29 | A | 4004 | BCR | C5-C6-C7-C8 |
| 29 | B | 4001 | BCR | C1-C6-C7-C8 |
| 29 | B | 4001 | BCR | C5-C6-C7-C8 |
| 29 | B | 4002 | BCR | C23-C24-C25-C26 |
| 29 | B | 4004 | BCR | C1-C6-C7-C8 |
| 29 | B | 4004 | BCR | C5-C6-C7-C8 |
| 29 | B | 4004 | BCR | C23-C24-C25-C26 |
| 29 | B | 4005 | BCR | C1-C6-C7-C8 |
| 29 | B | 4005 | BCR | C5-C6-C7-C8 |
| 29 | H | 4001 | BCR | C1-C6-C7-C8 |
| 29 | H | 4001 | BCR | C5-C6-C7-C8 |
| 29 | H | 4001 | BCR | C23-C24-C25-C26 |
| 29 | H | 4001 | BCR | C23-C24-C25-C30 |
| 29 | J | 4001 | BCR | C23-C24-C25-C26 |
| 29 | J | 4001 | BCR | C23-C24-C25-C30 |
| 29 | K | 4002 | BCR | C23-C24-C25-C26 |
| 29 | K | 4002 | BCR | C23-C24-C25-C30 |
| 29 | L | 4002 | BCR | C1-C6-C7-C8 |
| 29 | L | 4002 | BCR | C5-C6-C7-C8 |
| 29 | L | 4003 | BCR | C1-C6-C7-C8 |
| 29 | L | 4003 | BCR | C5-C6-C7-C8 |
| 29 | L | 4003 | BCR | C23-C24-C25-C26 |
| 29 | L | 4001 | BCR | C1-C6-C7-C8 |
| 29 | L | 4001 | BCR | C5-C6-C7-C8 |
| 29 | I | 4001 | BCR | C1-C6-C7-C8 |
| 29 | I | 4001 | BCR | C5-C6-C7-C8 |
| 29 | O | 4001 | BCR | C1-C6-C7-C8 |
| 29 | O | 4001 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | O | 4001 | BCR | C23-C24-C25-C26 |
| 29 | O | 4001 | BCR | C23-C24-C25-C30 |
| 29 | 3 | 503 | BCR | C1-C6-C7-C8 |
| 29 | 3 | 503 | BCR | C23-C24-C25-C26 |
| 29 | 3 | 505 | BCR | C23-C24-C25-C26 |
| 29 | 3 | 505 | BCR | C23-C24-C25-C30 |
| 29 | 4 | 503 | BCR | C1-C6-C7-C8 |
| 29 | 4 | 503 | BCR | C5-C6-C7-C8 |
| 29 | 5 | 503 | BCR | C1-C6-C7-C8 |
| 29 | 5 | 504 | BCR | C1-C6-C7-C8 |
| 29 | 5 | 504 | BCR | C5-C6-C7-C8 |
| 29 | 5 | 504 | BCR | C23-C24-C25-C26 |
| 29 | 5 | 504 | BCR | C23-C24-C25-C30 |
| 29 | 6 | 503 | BCR | C1-C6-C7-C8 |
| 29 | 6 | 503 | BCR | C5-C6-C7-C8 |
| 29 | 6 | 504 | BCR | C23-C24-C25-C26 |
| 29 | 6 | 504 | BCR | C23-C24-C25-C30 |
| 29 | 7 | 503 | BCR | C1-C6-C7-C8 |
| 29 | 7 | 503 | BCR | C5-C6-C7-C8 |
| 29 | 8 | 503 | BCR | C1-C6-C7-C8 |
| 40 | J | 4002 | RRX | C23-C24-C25-C26 |
| 42 | M | 4001 | ECH | C23-C24-C25-C26 |
| 43 | 1 | 501 | LUT | C1-C6-C7-C8 |
| 43 | a | 501 | LUT | C1-C6-C7-C8 |
| 43 | 6 | 501 | LUT | C1-C6-C7-C8 |
| 43 | 2 | 507 | LUT | C1-C6-C7-C8 |
| 43 | 2 | 507 | LUT | C5-C6-C7-C8 |
| 44 | 1 | 502 | AXT | C21-C26-C27-C28 |
| 44 | 7 | 504 | AXT | C21-C26-C27-C28 |
| 37 | K | 5002 | PCW | C32-C33-C34-C35 |
| 41 | J | 5002 | SPH | C10-C11-C12-C13 |
| 48 | 2 | 803 | DGA | CA9-CAA-CBA-CCA |
| 25 | A | 1137 | CLA | CBA-CGA-O2A-C1 |
| 25 | 1 | 605 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1127 | CLA | C13-C15-C16-C17 |
| 25 | B | 1205 | CLA | C13-C15-C16-C17 |
| 25 | B | 1216 | CLA | C15-C16-C17-C18 |
| 25 | B | 1231 | CLA | C13-C15-C16-C17 |
| 25 | B | 1235 | CLA | C5-C6-C7-C8 |
| 52 | 8 | 805 | P5S | C39-C38-O37-C2 |
| 33 | 9 | 803 | PTY | C11-C12-C13-C14 |
| 25 | A | 1121 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1209 | CLA | CBD-CGD-O2D-CED |
| 30 | F | 5002 | LHG | C7-C8-C9-C10 |
| 25 | A | 1108 | CLA | C8-C10-C11-C12 |
| 25 | A | 1126 | CLA | C15-C16-C17-C18 |
| 25 | 2 | 607 | CLA | C10-C11-C12-C13 |
| 30 | 3 | 801 | LHG | C26-C27-C28-C29 |
| 33 | a | 803 | PTY | C11-C12-C13-C14 |
| 34 | A | 5007 | 3PH | C27-C28-C29-C2A |
| 34 | A | 5007 | 3PH | C34-C35-C36-C37 |
| 37 | B | 5004 | PCW | C32-C33-C34-C35 |
| 45 | 8 | 808 | OLA | C11-C12-C13-C14 |
| 25 | A | 1103 | CLA | C4-C3-C5-C6 |
| 25 | A | 1109 | CLA | C4-C3-C5-C6 |
| 25 | B | 1234 | CLA | C4-C3-C5-C6 |
| 25 | 2 | 605 | CLA | C4-C3-C5-C6 |
| 25 | A | 1103 | CLA | C6-C7-C8-C10 |
| 25 | A | 1109 | CLA | C2-C3-C5-C6 |
| 25 | A | 1111 | CLA | C11-C10-C8-C7 |
| 25 | A | 1119 | CLA | C2-C3-C5-C6 |
| 25 | A | 1125 | CLA | C6-C7-C8-C10 |
| 25 | A | 1128 | CLA | C2-C3-C5-C6 |
| 25 | A | 1136 | CLA | C11-C10-C8-C7 |
| 25 | A | 1138 | CLA | C11-C10-C8-C7 |
| 25 | A | 1101 | CLA | C11-C10-C8-C7 |
| 25 | B | 1204 | CLA | C2-C3-C5-C6 |
| 25 | B | 1229 | CLA | C6-C7-C8-C10 |
| 25 | B | 1231 | CLA | C12-C13-C15-C16 |
| 25 | B | 1234 | CLA | C6-C7-C8-C10 |
| 25 | B | 1239 | CLA | C12-C13-C15-C16 |
| 25 | a | 607 | CLA | C6-C7-C8-C10 |
| 25 | 4 | 603 | CLA | C2-C3-C5-C6 |
| 25 | 5 | 612 | CLA | C2-C3-C5-C6 |
| 25 | 7 | 603 | CLA | C12-C13-C15-C16 |
| 25 | 7 | 604 | CLA | C12-C13-C15-C16 |
| 25 | 7 | 610 | CLA | C11-C10-C8-C7 |
| 25 | 7 | 612 | CLA | C6-C7-C8-C10 |
| 25 | 2 | 603 | CLA | C11-C10-C8-C7 |
| 25 | 2 | 605 | CLA | C2-C3-C5-C6 |
| 25 | 2 | 605 | CLA | C11-C10-C8-C7 |
| 25 | 2 | 607 | CLA | C12-C13-C15-C16 |
| 26 | A | 1114 | CHL | C11-C10-C8-C7 |
| 26 | 1 | 609 | CHL | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | 1 | 609 | CHL | C11-C12-C13-C15 |
| 26 | 9 | 603 | CHL | C12-C13-C15-C16 |
| 27 | A | 2001 | PQN | C17-C18-C20-C21 |
| 25 | A | 1122 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1137 | CLA | O1A-CGA-O2A-C1 |
| 25 | F | 1301 | CLA | O1A-CGA-O2A-C1 |
| 25 | 6 | 603 | CLA | O1A-CGA-O2A-C1 |
| 30 | 9 | 802 | LHG | C29-C30-C31-C32 |
| 25 | A | 1108 | CLA | C10-C11-C12-C13 |
| 25 | A | 1133 | CLA | C8-C10-C11-C12 |
| 25 | 7 | 603 | CLA | C13-C15-C16-C17 |
| 29 | A | 4004 | BCR | C13-C14-C15-C16 |
| 29 | B | 4003 | BCR | C19-C20-C21-C22 |
| 29 | B | 4006 | BCR | C19-C20-C21-C22 |
| 29 | I | 4001 | BCR | C13-C14-C15-C16 |
| 43 | 6 | 501 | LUT | C29-C30-C31-C32 |
| 25 | A | 1109 | CLA | C16-C17-C18-C20 |
| 25 | 7 | 601 | CLA | C11-C12-C13-C15 |
| 25 | B | 1217 | CLA | O1D-CGD-O2D-CED |
| 45 | 1 | 803 | OLA | C6-C7-C8-C9 |
| 30 | 9 | 802 | LHG | O9-C7-O7-C5 |
| 30 | 9 | 801 | LHG | O9-C7-O7-C5 |
| 33 | B | 5005 | PTY | O10-C8-O7-C6 |
| 52 | 8 | 805 | P5S | O47-C38-O37-C2 |
| 30 | 2 | 801 | LHG | C7-C8-C9-C10 |
| 25 | A | 1119 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1224 | CLA | CBA-CGA-O2A-C1 |
| 25 | 1 | 603 | CLA | CBA-CGA-O2A-C1 |
| 25 | 5 | 606 | CLA | CBA-CGA-O2A-C1 |
| 37 | K | 5002 | PCW | C12-C11-O3-C3 |
| 37 | 6 | 803 | PCW | C32-C33-C34-C35 |
| 25 | B | 1235 | CLA | C2A-CAA-CBA-CGA |
| 25 | 1 | 612 | CLA | C2A-CAA-CBA-CGA |
| 25 | a | 612 | CLA | C2A-CAA-CBA-CGA |
| 25 | 4 | 604 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 604 | CLA | C2A-CAA-CBA-CGA |
| 25 | 6 | 618 | CLA | C2A-CAA-CBA-CGA |
| 25 | 7 | 603 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 612 | CLA | C2A-CAA-CBA-CGA |
| 26 | 1 | 604 | CHL | C2A-CAA-CBA-CGA |
| 26 | 3 | 603 | CHL | C2A-CAA-CBA-CGA |
| 26 | 8 | 604 | CHL | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1013 | CLA | C5-C6-C7-C8 |
| 25 | A | 1104 | CLA | C8-C10-C11-C12 |
| 25 | A | 1117 | CLA | C13-C15-C16-C17 |
| 25 | A | 1131 | CLA | C15-C16-C17-C18 |
| 25 | a | 607 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 601 | CLA | C5-C6-C7-C8 |
| 30 | 1 | 802 | LHG | C13-C14-C15-C16 |
| 30 | 2 | 801 | LHG | C9-C10-C11-C12 |
| 32 | G | 5001 | SQD | C29-C30-C31-C32 |
| 25 | a | 607 | CLA | O1D-CGD-O2D-CED |
| 30 | a | 801 | LHG | C24-C25-C26-C27 |
| 33 | a | 803 | PTY | C31-C32-C33-C34 |
| 37 | B | 5004 | PCW | C33-C34-C35-C36 |
| 25 | A | 1133 | CLA | C5-C6-C7-C8 |
| 25 | A | 1136 | CLA | C8-C10-C11-C12 |
| 25 | B | 1203 | CLA | C13-C15-C16-C17 |
| 30 | 4 | 801 | LHG | C11-C12-C13-C14 |
| 30 | 2 | 802 | LHG | C9-C10-C11-C12 |
| 30 | 9 | 802 | LHG | C16-C17-C18-C19 |
| 32 | A | 5005 | SQD | C28-C29-C30-C31 |
| 47 | 4 | 804 | PLM | C9-CA-CB-CC |
| 48 | 8 | 804 | DGA | CA4-CA5-CA6-CA7 |
| 35 | 1 | 804 | LMT | C1-C2-C3-C4 |
| 25 | A | 1137 | CLA | C11-C12-C13-C15 |
| 26 | 3 | 611 | CHL | C11-C12-C13-C15 |
| 32 | H | 5001 | SQD | O5-C1-O6-C44 |
| 25 | A | 1126 | CLA | C5-C6-C7-C8 |
| 25 | A | 1130 | CLA | C5-C6-C7-C8 |
| 25 | 2 | 601 | CLA | C5-C6-C7-C8 |
| 37 | 6 | 803 | PCW | C33-C34-C35-C36 |
| 30 | 4 | 802 | LHG | C7-C8-C9-C10 |
| 30 | 6 | 802 | LHG | C7-C8-C9-C10 |
| 33 | B | 5005 | PTY | C30-C31-C32-C33 |
| 30 | 9 | 801 | LHG | C8-C7-O7-C5 |
| 32 | 7 | 805 | SQD | C8-C7-O47-C45 |
| 33 | B | 5005 | PTY | C11-C8-O7-C6 |
| 33 | a | 802 | PTY | C11-C8-O7-C6 |
| 48 | 2 | 803 | DGA | CB2-CB1-OG2-CG2 |
| 51 | 7 | 807 | 4RF | C24-C22-O21-C20 |
| 37 | B | 5004 | PCW | O3P-C1-C2-O2 |
| 30 | 7 | 801 | LHG | C25-C26-C27-C28 |
| 30 | 9 | 802 | LHG | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 9 | 804 | SPH | C7-C8-C9-C10 |
| 48 | 8 | 804 | DGA | CB7-CB8-CB9-CAB |
| 25 | B | 1209 | CLA | C10-C11-C12-C13 |
| 25 | B | 1223 | CLA | C8-C10-C11-C12 |
| 32 | I | 5001 | SQD | C28-C29-C30-C31 |
| 33 | 3 | 802 | PTY | C33-C34-C35-C36 |
| 33 | a | 802 | PTY | O10-C8-O7-C6 |
| 48 | 2 | 803 | DGA | OB1-CB1-OG2-CG2 |
| 25 | B | 1206 | CLA | C3-C5-C6-C7 |
| 25 | L | 1502 | CLA | C3-C5-C6-C7 |
| 25 | 7 | 603 | CLA | C3-C5-C6-C7 |
| 30 | A | 5002 | LHG | C11-C12-C13-C14 |
| 36 | B | 5003 | DGD | C7A-C8A-C9A-CAA |
| 35 | 1 | 804 | LMT | C2'-C1'-O1'-C1 |
| 33 | 5 | 802 | PTY | O4-C1-C6-O7 |
| 33 | a | 803 | PTY | C36-C37-C38-C39 |
| 25 | 2 | 605 | CLA | C11-C12-C13-C14 |
| 30 | 3 | 801 | LHG | C10-C11-C12-C13 |
| 30 | 5 | 801 | LHG | C11-C12-C13-C14 |
| 33 | a | 802 | PTY | C36-C37-C38-C39 |
| 41 | J | 5002 | SPH | C7-C8-C9-C10 |
| 47 | 4 | 803 | PLM | C4-C5-C6-C7 |
| 25 | B | 1021 | CLA | C15-C16-C17-C18 |
| 25 | B | 1210 | CLA | C10-C11-C12-C13 |
| 25 | A | 1119 | CLA | C4-C3-C5-C6 |
| 25 | A | 1123 | CLA | C4-C3-C5-C6 |
| 25 | B | 1216 | CLA | C4-C3-C5-C6 |
| 25 | 4 | 603 | CLA | C4-C3-C5-C6 |
| 25 | A | 1123 | CLA | C2-C3-C5-C6 |
| 25 | 6 | 602 | CLA | C2-C3-C5-C6 |
| 25 | 7 | 603 | CLA | C2-C3-C5-C6 |
| 30 | B | 5001 | LHG | C26-C27-C28-C29 |
| 25 | A | 1103 | CLA | C6-C7-C8-C9 |
| 25 | A | 1104 | CLA | C14-C13-C15-C16 |
| 25 | A | 1131 | CLA | C6-C7-C8-C9 |
| 25 | A | 1133 | CLA | C11-C10-C8-C9 |
| 25 | A | 1136 | CLA | C11-C10-C8-C9 |
| 25 | A | 1101 | CLA | C6-C7-C8-C9 |
| 25 | B | 1212 | CLA | C6-C7-C8-C9 |
| 25 | B | 1214 | CLA | C6-C7-C8-C9 |
| 25 | B | 1220 | CLA | C6-C7-C8-C9 |
| 25 | B | 1229 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 603 | CLA | C11-C12-C13-C14 |
| 25 | 1 | 612 | CLA | C11-C10-C8-C9 |
| 25 | 3 | 601 | CLA | C11-C12-C13-C14 |
| 25 | 7 | 603 | CLA | C14-C13-C15-C16 |
| 25 | 7 | 604 | CLA | C11-C10-C8-C9 |
| 25 | 7 | 604 | CLA | C14-C13-C15-C16 |
| 25 | 7 | 612 | CLA | C6-C7-C8-C9 |
| 25 | 8 | 606 | CLA | C11-C10-C8-C9 |
| 26 | A | 1114 | CHL | C11-C10-C8-C9 |
| 26 | 1 | 609 | CHL | C11-C12-C13-C14 |
| 26 | 9 | 601 | CHL | C14-C13-C15-C16 |
| 26 | 9 | 603 | CHL | C14-C13-C15-C16 |
| 27 | B | 2002 | PQN | C21-C22-C23-C24 |
| 25 | A | 1119 | CLA | C3-C5-C6-C7 |
| 25 | B | 1236 | CLA | C3-C5-C6-C7 |
| 25 | 4 | 601 | CLA | C3-C5-C6-C7 |
| 25 | A | 1116 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1122 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1129 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1130 | CLA | C2A-CAA-CBA-CGA |
| 25 | a | 611 | CLA | C2A-CAA-CBA-CGA |
| 26 | a | 604 | CHL | C2A-CAA-CBA-CGA |
| 30 | 7 | 801 | LHG | C10-C11-C12-C13 |
| 29 | A | 4003 | BCR | C37-C22-C23-C24 |
| 29 | L | 4002 | BCR | C36-C18-C19-C20 |
| 50 | 9 | 504 | XAT | C11-C12-C13-C20 |
| 25 | 3 | 610 | CLA | O1D-CGD-O2D-CED |
| 25 | A | 1104 | CLA | C13-C15-C16-C17 |
| 25 | 4 | 611 | CLA | C5-C6-C7-C8 |
| 30 | A | 5002 | LHG | C26-C27-C28-C29 |
| 30 | B | 5002 | LHG | C31-C32-C33-C34 |
| 30 | 2 | 801 | LHG | C16-C17-C18-C19 |
| 35 | A | 5008 | LMT | C4-C5-C6-C7 |
| 48 | 3 | 803 | DGA | CB3-CB4-CB5-CB6 |
| 53 | 8 | 810 | LAP | C7-C8-C9-C10 |
| 29 | A | 4002 | BCR | C17-C18-C19-C20 |
| 29 | A | 4003 | BCR | C21-C22-C23-C24 |
| 29 | B | 4005 | BCR | C7-C8-C9-C10 |
| 29 | K | 4002 | BCR | C17-C18-C19-C20 |
| 29 | 5 | 504 | BCR | C17-C18-C19-C20 |
| 43 | a | 503 | LUT | C31-C32-C33-C34 |
| 25 | 1 | 603 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 605 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1103 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1104 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1106 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1107 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1108 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1113 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1118 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1121 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1122 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1124 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1132 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1134 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1135 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1021 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1202 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1214 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1216 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1217 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1227 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1229 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1230 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1235 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1239 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1240 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1207 | CLA | C1A-C2A-CAA-CBA |
| 25 | F | 1301 | CLA | C1A-C2A-CAA-CBA |
| 25 | F | 1302 | CLA | C1A-C2A-CAA-CBA |
| 25 | H | 1701 | CLA | C1A-C2A-CAA-CBA |
| 25 | K | 1402 | CLA | C1A-C2A-CAA-CBA |
| 25 | L | 1502 | CLA | C1A-C2A-CAA-CBA |
| 25 | L | 1503 | CLA | C1A-C2A-CAA-CBA |
| 25 | L | 1504 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 602 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 607 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 608 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 612 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 602 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 607 | CLA | C1A-C2A-CAA-CBA |
| 25 | a | 612 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 3 | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | 3 | 610 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 610 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 611 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 616 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 617 | CLA | C1A-C2A-CAA-CBA |
| 25 | 5 | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | 5 | 607 | CLA | C1A-C2A-CAA-CBA |
| 25 | 6 | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | 7 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 7 | 608 | CLA | C1A-C2A-CAA-CBA |
| 25 | 7 | 610 | CLA | C1A-C2A-CAA-CBA |
| 25 | 7 | 612 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 605 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 612 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 615 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 620 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 601 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 603 | CLA | C1A-C2A-CAA-CBA |
| 26 | 1 | 604 | CHL | C1A-C2A-CAA-CBA |
| 26 | a | 604 | CHL | C1A-C2A-CAA-CBA |
| 26 | a | 606 | CHL | C1A-C2A-CAA-CBA |
| 26 | a | 613 | CHL | C1A-C2A-CAA-CBA |
| 26 | 3 | 604 | CHL | C1A-C2A-CAA-CBA |
| 26 | 4 | 613 | CHL | C1A-C2A-CAA-CBA |
| 26 | 8 | 604 | CHL | C1A-C2A-CAA-CBA |
| 26 | 8 | 610 | CHL | C1A-C2A-CAA-CBA |
| 26 | 9 | 601 | CHL | C1A-C2A-CAA-CBA |
| 24 | A | 1011 | CL0 | C16-C17-C18-C20 |
| 25 | A | 1117 | CLA | C16-C17-C18-C19 |
| 25 | A | 1137 | CLA | C11-C12-C13-C14 |
| 25 | B | 1221 | CLA | C16-C17-C18-C20 |
| 25 | B | 1238 | CLA | C16-C17-C18-C20 |
| 25 | B | 1207 | CLA | C11-C12-C13-C15 |
| 25 | 1 | 605 | CLA | C16-C17-C18-C20 |
| 25 | a | 605 | CLA | C6-C7-C8-C9 |
| 25 | 6 | 607 | CLA | C6-C7-C8-C9 |
| 25 | 7 | 601 | CLA | C11-C12-C13-C14 |
| 27 | A | 2001 | PQN | C26-C27-C28-C29 |
| 32 | 7 | 805 | SQD | O49-C7-O47-C45 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 5 | 801 | LHG | C8-C7-O7-C5 |
| 30 | a | 801 | LHG | C29-C30-C31-C32 |
| 30 | 6 | 801 | LHG | C9-C10-C11-C12 |
| 47 | a | 804 | PLM | CC-CD-CE-CF |
| 29 | A | 4003 | BCR | C15-C16-C17-C18 |
| 29 | 6 | 503 | BCR | C15-C16-C17-C18 |
| 29 | 6 | 504 | BCR | C9-C10-C11-C12 |
| 43 | a | 503 | LUT | C29-C30-C31-C32 |
| 43 | 6 | 502 | LUT | C29-C30-C31-C32 |
| 50 | 9 | 507 | XAT | C29-C30-C31-C32 |
| 25 | 1 | 607 | CLA | C13-C15-C16-C17 |
| 25 | 4 | 601 | CLA | C10-C11-C12-C13 |
| 25 | 6 | 615 | CLA | C10-C11-C12-C13 |
| 30 | 1 | 802 | LHG | C4-O6-P-O3 |
| 30 | 4 | 801 | LHG | C3-O3-P-O6 |
| 30 | 2 | 802 | LHG | C3-O3-P-O6 |
| 33 | G | 5002 | PTY | C5-O14-P1-O11 |
| 33 | 5 | 802 | PTY | C3-O11-P1-O14 |
| 33 | 9 | 803 | PTY | C3-O11-P1-O14 |
| 37 | K | 5002 | PCW | C1-O3P-P-O4P |
| 30 | 5 | 801 | LHG | C23-C24-C25-C26 |
| 36 | 7 | 806 | DGD | C1B-C2B-C3B-C4B |
| 25 | 6 | 607 | CLA | C3-C5-C6-C7 |
| 25 | A | 1106 | CLA | C5-C6-C7-C8 |
| 25 | A | 1136 | CLA | C13-C15-C16-C17 |
| 30 | 1 | 802 | LHG | O6-C4-C5-C6 |
| 30 | 6 | 802 | LHG | O6-C4-C5-C6 |
| 30 | 7 | 802 | LHG | O6-C4-C5-C6 |
| 30 | 8 | 801 | LHG | O6-C4-C5-C6 |
| 37 | K | 5001 | PCW | O3P-C1-C2-C3 |
| 30 | 7 | 801 | LHG | C29-C30-C31-C32 |
| 30 | 8 | 801 | LHG | C30-C31-C32-C33 |
| 33 | 9 | 803 | PTY | C38-C39-C40-C41 |
| 48 | 8 | 804 | DGA | CA6-CA7-CA8-CA9 |
| 30 | A | 5001 | LHG | C25-C26-C27-C28 |
| 25 | B | 1231 | CLA | C8-C10-C11-C12 |
| 25 | 4 | 610 | CLA | C13-C15-C16-C17 |
| 25 | 6 | 608 | CLA | C5-C6-C7-C8 |
| 25 | A | 1111 | CLA | C16-C17-C18-C19 |
| 25 | A | 1122 | CLA | C11-C12-C13-C15 |
| 32 | A | 5005 | SQD | C13-C14-C15-C16 |
| 32 | A | 5005 | SQD | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 2 | 803 | DGA | CA7-CA8-CA9-CAA |
| 30 | 4 | 801 | LHG | C13-C14-C15-C16 |
| 45 | a | 805 | OLA | C10-C11-C12-C13 |
| 45 | 8 | 808 | OLA | C10-C11-C12-C13 |
| 37 | 6 | 803 | PCW | C14-C15-C16-C17 |
| 25 | B | 1204 | CLA | C4-C3-C5-C6 |
| 25 | 7 | 603 | CLA | C4-C3-C5-C6 |
| 30 | 4 | 801 | LHG | C25-C26-C27-C28 |
| 30 | 7 | 801 | LHG | C9-C10-C11-C12 |
| 32 | G | 5001 | SQD | C12-C13-C14-C15 |
| 52 | 8 | 805 | P5S | C39-C40-C41-C42 |
| 25 | A | 1127 | CLA | C8-C10-C11-C12 |
| 25 | A | 1132 | CLA | C13-C15-C16-C17 |
| 25 | B | 1022 | CLA | C10-C11-C12-C13 |
| 25 | a | 603 | CLA | C8-C10-C11-C12 |
| 35 | 2 | 804 | LMT | O5B-C5B-C6B-O6B |
| 30 | F | 5001 | LHG | C25-C26-C27-C28 |
| 30 | 7 | 802 | LHG | C27-C28-C29-C30 |
| 25 | 5 | 606 | CLA | O1A-CGA-O2A-C1 |
| 37 | K | 5002 | PCW | O11-C11-O3-C3 |
| 25 | A | 1125 | CLA | C16-C17-C18-C20 |
| 25 | 9 | 605 | CLA | C11-C12-C13-C15 |
| 30 | A | 5002 | LHG | C25-C26-C27-C28 |
| 30 | B | 5001 | LHG | C4-C5-C6-O8 |
| 30 | F | 5001 | LHG | C4-C5-C6-O8 |
| 30 | 3 | 801 | LHG | C25-C26-C27-C28 |
| 30 | 6 | 801 | LHG | C4-C5-C6-O8 |
| 30 | 7 | 802 | LHG | C29-C30-C31-C32 |
| 30 | 8 | 801 | LHG | C4-C5-C6-O8 |
| 30 | 2 | 801 | LHG | C4-C5-C6-O8 |
| 32 | G | 5001 | SQD | O6-C44-C45-C46 |
| 32 | I | 5001 | SQD | C14-C15-C16-C17 |
| 32 | 7 | 805 | SQD | C11-C12-C13-C14 |
| 33 | 9 | 803 | PTY | O4-C1-C6-C5 |
| 36 | B | 5003 | DGD | O1G-C1G-C2G-C3G |
| 37 | K | 5002 | PCW | C1-C2-C3-O3 |
| 48 | 5 | 803 | DGA | OG1-CG1-CG2-CG3 |
| 48 | 2 | 803 | DGA | CBB-CAB-CB9-CB8 |
| 25 | B | 1228 | CLA | C5-C6-C7-C8 |
| 25 | 1 | 605 | CLA | C10-C11-C12-C13 |
| 25 | 7 | 603 | CLA | C10-C11-C12-C13 |
| 30 | 7 | 803 | LHG | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 36 | 8 | 803 | DGD | O6D-C5D-C6D-O5D |
| 36 | 8 | 802 | DGD | C5D-C6D-O5D-C1E |
| 36 | 8 | 803 | DGD | C5D-C6D-O5D-C1E |
| 33 | 5 | 802 | PTY | C37-C38-C39-C40 |
| 36 | B | 5003 | DGD | O6E-C5E-C6E-O5E |
| 25 | A | 1101 | CLA | C8-C10-C11-C12 |
| 30 | 6 | 802 | LHG | C9-C10-C11-C12 |
| 30 | 2 | 802 | LHG | C35-C36-C37-C38 |
| 37 | B | 5004 | PCW | C42-C43-C44-C45 |
| 52 | 8 | 805 | P5S | C45-C46-C48-C49 |
| 25 | B | 1227 | CLA | CAA-CBA-CGA-O2A |
| 26 | 6 | 610 | CHL | CAA-CBA-CGA-O2A |
| 30 | 1 | 802 | LHG | O8-C23-C24-C25 |
| 30 | B | 5001 | LHG | C9-C10-C11-C12 |
| 30 | F | 5001 | LHG | C11-C10-C9-C8 |
| 32 | I | 5001 | SQD | C11-C10-C9-C8 |
| 48 | 2 | 803 | DGA | CBB-CCB-CDB-CEB |
| 25 | 6 | 606 | CLA | C3-C5-C6-C7 |
| 30 | A | 5002 | LHG | C16-C17-C18-C19 |
| 48 | 3 | 803 | DGA | CA6-CA7-CA8-CA9 |
| 48 | 5 | 803 | DGA | CA6-CA7-CA8-CA9 |
| 30 | A | 5002 | LHG | O1-C1-C2-O2 |
| 30 | 1 | 802 | LHG | O1-C1-C2-O2 |
| 30 | 3 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 6 | 802 | LHG | O1-C1-C2-O2 |
| 30 | 2 | 802 | LHG | O1-C1-C2-O2 |
| 30 | 9 | 801 | LHG | O1-C1-C2-O2 |
| 25 | 4 | 602 | CLA | C3-C5-C6-C7 |
| 36 | 8 | 803 | DGD | C2G-C1G-O1G-C1A |
| 30 | 3 | 801 | LHG | C28-C29-C30-C31 |
| 30 | 3 | 801 | LHG | C32-C33-C34-C35 |
| 25 | 6 | 604 | CLA | C8-C10-C11-C12 |
| 25 | A | 1119 | CLA | O1A-CGA-O2A-C1 |
| 30 | A | 5003 | LHG | C30-C31-C32-C33 |
| 30 | 7 | 802 | LHG | C11-C12-C13-C14 |
| 30 | 9 | 801 | LHG | C11-C12-C13-C14 |
| 30 | B | 5001 | LHG | C8-C7-O7-C5 |
| 30 | 3 | 801 | LHG | C35-C36-C37-C38 |
| 30 | 2 | 802 | LHG | C11-C10-C9-C8 |
| 33 | a | 802 | PTY | C31-C32-C33-C34 |
| 48 | 8 | 804 | DGA | CCB-CDB-CEB-CFB |
| 48 | 2 | 803 | DGA | CA6-CA7-CA8-CA9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 51 | 7 | 807 | 4RF | C26-C27-C28-C29 |
| 25 | 1 | 607 | CLA | C10-C11-C12-C13 |
| 36 | 7 | 806 | DGD | O6E-C5E-C6E-O5E |
| 25 | 4 | 605 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1101 | CLA | C4-C3-C5-C6 |
| 25 | 1 | 603 | CLA | C4-C3-C5-C6 |
| 30 | 2 | 801 | LHG | C34-C35-C36-C37 |
| 48 | 5 | 803 | DGA | CB3-CB4-CB5-CB6 |
| 48 | 2 | 803 | DGA | CA8-CA9-CAA-CBA |
| 25 | 1 | 603 | CLA | C2-C3-C5-C6 |
| 25 | 3 | 601 | CLA | C16-C17-C18-C20 |
| 25 | B | 1227 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 601 | CLA | CBA-CGA-O2A-C1 |
| 34 | A | 5007 | 3PH | C32-C31-O31-C3 |
| 36 | B | 5003 | DGD | C2A-C1A-O1G-C1G |
| 25 | A | 1115 | CLA | C8-C10-C11-C12 |
| 25 | 8 | 618 | CLA | C10-C11-C12-C13 |
| 30 | B | 5002 | LHG | C29-C30-C31-C32 |
| 30 | B | 5002 | LHG | C35-C36-C37-C38 |
| 33 | B | 5005 | PTY | C26-C27-C28-C29 |
| 25 | 3 | 618 | CLA | O1A-CGA-O2A-C1 |
| 33 | 3 | 802 | PTY | C5-C6-O7-C8 |
| 33 | 5 | 802 | PTY | C5-C6-O7-C8 |
| 25 | A | 1013 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1141 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 602 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 607 | CLA | C2A-CAA-CBA-CGA |
| 26 | 1 | 609 | CHL | C2A-CAA-CBA-CGA |
| 25 | B | 1224 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1237 | CLA | C10-C11-C12-C13 |
| 25 | A | 1127 | CLA | C2-C1-O2A-CGA |
| 25 | 6 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 604 | CLA | C2-C1-O2A-CGA |
| 25 | 8 | 612 | CLA | C2-C1-O2A-CGA |
| 25 | 8 | 618 | CLA | C2-C1-O2A-CGA |
| 25 | 2 | 602 | CLA | C2-C1-O2A-CGA |
| 26 | 8 | 610 | CHL | C2-C1-O2A-CGA |
| 30 | B | 5001 | LHG | C35-C36-C37-C38 |
| 30 | 3 | 801 | LHG | C27-C28-C29-C30 |
| 30 | 8 | 801 | LHG | C27-C28-C29-C30 |
| 45 | 8 | 808 | OLA | C13-C14-C15-C16 |
| 30 | 2 | 802 | LHG | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1224 | CLA | C10-C11-C12-C13 |
| 30 | A | 5003 | LHG | C26-C27-C28-C29 |
| 33 | A | 5006 | PTY | C31-C32-C33-C34 |
| 25 | B | 1235 | CLA | CBA-CGA-O2A-C1 |
| 30 | 1 | 801 | LHG | O6-C4-C5-O7 |
| 33 | J | 5001 | PTY | O14-C5-C6-O7 |
| 48 | 3 | 803 | DGA | OG1-CA1-CA2-CA3 |
| 25 | A | 1109 | CLA | C16-C17-C18-C19 |
| 25 | a | 605 | CLA | C6-C7-C8-C10 |
| 25 | 8 | 618 | CLA | C11-C12-C13-C15 |
| 30 | A | 5002 | LHG | C13-C14-C15-C16 |
| 30 | 2 | 801 | LHG | C35-C36-C37-C38 |
| 32 | G | 5001 | SQD | C27-C28-C29-C30 |
| 25 | A | 1117 | CLA | C8-C10-C11-C12 |
| 25 | B | 1222 | CLA | C8-C10-C11-C12 |
| 25 | 1 | 608 | CLA | C8-C10-C11-C12 |
| 26 | 1 | 609 | CHL | C5-C6-C7-C8 |
| 29 | 5 | 504 | BCR | C11-C10-C9-C8 |
| 36 | 7 | 806 | DGD | C2E-C1E-O5D-C6D |
| 47 | a | 804 | PLM | CD-CE-CF-CG |
| 30 | 1 | 801 | LHG | O7-C5-C6-O8 |
| 30 | 8 | 801 | LHG | O7-C5-C6-O8 |
| 32 | 7 | 805 | SQD | O47-C45-C46-O48 |
| 30 | 6 | 802 | LHG | C11-C12-C13-C14 |
| 32 | 7 | 805 | SQD | C13-C14-C15-C16 |
| 36 | B | 5003 | DGD | C4B-C5B-C6B-C7B |
| 41 | 9 | 804 | SPH | C6-C7-C8-C9 |
| 48 | 8 | 804 | DGA | CA9-CAA-CBA-CCA |
| 51 | 7 | 807 | 4RF | C45-C46-C47-C48 |
| 51 | 7 | 807 | 4RF | O23-C22-O21-C20 |
| 25 | 2 | 621 | CLA | C5-C6-C7-C8 |
| 25 | B | 1207 | CLA | C11-C12-C13-C14 |
| 30 | 3 | 801 | LHG | C29-C30-C31-C32 |
| 33 | 9 | 803 | PTY | C24-C25-C26-C27 |
| 33 | B | 5005 | PTY | C11-C12-C13-C14 |
| 25 | A | 1013 | CLA | C11-C12-C13-C15 |
| 25 | A | 1104 | CLA | C11-C10-C8-C7 |
| 25 | A | 1104 | CLA | C12-C13-C15-C16 |
| 25 | A | 1106 | CLA | C11-C12-C13-C15 |
| 25 | A | 1109 | CLA | C11-C12-C13-C15 |
| 25 | A | 1119 | CLA | C6-C7-C8-C10 |
| 25 | A | 1121 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1122 | CLA | C6-C7-C8-C10 |
| 25 | A | 1123 | CLA | C11-C10-C8-C7 |
| 25 | A | 1126 | CLA | C12-C13-C15-C16 |
| 25 | A | 1128 | CLA | C11-C10-C8-C7 |
| 25 | A | 1131 | CLA | C6-C7-C8-C10 |
| 25 | A | 1101 | CLA | C2-C3-C5-C6 |
| 25 | A | 1101 | CLA | C6-C7-C8-C10 |
| 25 | B | 1022 | CLA | C11-C10-C8-C7 |
| 25 | B | 1023 | CLA | C11-C10-C8-C7 |
| 25 | B | 1204 | CLA | C12-C13-C15-C16 |
| 25 | B | 1206 | CLA | C6-C7-C8-C10 |
| 25 | B | 1210 | CLA | C11-C10-C8-C7 |
| 25 | B | 1212 | CLA | C6-C7-C8-C10 |
| 25 | B | 1221 | CLA | C6-C7-C8-C10 |
| 25 | B | 1235 | CLA | C11-C10-C8-C7 |
| 25 | B | 1235 | CLA | C12-C13-C15-C16 |
| 25 | K | 1402 | CLA | C6-C7-C8-C10 |
| 25 | 3 | 601 | CLA | C11-C12-C13-C15 |
| 25 | 3 | 605 | CLA | C6-C7-C8-C10 |
| 25 | 3 | 605 | CLA | C12-C13-C15-C16 |
| 25 | 3 | 606 | CLA | C11-C10-C8-C7 |
| 25 | 3 | 613 | CLA | C6-C7-C8-C10 |
| 25 | 7 | 601 | CLA | C6-C7-C8-C10 |
| 25 | 7 | 601 | CLA | C11-C10-C8-C7 |
| 25 | 7 | 603 | CLA | C11-C10-C8-C7 |
| 25 | 7 | 604 | CLA | C11-C10-C8-C7 |
| 25 | 8 | 606 | CLA | C6-C7-C8-C10 |
| 25 | 8 | 606 | CLA | C11-C10-C8-C7 |
| 26 | 3 | 604 | CHL | C6-C7-C8-C10 |
| 26 | 3 | 604 | CHL | C11-C12-C13-C15 |
| 26 | 4 | 609 | CHL | C11-C12-C13-C15 |
| 26 | 5 | 610 | CHL | C12-C13-C15-C16 |
| 26 | 2 | 609 | CHL | C12-C13-C15-C16 |
| 27 | A | 2001 | PQN | C21-C22-C23-C25 |
| 27 | B | 2002 | PQN | C17-C18-C20-C21 |
| 25 | A | 1127 | CLA | C3-C5-C6-C7 |
| 25 | A | 1104 | CLA | C11-C10-C8-C9 |
| 25 | A | 1106 | CLA | C11-C12-C13-C14 |
| 25 | A | 1109 | CLA | C11-C12-C13-C14 |
| 25 | A | 1111 | CLA | C6-C7-C8-C9 |
| 25 | A | 1119 | CLA | C6-C7-C8-C9 |
| 25 | A | 1122 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1123 | CLA | C11-C10-C8-C9 |
| 25 | A | 1125 | CLA | C11-C10-C8-C9 |
| 25 | A | 1126 | CLA | C11-C10-C8-C9 |
| 25 | A | 1126 | CLA | C14-C13-C15-C16 |
| 25 | A | 1128 | CLA | C11-C10-C8-C9 |
| 25 | B | 1237 | CLA | C6-C7-C8-C9 |
| 25 | B | 1021 | CLA | C11-C10-C8-C9 |
| 25 | B | 1022 | CLA | C11-C10-C8-C9 |
| 25 | B | 1023 | CLA | C11-C10-C8-C9 |
| 25 | B | 1204 | CLA | C14-C13-C15-C16 |
| 25 | B | 1210 | CLA | C11-C10-C8-C9 |
| 25 | B | 1215 | CLA | C11-C10-C8-C9 |
| 25 | B | 1216 | CLA | C11-C12-C13-C14 |
| 25 | B | 1221 | CLA | C6-C7-C8-C9 |
| 25 | B | 1223 | CLA | C11-C10-C8-C9 |
| 25 | B | 1224 | CLA | C11-C10-C8-C9 |
| 25 | B | 1230 | CLA | C6-C7-C8-C9 |
| 25 | B | 1231 | CLA | C11-C10-C8-C9 |
| 25 | K | 1402 | CLA | C6-C7-C8-C9 |
| 25 | L | 1502 | CLA | C6-C7-C8-C9 |
| 25 | 1 | 607 | CLA | C11-C12-C13-C14 |
| 25 | 3 | 605 | CLA | C11-C12-C13-C14 |
| 25 | 3 | 605 | CLA | C14-C13-C15-C16 |
| 25 | 3 | 606 | CLA | C11-C10-C8-C9 |
| 25 | 4 | 610 | CLA | C11-C12-C13-C14 |
| 25 | 5 | 604 | CLA | C14-C13-C15-C16 |
| 25 | 6 | 604 | CLA | C11-C10-C8-C9 |
| 25 | 7 | 603 | CLA | C11-C10-C8-C9 |
| 25 | 7 | 603 | CLA | C11-C12-C13-C14 |
| 25 | 8 | 606 | CLA | C6-C7-C8-C9 |
| 26 | 1 | 609 | CHL | C14-C13-C15-C16 |
| 26 | 4 | 609 | CHL | C11-C12-C13-C14 |
| 26 | 6 | 609 | CHL | C11-C12-C13-C14 |
| 26 | 6 | 619 | CHL | C11-C10-C8-C9 |
| 26 | 8 | 604 | CHL | C11-C10-C8-C9 |
| 26 | 8 | 604 | CHL | C11-C12-C13-C14 |
| 43 | 3 | 502 | LUT | C29-C30-C31-C32 |
| 33 | B | 5005 | PTY | C25-C26-C27-C28 |
| 24 | A | 1011 | CL0 | CBA-CGA-O2A-C1 |
| 25 | B | 1224 | CLA | C2A-CAA-CBA-CGA |
| 25 | 6 | 604 | CLA | C2A-CAA-CBA-CGA |
| 31 | A | 5004 | LMG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | G | 5002 | PTY | C11-C12-C13-C14 |
| 29 | B | 4006 | BCR | C37-C22-C23-C24 |
| 29 | L | 4002 | BCR | C37-C22-C23-C24 |
| 29 | 7 | 503 | BCR | C11-C12-C13-C35 |
| 42 | M | 4001 | ECH | C37-C22-C23-C24 |
| 25 | 1 | 601 | CLA | C11-C12-C13-C15 |
| 25 | 9 | 605 | CLA | C11-C12-C13-C14 |
| 30 | 5 | 801 | LHG | C28-C29-C30-C31 |
| 29 | B | 4004 | BCR | C7-C8-C9-C10 |
| 29 | L | 4002 | BCR | C21-C22-C23-C24 |
| 30 | 4 | 801 | LHG | C35-C36-C37-C38 |
| 30 | 1 | 801 | LHG | C31-C32-C33-C34 |
| 30 | 2 | 802 | LHG | C33-C34-C35-C36 |
| 35 | A | 5008 | LMT | C5-C6-C7-C8 |
| 25 | B | 1203 | CLA | CBA-CGA-O2A-C1 |
| 25 | H | 1701 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 602 | CLA | CBA-CGA-O2A-C1 |
| 26 | 1 | 611 | CHL | C2C-C3C-CAC-CBC |
| 36 | 8 | 802 | DGD | CDA-CEA-CFA-CGA |
| 47 | 4 | 804 | PLM | C2-C3-C4-C5 |
| 25 | A | 1121 | CLA | C5-C6-C7-C8 |
| 25 | B | 1224 | CLA | C13-C15-C16-C17 |
| 25 | 3 | 601 | CLA | C15-C16-C17-C18 |
| 25 | 5 | 612 | CLA | C13-C15-C16-C17 |
| 27 | B | 2002 | PQN | C23-C25-C26-C27 |
| 25 | B | 1209 | CLA | O1D-CGD-O2D-CED |
| 30 | A | 5003 | LHG | C15-C16-C17-C18 |
| 37 | K | 5002 | PCW | C13-C14-C15-C16 |
| 25 | 5 | 614 | CLA | CAA-CBA-CGA-O2A |
| 36 | B | 5003 | DGD | O1A-C1A-O1G-C1G |
| 47 | 8 | 806 | PLM | CA-CB-CC-CD |
| 25 | A | 1106 | CLA | C8-C10-C11-C12 |
| 25 | B | 1023 | CLA | C13-C15-C16-C17 |
| 25 | 2 | 607 | CLA | C13-C15-C16-C17 |
| 30 | A | 5001 | LHG | O6-C4-C5-C6 |
| 30 | F | 5001 | LHG | O6-C4-C5-C6 |
| 30 | 1 | 801 | LHG | O6-C4-C5-C6 |
| 30 | 4 | 801 | LHG | O6-C4-C5-C6 |
| 33 | J | 5001 | PTY | O14-C5-C6-C1 |
| 33 | 3 | 802 | PTY | O14-C5-C6-C1 |
| 33 | 5 | 802 | PTY | O14-C5-C6-C1 |
| 34 | A | 5007 | 3PH | O11-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 5004 | PCW | O3P-C1-C2-C3 |
| 25 | A | 1101 | CLA | C3-C5-C6-C7 |
| 33 | A | 5006 | PTY | C11-C12-C13-C14 |
| 30 | a | 801 | LHG | C23-C24-C25-C26 |
| 33 | 5 | 802 | PTY | N1-C2-C3-O11 |
| 25 | 5 | 614 | CLA | CBA-CGA-O2A-C1 |
| 41 | J | 5002 | SPH | C11-C10-C9-C8 |
| 30 | A | 5002 | LHG | C12-C13-C14-C15 |
| 30 | 2 | 801 | LHG | C13-C14-C15-C16 |
| 25 | A | 1125 | CLA | C4-C3-C5-C6 |
| 25 | B | 1214 | CLA | C4-C3-C5-C6 |
| 25 | 1 | 608 | CLA | C4-C3-C5-C6 |
| 25 | 7 | 610 | CLA | C4-C3-C5-C6 |
| 25 | 2 | 602 | CLA | C4-C3-C5-C6 |
| 26 | 8 | 603 | CHL | C4-C3-C5-C6 |
| 30 | 7 | 802 | LHG | C24-C25-C26-C27 |
| 52 | 8 | 805 | P5S | C43-C44-C45-C46 |
| 25 | 5 | 603 | CLA | C11-C10-C8-C9 |
| 25 | B | 1227 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1219 | CLA | C10-C11-C12-C13 |
| 30 | 5 | 801 | LHG | C19-C20-C21-C22 |
| 30 | 5 | 801 | LHG | C35-C36-C37-C38 |
| 48 | 2 | 803 | DGA | CA2-CA3-CA4-CA5 |
| 25 | 7 | 604 | CLA | C16-C17-C18-C20 |
| 25 | 4 | 612 | CLA | C13-C15-C16-C17 |
| 37 | B | 5004 | PCW | C41-C42-C43-C44 |
| 25 | 4 | 610 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 611 | CLA | CBA-CGA-O2A-C1 |
| 25 | 6 | 618 | CLA | CAA-CBA-CGA-O2A |
| 37 | K | 5001 | PCW | C42-C43-C44-C45 |
| 47 | 8 | 806 | PLM | C6-C7-C8-C9 |
| 30 | a | 801 | LHG | C2-C3-O3-P |
| 25 | A | 1124 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1021 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1227 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1235 | CLA | C3A-C2A-CAA-CBA |
| 25 | 2 | 604 | CLA | C3A-C2A-CAA-CBA |
| 26 | 7 | 611 | CHL | C3A-C2A-CAA-CBA |
| 30 | 8 | 801 | LHG | C28-C29-C30-C31 |
| 33 | J | 5001 | PTY | C11-C12-C13-C14 |
| 29 | A | 4003 | BCR | C13-C14-C15-C16 |
| 29 | L | 4003 | BCR | C9-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | O | 4001 | BCR | C19-C20-C21-C22 |
| 43 | 3 | 501 | LUT | C29-C30-C31-C32 |
| 50 | 9 | 507 | XAT | C33-C34-C35-C15 |
| 35 | A | 5008 | LMT | C2-C1-O1'-C1' |
| 35 | 1 | 804 | LMT | C2-C1-O1'-C1' |
| 30 | B | 5001 | LHG | C25-C26-C27-C28 |
| 41 | 4 | 805 | SPH | C11-C12-C13-C14 |
| 25 | 8 | 618 | CLA | C3-C5-C6-C7 |
| 30 | F | 5001 | LHG | C29-C30-C31-C32 |
| 30 | 3 | 801 | LHG | C34-C35-C36-C37 |
| 33 | 3 | 802 | PTY | C34-C35-C36-C37 |
| 36 | B | 5003 | DGD | C5A-C6A-C7A-C8A |
| 25 | A | 1122 | CLA | C11-C12-C13-C14 |
| 25 | A | 1125 | CLA | C16-C17-C18-C19 |
| 37 | 6 | 803 | PCW | C12-C11-O3-C3 |
| 25 | 5 | 602 | CLA | C3-C5-C6-C7 |
| 25 | 4 | 604 | CLA | C8-C10-C11-C12 |
| 25 | 8 | 605 | CLA | C5-C6-C7-C8 |
| 25 | 2 | 621 | CLA | C15-C16-C17-C18 |
| 30 | 1 | 801 | LHG | C4-C5-C6-O8 |
| 30 | 4 | 801 | LHG | C4-C5-C6-O8 |
| 30 | 7 | 803 | LHG | C4-C5-C6-O8 |
| 32 | 7 | 805 | SQD | C44-C45-C46-O48 |
| 33 | J | 5001 | PTY | O4-C1-C6-C5 |
| 37 | B | 5004 | PCW | C1-C2-C3-O3 |
| 37 | 6 | 803 | PCW | C1-C2-C3-O3 |
| 51 | 7 | 807 | 4RF | O18-C19-C20-C39 |
| 52 | 8 | 805 | P5S | O19-C1-C2-C3 |
| 41 | J | 5002 | SPH | C13-C14-C15-C16 |
| 24 | A | 1011 | CL0 | O1A-CGA-O2A-C1 |
| 51 | 7 | 807 | 4RF | C28-C29-C30-C31 |
| 25 | 2 | 604 | CLA | CAA-CBA-CGA-O2A |
| 37 | K | 5001 | PCW | C12-C13-C14-C15 |
| 25 | 1 | 608 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1112 | CLA | C6-C7-C8-C9 |
| 25 | B | 1214 | CLA | C2-C3-C5-C6 |
| 25 | 7 | 610 | CLA | C2-C3-C5-C6 |
| 26 | 8 | 603 | CHL | C2-C3-C5-C6 |
| 30 | A | 5003 | LHG | C25-C26-C27-C28 |
| 30 | F | 5001 | LHG | C16-C17-C18-C19 |
| 30 | 4 | 801 | LHG | C31-C32-C33-C34 |
| 30 | B | 5002 | LHG | C3-O3-P-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 7 | 802 | LHG | C3-O3-P-O6 |
| 30 | 2 | 802 | LHG | C4-O6-P-O3 |
| 25 | 7 | 601 | CLA | O1A-CGA-O2A-C1 |
| 34 | A | 5007 | 3PH | O32-C31-O31-C3 |
| 30 | a | 801 | LHG | C9-C10-C11-C12 |
| 30 | 7 | 803 | LHG | C25-C26-C27-C28 |
| 51 | 7 | 807 | 4RF | C44-C45-C46-C47 |
| 25 | A | 1104 | CLA | C3-C5-C6-C7 |
| 25 | 3 | 606 | CLA | C2A-CAA-CBA-CGA |
| 34 | A | 5007 | 3PH | C22-C23-C24-C25 |
| 53 | 8 | 810 | LAP | C6-C7-C8-C9 |
| 30 | B | 5001 | LHG | O6-C4-C5-O7 |
| 30 | B | 5002 | LHG | O6-C4-C5-O7 |
| 30 | F | 5002 | LHG | O6-C4-C5-O7 |
| 30 | F | 5001 | LHG | O6-C4-C5-O7 |
| 30 | a | 801 | LHG | O6-C4-C5-O7 |
| 30 | 4 | 802 | LHG | O6-C4-C5-O7 |
| 30 | 7 | 802 | LHG | O6-C4-C5-O7 |
| 52 | 8 | 805 | P5S | O37-C2-C3-O16 |
| 25 | 4 | 602 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 608 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 1235 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1201 | CLA | C16-C17-C18-C19 |
| 25 | 1 | 601 | CLA | C11-C12-C13-C14 |
| 25 | 5 | 612 | CLA | C16-C17-C18-C20 |
| 25 | 7 | 604 | CLA | C16-C17-C18-C19 |
| 30 | A | 5001 | LHG | C35-C36-C37-C38 |
| 30 | A | 5002 | LHG | C11-C10-C9-C8 |
| 30 | 1 | 802 | LHG | C33-C34-C35-C36 |
| 30 | 2 | 801 | LHG | C26-C27-C28-C29 |
| 33 | 7 | 804 | PTY | C15-C16-C17-C18 |
| 25 | H | 1701 | CLA | O1A-CGA-O2A-C1 |
| 30 | B | 5001 | LHG | C24-C25-C26-C27 |
| 30 | a | 801 | LHG | C28-C29-C30-C31 |
| 48 | 8 | 804 | DGA | CAA-CBA-CCA-CDA |
| 30 | B | 5002 | LHG | O7-C5-C6-O8 |
| 30 | 4 | 801 | LHG | O7-C5-C6-O8 |
| 30 | 2 | 801 | LHG | O7-C5-C6-O8 |
| 32 | G | 5001 | SQD | O47-C45-C46-O48 |
| 33 | 9 | 803 | PTY | O4-C1-C6-O7 |
| 37 | B | 5004 | PCW | O2-C2-C3-O3 |
| 25 | 1 | 601 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 6 | 601 | CLA | C5-C6-C7-C8 |
| 30 | 4 | 801 | LHG | C9-C10-C11-C12 |
| 29 | 5 | 504 | BCR | C13-C14-C15-C16 |
| 33 | J | 5001 | PTY | C11-C8-O7-C6 |
| 25 | B | 1209 | CLA | C16-C17-C18-C20 |
| 25 | 4 | 610 | CLA | C16-C17-C18-C20 |
| 25 | 8 | 618 | CLA | C11-C12-C13-C14 |
| 30 | 1 | 802 | LHG | C26-C27-C28-C29 |
| 30 | 5 | 801 | LHG | C17-C18-C19-C20 |
| 45 | a | 805 | OLA | C13-C14-C15-C16 |
| 30 | B | 5002 | LHG | C1-C2-C3-O3 |
| 48 | 8 | 804 | DGA | CG1-CG2-CG3-OXT |
| 53 | 8 | 810 | LAP | C13-C14-C15-O4 |
| 30 | 1 | 802 | LHG | C35-C36-C37-C38 |
| 30 | 4 | 801 | LHG | C34-C35-C36-C37 |
| 30 | B | 5001 | LHG | O9-C7-O7-C5 |
| 30 | 5 | 801 | LHG | O9-C7-O7-C5 |
| 25 | B | 1226 | CLA | C2-C1-O2A-CGA |
| 25 | 6 | 604 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 601 | CLA | C2-C1-O2A-CGA |
| 25 | 8 | 605 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1125 | CLA | C2-C3-C5-C6 |
| 25 | 1 | 608 | CLA | C2-C3-C5-C6 |
| 26 | 2 | 609 | CHL | CAA-CBA-CGA-O2A |
| 25 | A | 1013 | CLA | C6-C7-C8-C9 |
| 25 | A | 1103 | CLA | C11-C10-C8-C9 |
| 25 | A | 1106 | CLA | C11-C10-C8-C9 |
| 25 | A | 1117 | CLA | C11-C12-C13-C14 |
| 25 | A | 1132 | CLA | C6-C7-C8-C9 |
| 25 | A | 1137 | CLA | C6-C7-C8-C9 |
| 25 | B | 1021 | CLA | C14-C13-C15-C16 |
| 25 | B | 1023 | CLA | C11-C12-C13-C14 |
| 25 | B | 1204 | CLA | C6-C7-C8-C9 |
| 25 | B | 1210 | CLA | C6-C7-C8-C9 |
| 25 | B | 1219 | CLA | C6-C7-C8-C9 |
| 25 | B | 1223 | CLA | C11-C12-C13-C14 |
| 25 | B | 1234 | CLA | C11-C10-C8-C9 |
| 25 | B | 1235 | CLA | C14-C13-C15-C16 |
| 25 | B | 1239 | CLA | C11-C10-C8-C9 |
| 25 | B | 1240 | CLA | C14-C13-C15-C16 |
| 25 | G | 1602 | CLA | C11-C10-C8-C9 |
| 25 | 1 | 601 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 607 | CLA | C14-C13-C15-C16 |
| 25 | 5 | 603 | CLA | C6-C7-C8-C9 |
| 25 | 6 | 604 | CLA | C14-C13-C15-C16 |
| 26 | 1 | 604 | CHL | C11-C12-C13-C14 |
| 26 | 1 | 604 | CHL | C14-C13-C15-C16 |
| 26 | 3 | 604 | CHL | C11-C12-C13-C14 |
| 26 | 3 | 611 | CHL | C6-C7-C8-C9 |
| 26 | 5 | 610 | CHL | C11-C10-C8-C9 |
| 27 | A | 2001 | PQN | C21-C22-C23-C24 |
| 33 | A | 5006 | PTY | C13-C14-C15-C16 |
| 30 | 9 | 801 | LHG | C25-C26-C27-C28 |
| 38 | F | 5003 | LPX | C11-C10-C9-C8 |
| 25 | A | 1125 | CLA | C10-C11-C12-C13 |
| 25 | B | 1234 | CLA | C10-C11-C12-C13 |
| 25 | 3 | 610 | CLA | C5-C6-C7-C8 |
| 25 | 8 | 618 | CLA | C5-C6-C7-C8 |
| 30 | B | 5002 | LHG | C5-C4-O6-P |
| 30 | 4 | 801 | LHG | C2-C3-O3-P |
| 30 | 7 | 803 | LHG | C2-C3-O3-P |
| 30 | A | 5002 | LHG | C28-C29-C30-C31 |
| 30 | 1 | 801 | LHG | C28-C29-C30-C31 |
| 30 | 7 | 802 | LHG | C11-C10-C9-C8 |
| 33 | A | 5006 | PTY | C34-C35-C36-C37 |
| 25 | A | 1134 | CLA | C2A-CAA-CBA-CGA |
| 25 | 1 | 606 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1121 | CLA | C11-C12-C13-C15 |
| 25 | 3 | 601 | CLA | C16-C17-C18-C19 |
| 26 | 8 | 601 | CHL | C11-C12-C13-C15 |
| 25 | K | 1402 | CLA | C3-C5-C6-C7 |
| 29 | A | 4001 | BCR | C5-C6-C7-C8 |
| 29 | A | 4003 | BCR | C23-C24-C25-C26 |
| 29 | B | 4001 | BCR | C23-C24-C25-C26 |
| 29 | B | 4001 | BCR | C23-C24-C25-C30 |
| 29 | B | 4003 | BCR | C23-C24-C25-C26 |
| 29 | B | 4005 | BCR | C23-C24-C25-C26 |
| 29 | B | 4005 | BCR | C23-C24-C25-C30 |
| 29 | B | 4006 | BCR | C23-C24-C25-C26 |
| 29 | B | 4006 | BCR | C23-C24-C25-C30 |
| 29 | G | 4001 | BCR | C1-C6-C7-C8 |
| 29 | K | 4001 | BCR | C1-C6-C7-C8 |
| 29 | K | 4001 | BCR | C5-C6-C7-C8 |
| 29 | K | 4002 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | 5 | 503 | BCR | C23-C24-C25-C26 |
| 29 | 5 | 503 | BCR | C23-C24-C25-C30 |
| 40 | J | 4002 | RRX | C1-C6-C7-C8 |
| 40 | 3 | 506 | RRX | C23-C24-C25-C26 |
| 42 | M | 4001 | ECH | C5-C6-C7-C8 |
| 42 | M | 4001 | ECH | C23-C24-C25-C30 |
| 43 | 1 | 501 | LUT | C5-C6-C7-C8 |
| 43 | 4 | 501 | LUT | C5-C6-C7-C8 |
| 43 | 5 | 502 | LUT | C5-C6-C7-C8 |
| 43 | 5 | 505 | LUT | C1-C6-C7-C8 |
| 43 | 6 | 501 | LUT | C5-C6-C7-C8 |
| 43 | 6 | 502 | LUT | C5-C6-C7-C8 |
| 43 | 7 | 501 | LUT | C1-C6-C7-C8 |
| 43 | 7 | 501 | LUT | C5-C6-C7-C8 |
| 43 | 8 | 502 | LUT | C5-C6-C7-C8 |
| 43 | 9 | 502 | LUT | C1-C6-C7-C8 |
| 43 | 9 | 502 | LUT | C5-C6-C7-C8 |
| 25 | A | 1138 | CLA | C5-C6-C7-C8 |
| 25 | 6 | 603 | CLA | C8-C10-C11-C12 |
| 41 | 4 | 805 | SPH | C14-C15-C16-C17 |
| 29 | A | 4001 | BCR | C17-C18-C19-C20 |
| 29 | A | 4005 | BCR | C7-C8-C9-C10 |
| 29 | B | 4005 | BCR | C21-C22-C23-C24 |
| 29 | J | 4001 | BCR | C21-C22-C23-C24 |
| 42 | M | 4001 | ECH | C21-C22-C23-C24 |
| 25 | A | 1012 | CLA | C10-C11-C12-C13 |
| 47 | 4 | 804 | PLM | CD-CE-CF-CG |
| 30 | 9 | 802 | LHG | C7-C8-C9-C10 |
| 25 | B | 1206 | CLA | C2C-C3C-CAC-CBC |
| 30 | B | 5002 | LHG | C30-C31-C32-C33 |
| 30 | 1 | 801 | LHG | C9-C10-C11-C12 |
| 47 | 8 | 806 | PLM | C9-CA-CB-CC |
| 25 | B | 1021 | CLA | C13-C15-C16-C17 |
| 25 | B | 1203 | CLA | O1A-CGA-O2A-C1 |
| 30 | a | 801 | LHG | C31-C32-C33-C34 |
| 25 | 5 | 612 | CLA | C8-C10-C11-C12 |
| 30 | A | 5003 | LHG | O6-C4-C5-C6 |
| 30 | 2 | 802 | LHG | O6-C4-C5-C6 |
| 33 | 9 | 803 | PTY | O14-C5-C6-C1 |
| 25 | A | 1106 | CLA | C11-C10-C8-C7 |
| 25 | A | 1111 | CLA | C6-C7-C8-C10 |
| 25 | A | 1125 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1126 | CLA | C11-C10-C8-C7 |
| 25 | A | 1128 | CLA | C6-C7-C8-C10 |
| 25 | A | 1134 | CLA | C6-C7-C8-C10 |
| 25 | A | 1137 | CLA | C6-C7-C8-C10 |
| 25 | A | 1137 | CLA | C11-C10-C8-C7 |
| 25 | B | 1237 | CLA | C6-C7-C8-C10 |
| 25 | B | 1237 | CLA | C11-C10-C8-C7 |
| 25 | B | 1021 | CLA | C11-C10-C8-C7 |
| 25 | B | 1022 | CLA | C6-C7-C8-C10 |
| 25 | B | 1023 | CLA | C12-C13-C15-C16 |
| 25 | B | 1201 | CLA | C11-C10-C8-C7 |
| 25 | B | 1201 | CLA | C12-C13-C15-C16 |
| 25 | B | 1202 | CLA | C11-C12-C13-C15 |
| 25 | B | 1203 | CLA | C6-C7-C8-C10 |
| 25 | B | 1204 | CLA | C6-C7-C8-C10 |
| 25 | B | 1206 | CLA | C11-C12-C13-C15 |
| 25 | B | 1215 | CLA | C11-C10-C8-C7 |
| 25 | B | 1216 | CLA | C11-C12-C13-C15 |
| 25 | B | 1217 | CLA | C6-C7-C8-C10 |
| 25 | B | 1223 | CLA | C11-C10-C8-C7 |
| 25 | B | 1223 | CLA | C11-C12-C13-C15 |
| 25 | B | 1224 | CLA | C6-C7-C8-C10 |
| 25 | B | 1226 | CLA | C11-C10-C8-C7 |
| 25 | B | 1230 | CLA | C6-C7-C8-C10 |
| 25 | B | 1231 | CLA | C11-C10-C8-C7 |
| 25 | B | 1234 | CLA | C11-C10-C8-C7 |
| 25 | B | 1240 | CLA | C12-C13-C15-C16 |
| 25 | B | 1207 | CLA | C6-C7-C8-C10 |
| 25 | L | 1502 | CLA | C11-C10-C8-C7 |
| 25 | 1 | 607 | CLA | C11-C12-C13-C15 |
| 25 | 1 | 612 | CLA | C12-C13-C15-C16 |
| 25 | a | 603 | CLA | C6-C7-C8-C10 |
| 25 | 3 | 605 | CLA | C11-C12-C13-C15 |
| 25 | 3 | 607 | CLA | C6-C7-C8-C10 |
| 25 | 3 | 607 | CLA | C11-C10-C8-C7 |
| 25 | 3 | 610 | CLA | C6-C7-C8-C10 |
| 25 | 5 | 601 | CLA | C11-C10-C8-C7 |
| 25 | 5 | 603 | CLA | C6-C7-C8-C10 |
| 25 | 5 | 604 | CLA | C12-C13-C15-C16 |
| 25 | 5 | 612 | CLA | C6-C7-C8-C10 |
| 25 | 6 | 604 | CLA | C11-C10-C8-C7 |
| 25 | 7 | 603 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 2 | 621 | CLA | C6-C7-C8-C10 |
| 26 | 1 | 604 | CHL | C11-C10-C8-C7 |
| 26 | 1 | 609 | CHL | C12-C13-C15-C16 |
| 26 | 3 | 603 | CHL | C12-C13-C15-C16 |
| 26 | 3 | 611 | CHL | C11-C10-C8-C7 |
| 26 | 5 | 610 | CHL | C11-C10-C8-C7 |
| 26 | 6 | 609 | CHL | C11-C12-C13-C15 |
| 26 | 6 | 609 | CHL | C12-C13-C15-C16 |
| 26 | 8 | 604 | CHL | C11-C10-C8-C7 |
| 26 | 2 | 609 | CHL | C11-C12-C13-C15 |
| 26 | 9 | 603 | CHL | C11-C10-C8-C7 |
| 32 | I | 5001 | SQD | C27-C28-C29-C30 |
| 45 | 8 | 809 | OLA | C2-C3-C4-C5 |
| 25 | B | 1204 | CLA | C13-C15-C16-C17 |
| 29 | B | 4002 | BCR | C9-C10-C11-C12 |
| 29 | B | 4004 | BCR | C19-C20-C21-C22 |
| 29 | B | 4005 | BCR | C19-C20-C21-C22 |
| 29 | B | 4006 | BCR | C15-C16-C17-C18 |
| 29 | L | 4002 | BCR | C13-C14-C15-C16 |
| 29 | L | 4001 | BCR | C13-C14-C15-C16 |
| 29 | I | 4001 | BCR | C19-C20-C21-C22 |
| 29 | 3 | 503 | BCR | C19-C20-C21-C22 |
| 29 | 3 | 504 | BCR | C9-C10-C11-C12 |
| 29 | 5 | 504 | BCR | C19-C20-C21-C22 |
| 43 | a | 501 | LUT | C29-C30-C31-C32 |
| 43 | a | 502 | LUT | C29-C30-C31-C32 |
| 43 | 4 | 502 | LUT | C29-C30-C31-C32 |
| 43 | 5 | 501 | LUT | C29-C30-C31-C32 |
| 43 | 5 | 502 | LUT | C29-C30-C31-C32 |
| 43 | 2 | 507 | LUT | C29-C30-C31-C32 |
| 43 | 2 | 507 | LUT | C33-C34-C35-C15 |
| 43 | 9 | 502 | LUT | C29-C30-C31-C32 |
| 44 | 7 | 504 | AXT | C33-C34-C35-C15 |
| 25 | A | 1112 | CLA | C6-C7-C8-C10 |
| 25 | A | 1121 | CLA | C11-C12-C13-C14 |
| 25 | B | 1201 | CLA | C16-C17-C18-C20 |
| 30 | 2 | 802 | LHG | C24-C25-C26-C27 |
| 30 | 5 | 801 | LHG | C34-C35-C36-C37 |
| 33 | a | 802 | PTY | C35-C36-C37-C38 |
| 25 | A | 1107 | CLA | C5-C6-C7-C8 |
| 25 | A | 1139 | CLA | C5-C6-C7-C8 |
| 25 | B | 1228 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1234 | CLA | C5-C6-C7-C8 |
| 26 | 4 | 609 | CHL | CAA-CBA-CGA-O2A |
| 26 | 9 | 610 | CHL | C2A-CAA-CBA-CGA |
| 35 | A | 5008 | LMT | C1-C2-C3-C4 |
| 25 | B | 1220 | CLA | C5-C6-C7-C8 |
| 33 | a | 803 | PTY | C32-C33-C34-C35 |
| 34 | A | 5007 | 3PH | C1-O11-P-O13 |
| 30 | 8 | 801 | LHG | C7-C8-C9-C10 |
| 25 | B | 1234 | CLA | C3-C5-C6-C7 |
| 25 | 5 | 601 | CLA | C5-C6-C7-C8 |
| 26 | 7 | 609 | CHL | C12-C13-C15-C16 |
| 32 | A | 5005 | SQD | C34-C35-C36-C37 |
| 48 | 8 | 804 | DGA | CB9-CAB-CBB-CCB |
| 25 | A | 1119 | CLA | C5-C6-C7-C8 |
| 25 | 7 | 601 | CLA | C8-C10-C11-C12 |
| 25 | 9 | 605 | CLA | C8-C10-C11-C12 |
| 33 | 9 | 803 | PTY | C36-C37-C38-C39 |
| 41 | J | 5002 | SPH | C6-C7-C8-C9 |
| 48 | 8 | 804 | DGA | CBB-CAB-CB9-CB8 |
| 48 | 8 | 804 | DGA | CAB-CBB-CCB-CDB |
| 25 | A | 1102 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 1103 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 1104 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 1123 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 1133 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 1135 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 1201 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 1217 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 1240 | CLA | CAD-CBD-CGD-O2D |
| 25 | K | 1402 | CLA | CAD-CBD-CGD-O2D |
| 25 | L | 1503 | CLA | CAD-CBD-CGD-O2D |
| 25 | 4 | 604 | CLA | CAD-CBD-CGD-O2D |
| 25 | 4 | 605 | CLA | CAD-CBD-CGD-O2D |
| 25 | 5 | 605 | CLA | CAD-CBD-CGD-O2D |
| 25 | 8 | 605 | CLA | CAD-CBD-CGD-O2D |
| 25 | 2 | 602 | CLA | CAD-CBD-CGD-O2D |
| 26 | A | 1114 | CHL | CAD-CBD-CGD-O2D |
| 26 | 7 | 617 | CHL | CAD-CBD-CGD-O2D |
| 30 | 2 | 801 | LHG | C4-C5-O7-C7 |
| 32 | G | 5001 | SQD | C46-C45-O47-C7 |
| 30 | F | 5002 | LHG | C10-C11-C12-C13 |
| 32 | I | 5001 | SQD | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | A | 1011 | CL0 | CBD-CGD-O2D-CED |
| 30 | 3 | 801 | LHG | C24-C23-O8-C6 |
| 33 | J | 5001 | PTY | C31-C30-O4-C1 |
| 25 | a | 603 | CLA | C16-C17-C18-C20 |
| 25 | 7 | 604 | CLA | C8-C10-C11-C12 |
| 30 | A | 5003 | LHG | C2-C3-O3-P |
| 30 | A | 5003 | LHG | C4-C5-C6-O8 |
| 30 | B | 5002 | LHG | C2-C3-O3-P |
| 30 | B | 5002 | LHG | C4-C5-C6-O8 |
| 30 | 1 | 802 | LHG | C2-C3-O3-P |
| 30 | 1 | 802 | LHG | C4-C5-C6-O8 |
| 30 | 3 | 801 | LHG | C2-C3-O3-P |
| 30 | 9 | 801 | LHG | C4-C5-C6-O8 |
| 32 | G | 5001 | SQD | C44-C45-C46-O48 |
| 36 | 7 | 806 | DGD | C1G-C2G-C3G-O3G |
| 37 | K | 5001 | PCW | C1-C2-C3-O3 |
| 48 | 2 | 803 | DGA | OG1-CG1-CG2-CG3 |
| 25 | 4 | 610 | CLA | O1A-CGA-O2A-C1 |
| 25 | 2 | 602 | CLA | O1A-CGA-O2A-C1 |
| 30 | 4 | 801 | LHG | O6-C4-C5-O7 |
| 30 | 2 | 801 | LHG | O6-C4-C5-O7 |
| 33 | 3 | 802 | PTY | O14-C5-C6-O7 |
| 33 | 9 | 803 | PTY | O14-C5-C6-O7 |
| 34 | A | 5007 | 3PH | O11-C1-C2-O21 |
| 37 | 6 | 803 | PCW | O3P-C1-C2-O2 |
| 25 | B | 1201 | CLA | C10-C11-C12-C13 |
| 25 | A | 1128 | CLA | C3-C5-C6-C7 |
| 25 | a | 607 | CLA | C3-C5-C6-C7 |
| 31 | A | 5004 | LMG | C32-C33-C34-C35 |
| 25 | A | 1132 | CLA | C2A-CAA-CBA-CGA |
| 25 | 1 | 608 | CLA | O1A-CGA-O2A-C1 |
| 26 | 3 | 611 | CHL | C11-C12-C13-C14 |
| 33 | J | 5001 | PTY | O10-C8-O7-C6 |
| 25 | A | 1106 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1106 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1112 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1115 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1117 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1117 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1119 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1119 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1128 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1129 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1136 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1136 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1205 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1213 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1213 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1219 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1223 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1227 | CLA | CHA-CBD-CGD-O1D |
| 25 | L | 1501 | CLA | CHA-CBD-CGD-O2D |
| 25 | O | 1802 | CLA | CHA-CBD-CGD-O1D |
| 25 | O | 1802 | CLA | CHA-CBD-CGD-O2D |
| 25 | a | 601 | CLA | CHA-CBD-CGD-O1D |
| 25 | a | 601 | CLA | CHA-CBD-CGD-O2D |
| 25 | a | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 4 | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | 4 | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 4 | 615 | CLA | CHA-CBD-CGD-O1D |
| 25 | 4 | 615 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 608 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 608 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 609 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 609 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 620 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 620 | CLA | CHA-CBD-CGD-O2D |
| 25 | 2 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 2 | 607 | CLA | CHA-CBD-CGD-O2D |
| 26 | a | 604 | CHL | CHA-CBD-CGD-O1D |
| 26 | 7 | 609 | CHL | CHA-CBD-CGD-O1D |
| 26 | 2 | 609 | CHL | CHA-CBD-CGD-O1D |
| 36 | B | 5003 | DGD | C9B-CAB-CBB-CCB |
| 36 | 7 | 806 | DGD | C9A-CAA-CBA-CCA |
| 25 | 1 | 601 | CLA | O1A-CGA-O2A-C1 |
| 25 | 8 | 611 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1104 | CLA | C10-C11-C12-C13 |
| 25 | 3 | 607 | CLA | C5-C6-C7-C8 |
| 30 | 7 | 803 | LHG | O7-C5-C6-O8 |
| 32 | I | 5001 | SQD | O47-C45-C46-O48 |
| 36 | B | 5003 | DGD | O1G-C1G-C2G-O2G |
| 36 | 7 | 806 | DGD | O2G-C2G-C3G-O3G |
| 48 | 2 | 803 | DGA | OG1-CG1-CG2-OG2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 6 | 803 | PCW | O11-C11-O3-C3 |
| 30 | 6 | 801 | LHG | C19-C20-C21-C22 |
| 30 | 5 | 801 | LHG | O1-C1-C2-O2 |
| 30 | 7 | 803 | LHG | C11-C10-C9-C8 |
| 25 | 5 | 607 | CLA | C4-C3-C5-C6 |
| 25 | 4 | 602 | CLA | O1A-CGA-O2A-C1 |
| 25 | 7 | 608 | CLA | O1A-CGA-O2A-C1 |
| 33 | a | 802 | PTY | C30-C31-C32-C33 |
| 26 | 6 | 609 | CHL | C8-C10-C11-C12 |
| 25 | 9 | 607 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1108 | CLA | C11-C10-C8-C9 |
| 25 | B | 1239 | CLA | C6-C7-C8-C9 |
| 25 | a | 603 | CLA | C11-C12-C13-C14 |
| 25 | 4 | 612 | CLA | C11-C12-C13-C14 |
| 25 | 2 | 621 | CLA | C6-C7-C8-C9 |
| 26 | 6 | 609 | CHL | C11-C10-C8-C9 |
| 30 | 8 | 801 | LHG | C11-C10-C9-C8 |
| 38 | F | 5003 | LPX | C14-C15-C16-C17 |
| 25 | 2 | 601 | CLA | O1A-CGA-O2A-C1 |
| 30 | B | 5002 | LHG | C9-C10-C11-C12 |
| 30 | 9 | 802 | LHG | C30-C31-C32-C33 |
| 32 | 7 | 805 | SQD | C4-C5-C6-S |
| 30 | B | 5001 | LHG | C19-C20-C21-C22 |
| 25 | A | 1109 | CLA | C2A-CAA-CBA-CGA |
| 25 | 5 | 612 | CLA | C2A-CAA-CBA-CGA |
| 25 | 6 | 601 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1103 | CLA | CAA-CBA-CGA-O2A |
| 30 | 3 | 801 | LHG | C11-C10-C9-C8 |
| 25 | 8 | 605 | CLA | CBA-CGA-O2A-C1 |
| 29 | 6 | 504 | BCR | C36-C18-C19-C20 |
| 40 | J | 4002 | RRX | C37-C22-C23-C24 |
| 43 | 8 | 502 | LUT | C7-C8-C9-C19 |
| 35 | 1 | 804 | LMT | C5'-C4'-O1B-C1B |
| 25 | 6 | 601 | CLA | C8-C10-C11-C12 |
| 25 | 8 | 609 | CLA | C8-C10-C11-C12 |
| 30 | 4 | 802 | LHG | C9-C10-C11-C12 |
| 29 | A | 4004 | BCR | C17-C18-C19-C20 |
| 29 | 7 | 503 | BCR | C11-C12-C13-C14 |
| 40 | J | 4002 | RRX | C21-C22-C23-C24 |
| 43 | 5 | 505 | LUT | C7-C8-C9-C10 |
| 43 | 5 | 505 | LUT | C27-C28-C29-C30 |
| 25 | B | 1209 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1211 | CLA | C1A-C2A-CAA-CBA |
| 25 | 1 | 605 | CLA | C1A-C2A-CAA-CBA |
| 25 | 4 | 612 | CLA | C1A-C2A-CAA-CBA |
| 25 | 6 | 607 | CLA | C1A-C2A-CAA-CBA |
| 25 | 7 | 607 | CLA | C1A-C2A-CAA-CBA |
| 25 | 9 | 606 | CLA | C1A-C2A-CAA-CBA |
| 26 | 7 | 617 | CHL | C1A-C2A-CAA-CBA |
| 25 | A | 1126 | CLA | C16-C17-C18-C19 |
| 25 | B | 1021 | CLA | C16-C17-C18-C20 |
| 25 | 6 | 604 | CLA | C16-C17-C18-C19 |
| 25 | 2 | 621 | CLA | C16-C17-C18-C19 |
| 25 | 1 | 612 | CLA | C13-C15-C16-C17 |
| 25 | A | 1109 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1115 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1215 | CLA | C2-C1-O2A-CGA |
| 25 | 5 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 607 | CLA | C2-C1-O2A-CGA |
| 25 | A | 1012 | CLA | CBA-CGA-O2A-C1 |
| 30 | 9 | 801 | LHG | C26-C27-C28-C29 |
| 29 | A | 4002 | BCR | C15-C16-C17-C18 |
| 29 | A | 4005 | BCR | C19-C20-C21-C22 |
| 29 | B | 4006 | BCR | C13-C14-C15-C16 |
| 29 | 6 | 503 | BCR | C9-C10-C11-C12 |
| 24 | A | 1011 | CL0 | O1D-CGD-O2D-CED |
| 30 | 2 | 801 | LHG | C3-O3-P-O6 |
| 30 | 2 | 801 | LHG | C4-O6-P-O3 |
| 30 | 9 | 801 | LHG | C3-O3-P-O6 |
| 33 | A | 5006 | PTY | C5-O14-P1-O11 |
| 33 | a | 803 | PTY | C3-O11-P1-O14 |
| 37 | K | 5001 | PCW | C4-O4P-P-O3P |
| 38 | F | 5003 | LPX | C3-O1-P1-O2 |
| 36 | B | 5003 | DGD | CFB-CGB-CHB-CIB |
| 25 | A | 1012 | CLA | C4-C3-C5-C6 |
| 25 | A | 1116 | CLA | C4-C3-C5-C6 |
| 25 | A | 1126 | CLA | C4-C3-C5-C6 |
| 25 | B | 1229 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1115 | CLA | C3-C5-C6-C7 |
| 25 | 5 | 612 | CLA | C3-C5-C6-C7 |
| 30 | F | 5002 | LHG | C2-C3-O3-P |
| 30 | 6 | 801 | LHG | C2-C3-O3-P |
| 30 | 7 | 802 | LHG | C2-C3-O3-P |
| 25 | B | 1216 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 2 | 802 | LHG | C10-C11-C12-C13 |
| 45 | 8 | 809 | OLA | C13-C14-C15-C16 |
| 30 | A | 5002 | LHG | C3-O3-P-O4 |
| 30 | B | 5002 | LHG | C4-O6-P-O4 |
| 30 | F | 5001 | LHG | C3-O3-P-O4 |
| 30 | 3 | 801 | LHG | C3-O3-P-O5 |
| 30 | 3 | 801 | LHG | C4-O6-P-O4 |
| 30 | 4 | 801 | LHG | C3-O3-P-O4 |
| 30 | 6 | 802 | LHG | C3-O3-P-O5 |
| 30 | 6 | 801 | LHG | C3-O3-P-O5 |
| 30 | 6 | 801 | LHG | C4-O6-P-O5 |
| 30 | 7 | 803 | LHG | C4-O6-P-O5 |
| 30 | 8 | 801 | LHG | C3-O3-P-O5 |
| 30 | 2 | 802 | LHG | C3-O3-P-O5 |
| 30 | 9 | 802 | LHG | C4-O6-P-O5 |
| 33 | B | 5005 | PTY | C5-O14-P1-O12 |
| 33 | G | 5003 | PTY | C3-O11-P1-O13 |
| 33 | G | 5002 | PTY | C3-O11-P1-O13 |
| 33 | J | 5001 | PTY | C5-O14-P1-O12 |
| 33 | a | 803 | PTY | C3-O11-P1-O13 |
| 33 | a | 803 | PTY | C5-O14-P1-O12 |
| 33 | a | 803 | PTY | C5-O14-P1-O13 |
| 33 | a | 802 | PTY | C5-O14-P1-O12 |
| 33 | 3 | 802 | PTY | C3-O11-P1-O13 |
| 33 | 5 | 802 | PTY | C3-O11-P1-O13 |
| 33 | 7 | 804 | PTY | C3-O11-P1-O12 |
| 33 | 7 | 804 | PTY | C3-O11-P1-O13 |
| 33 | 9 | 803 | PTY | C3-O11-P1-O12 |
| 37 | B | 5004 | PCW | C1-O3P-P-O1P |
| 37 | B | 5004 | PCW | C1-O3P-P-O2P |
| 37 | K | 5002 | PCW | C1-O3P-P-O1P |
| 37 | 6 | 803 | PCW | C1-O3P-P-O1P |
| 38 | F | 5003 | LPX | C1-O2-P1-O3 |
| 52 | 8 | 805 | P5S | C3-O16-P12-O15 |
| 53 | 8 | 810 | LAP | C15-O4-P9-O5 |
| 32 | A | 5005 | SQD | C31-C32-C33-C34 |
| 32 | I | 5001 | SQD | O5-C1-O6-C44 |
| 25 | 1 | 605 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 604 | CLA | C10-C11-C12-C13 |
| 25 | L | 1504 | CLA | CBA-CGA-O2A-C1 |
| 25 | 2 | 601 | CLA | CBA-CGA-O2A-C1 |
| 30 | A | 5002 | LHG | O6-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | B | 5001 | LHG | O6-C4-C5-C6 |
| 30 | B | 5002 | LHG | O6-C4-C5-C6 |
| 30 | F | 5002 | LHG | O6-C4-C5-C6 |
| 30 | a | 801 | LHG | O6-C4-C5-C6 |
| 30 | 4 | 802 | LHG | O6-C4-C5-C6 |
| 30 | 9 | 802 | LHG | O6-C4-C5-C6 |
| 33 | a | 803 | PTY | O14-C5-C6-C1 |
| 37 | 6 | 803 | PCW | O3P-C1-C2-C3 |
| 52 | 8 | 805 | P5S | C1-C2-C3-O16 |
| 48 | 5 | 803 | DGA | CA5-CA6-CA7-CA8 |
| 33 | J | 5001 | PTY | O30-C30-O4-C1 |
| 26 | a | 613 | CHL | C2C-C3C-CAC-CBC |
| 47 | 6 | 804 | PLM | C3-C4-C5-C6 |
| 26 | 2 | 609 | CHL | C2C-C3C-CAC-CBC |
| 30 | 2 | 801 | LHG | C24-C25-C26-C27 |
| 30 | 2 | 802 | LHG | C25-C26-C27-C28 |
| 25 | B | 1206 | CLA | C4C-C3C-CAC-CBC |
| 25 | A | 1012 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1021 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1136 | CLA | C16-C17-C18-C19 |
| 25 | B | 1240 | CLA | C16-C17-C18-C20 |
| 25 | 5 | 604 | CLA | C16-C17-C18-C20 |
| 25 | 7 | 603 | CLA | C16-C17-C18-C20 |
| 30 | a | 801 | LHG | C30-C31-C32-C33 |
| 25 | A | 1112 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1125 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1129 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1136 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 1210 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 1223 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 1227 | CLA | CAD-CBD-CGD-O1D |
| 25 | 1 | 605 | CLA | CAD-CBD-CGD-O1D |
| 25 | 4 | 606 | CLA | CAD-CBD-CGD-O1D |
| 25 | 6 | 605 | CLA | CAD-CBD-CGD-O1D |
| 25 | 6 | 615 | CLA | CAD-CBD-CGD-O1D |
| 25 | 8 | 609 | CLA | CAD-CBD-CGD-O1D |
| 26 | a | 609 | CHL | CAD-CBD-CGD-O1D |
| 26 | 6 | 609 | CHL | CAD-CBD-CGD-O1D |
| 26 | 7 | 609 | CHL | CAD-CBD-CGD-O1D |
| 32 | G | 5001 | SQD | C5-C6-S-O7 |
| 37 | K | 5001 | PCW | C5-C4-O4P-P |
| 37 | 6 | 803 | PCW | C5-C4-O4P-P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 38 | F | 5003 | LPX | C2-C1-O2-P1 |
| 30 | 3 | 801 | LHG | O10-C23-O8-C6 |
| 30 | 4 | 801 | LHG | C19-C20-C21-C22 |
| 24 | A | 1011 | CL0 | C3-C5-C6-C7 |
| 25 | A | 1116 | CLA | C8-C10-C11-C12 |
| 35 | B | 5006 | LMT | C4-C5-C6-C7 |
| 30 | 4 | 801 | LHG | C7-C8-C9-C10 |
| 25 | B | 1021 | CLA | CBA-CGA-O2A-C1 |
| 25 | a | 601 | CLA | CBA-CGA-O2A-C1 |
| 32 | H | 5001 | SQD | C15-C16-C17-C18 |
| 51 | 7 | 807 | 4RF | C11-C12-C13-C14 |
| 25 | A | 1131 | CLA | C16-C17-C18-C19 |
| 25 | A | 1013 | CLA | C12-C13-C15-C16 |
| 25 | A | 1117 | CLA | C11-C12-C13-C15 |
| 25 | A | 1122 | CLA | C11-C10-C8-C7 |
| 25 | A | 1125 | CLA | C11-C12-C13-C15 |
| 25 | A | 1132 | CLA | C6-C7-C8-C10 |
| 25 | B | 1209 | CLA | C11-C10-C8-C7 |
| 25 | B | 1229 | CLA | C11-C10-C8-C7 |
| 25 | B | 1239 | CLA | C6-C7-C8-C10 |
| 25 | B | 1240 | CLA | C6-C7-C8-C10 |
| 25 | B | 1207 | CLA | C11-C10-C8-C7 |
| 25 | 1 | 601 | CLA | C11-C10-C8-C7 |
| 25 | 1 | 605 | CLA | C6-C7-C8-C10 |
| 25 | 1 | 607 | CLA | C12-C13-C15-C16 |
| 25 | 1 | 608 | CLA | C6-C7-C8-C10 |
| 25 | a | 603 | CLA | C11-C12-C13-C15 |
| 25 | 3 | 606 | CLA | C6-C7-C8-C10 |
| 25 | 3 | 613 | CLA | C11-C12-C13-C15 |
| 25 | 4 | 610 | CLA | C12-C13-C15-C16 |
| 25 | 4 | 611 | CLA | C6-C7-C8-C10 |
| 25 | 4 | 612 | CLA | C11-C12-C13-C15 |
| 25 | 6 | 615 | CLA | C11-C10-C8-C7 |
| 26 | 3 | 603 | CHL | C6-C7-C8-C10 |
| 26 | 3 | 611 | CHL | C6-C7-C8-C10 |
| 26 | 6 | 609 | CHL | C11-C10-C8-C7 |
| 26 | 7 | 609 | CHL | C11-C10-C8-C7 |
| 30 | A | 5002 | LHG | O6-C4-C5-O7 |
| 30 | A | 5003 | LHG | O6-C4-C5-O7 |
| 30 | 1 | 802 | LHG | O6-C4-C5-O7 |
| 30 | 6 | 802 | LHG | O6-C4-C5-O7 |
| 30 | 2 | 802 | LHG | O6-C4-C5-O7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 9 | 802 | LHG | O6-C4-C5-O7 |
| 33 | a | 803 | PTY | O14-C5-C6-O7 |
| 33 | 5 | 802 | PTY | O14-C5-C6-O7 |
| 37 | K | 5001 | PCW | O3P-C1-C2-O2 |
| 43 | 2 | 507 | LUT | C25-C26-C27-C28 |
| 34 | A | 5007 | 3PH | C26-C27-C28-C29 |
| 48 | 2 | 803 | DGA | CB4-CB5-CB6-CB7 |
| 25 | B | 1207 | CLA | C5-C6-C7-C8 |
| 29 | G | 4001 | BCR | C15-C16-C17-C18 |
| 43 | 5 | 505 | LUT | C29-C30-C31-C32 |
| 43 | 8 | 502 | LUT | C29-C30-C31-C32 |
| 45 | 1 | 803 | OLA | C4-C5-C6-C7 |
| 25 | B | 1202 | CLA | C16-C17-C18-C20 |
| 35 | B | 5006 | LMT | C7-C8-C9-C10 |
| 30 | B | 5002 | LHG | O8-C23-C24-C25 |
| 32 | I | 5001 | SQD | C44-C45-C46-O48 |
| 37 | B | 5004 | PCW | O4P-C4-C5-N |
| 37 | K | 5001 | PCW | O4P-C4-C5-N |
| 47 | a | 804 | PLM | C1-C2-C3-C4 |
| 30 | A | 5002 | LHG | O7-C5-C6-O8 |
| 30 | A | 5003 | LHG | O7-C5-C6-O8 |
| 30 | 6 | 801 | LHG | O7-C5-C6-O8 |
| 30 | 7 | 801 | LHG | O7-C5-C6-O8 |
| 30 | 2 | 802 | LHG | O7-C5-C6-O8 |
| 32 | G | 5001 | SQD | O6-C44-C45-O47 |
| 36 | 8 | 802 | DGD | O2G-C2G-C3G-O3G |
| 48 | 5 | 803 | DGA | OG1-CG1-CG2-OG2 |
| 52 | 8 | 805 | P5S | O19-C1-C2-O37 |
| 45 | 8 | 809 | OLA | C10-C11-C12-C13 |
| 36 | B | 5003 | DGD | C1B-C2B-C3B-C4B |
| 25 | 8 | 605 | CLA | O1A-CGA-O2A-C1 |
| 30 | 2 | 802 | LHG | C28-C29-C30-C31 |
| 30 | 9 | 802 | LHG | C19-C20-C21-C22 |
| 30 | 2 | 802 | LHG | C2-C3-O3-P |
| 33 | 3 | 802 | PTY | C6-C5-O14-P1 |
| 25 | B | 1214 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1122 | CLA | C4-C3-C5-C6 |
| 25 | B | 1214 | CLA | CBA-CGA-O2A-C1 |
| 30 | 6 | 801 | LHG | C11-C10-C9-C8 |
| 30 | 9 | 801 | LHG | C10-C11-C12-C13 |
| 26 | 8 | 603 | CHL | C10-C11-C12-C13 |
| 25 | A | 1111 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1134 | CLA | C6-C7-C8-C9 |
| 25 | A | 1101 | CLA | C11-C12-C13-C14 |
| 25 | B | 1237 | CLA | C11-C10-C8-C9 |
| 25 | B | 1022 | CLA | C6-C7-C8-C9 |
| 25 | B | 1023 | CLA | C14-C13-C15-C16 |
| 25 | B | 1201 | CLA | C14-C13-C15-C16 |
| 25 | B | 1202 | CLA | C11-C12-C13-C14 |
| 25 | B | 1206 | CLA | C11-C12-C13-C14 |
| 25 | B | 1216 | CLA | C6-C7-C8-C9 |
| 25 | B | 1217 | CLA | C6-C7-C8-C9 |
| 25 | B | 1226 | CLA | C11-C10-C8-C9 |
| 25 | B | 1235 | CLA | C11-C10-C8-C9 |
| 25 | 1 | 612 | CLA | C11-C12-C13-C14 |
| 25 | 3 | 607 | CLA | C6-C7-C8-C9 |
| 25 | 3 | 607 | CLA | C11-C10-C8-C9 |
| 25 | 3 | 610 | CLA | C6-C7-C8-C9 |
| 25 | 5 | 601 | CLA | C11-C10-C8-C9 |
| 25 | 5 | 612 | CLA | C6-C7-C8-C9 |
| 25 | 2 | 604 | CLA | C6-C7-C8-C9 |
| 25 | 9 | 612 | CLA | C14-C13-C15-C16 |
| 26 | 3 | 603 | CHL | C14-C13-C15-C16 |
| 26 | 2 | 609 | CHL | C11-C12-C13-C14 |
| 26 | 9 | 603 | CHL | C11-C10-C8-C9 |
| 37 | K | 5002 | PCW | C15-C16-C17-C18 |
| 33 | 9 | 803 | PTY | C32-C33-C34-C35 |
| 30 | 6 | 801 | LHG | C31-C32-C33-C34 |
| 25 | L | 1504 | CLA | O1A-CGA-O2A-C1 |
| 25 | a | 601 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1012 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1107 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 608 | CLA | O1D-CGD-O2D-CED |
| 29 | H | 4001 | BCR | C18-C19-C20-C21 |
| 43 | 2 | 507 | LUT | C10-C11-C12-C13 |
| 43 | 2 | 507 | LUT | C30-C31-C32-C33 |
| 44 | 7 | 504 | AXT | C30-C31-C32-C33 |
| 29 | 8 | 503 | BCR | C11-C12-C13-C35 |
| 25 | 6 | 615 | CLA | C5-C6-C7-C8 |
| 30 | 7 | 801 | LHG | C30-C31-C32-C33 |
| 33 | J | 5001 | PTY | C8-C11-C12-C13 |
| 38 | F | 5003 | LPX | C6-C7-C8-C9 |
| 29 | L | 4002 | BCR | C17-C18-C19-C20 |
| 26 | 1 | 610 | CHL | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1108 | CLA | C15-C16-C17-C18 |
| 30 | A | 5001 | LHG | C9-C10-C11-C12 |
| 25 | 2 | 601 | CLA | C8-C10-C11-C12 |
| 25 | A | 1127 | CLA | CAA-CBA-CGA-O2A |
| 30 | 7 | 803 | LHG | C28-C29-C30-C31 |
| 37 | 6 | 803 | PCW | C12-C13-C14-C15 |
| 25 | A | 1111 | CLA | C13-C15-C16-C17 |
| 25 | A | 1138 | CLA | C8-C10-C11-C12 |
| 25 | A | 1115 | CLA | C11-C12-C13-C15 |
| 25 | 6 | 604 | CLA | C16-C17-C18-C20 |
| 25 | A | 1120 | CLA | C1-C2-C3-C4 |
| 25 | O | 1802 | CLA | CAA-CBA-CGA-O2A |
| 34 | A | 5007 | 3PH | O21-C21-C22-C23 |
| 30 | 4 | 801 | LHG | C30-C31-C32-C33 |
| 30 | 5 | 801 | LHG | C30-C31-C32-C33 |
| 33 | a | 803 | PTY | C33-C34-C35-C36 |
| 25 | 7 | 603 | CLA | C15-C16-C17-C18 |
| 27 | B | 2002 | PQN | C15-C16-C17-C18 |
| 30 | 2 | 801 | LHG | O6-C4-C5-C6 |
| 25 | H | 1702 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 611 | CLA | C2A-CAA-CBA-CGA |
| 25 | 2 | 604 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1224 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1239 | CLA | C2-C1-O2A-CGA |
| 26 | a | 606 | CHL | C2-C1-O2A-CGA |
| 26 | 7 | 611 | CHL | C2-C1-O2A-CGA |
| 33 | 3 | 802 | PTY | C12-C11-C8-O7 |
| 25 | 1 | 607 | CLA | C3-C5-C6-C7 |
| 30 | 5 | 801 | LHG | C2-C3-O3-P |
| 30 | 5 | 801 | LHG | C5-C4-O6-P |
| 30 | 2 | 802 | LHG | C5-C4-O6-P |
| 30 | 7 | 801 | LHG | O6-C4-C5-O7 |
| 30 | 8 | 801 | LHG | O6-C4-C5-O7 |
| 32 | G | 5001 | SQD | C9-C10-C11-C12 |
| 25 | B | 1224 | CLA | CAA-CBA-CGA-O2A |
| 30 | 5 | 801 | LHG | C18-C19-C20-C21 |
| 36 | 8 | 802 | DGD | CAA-CBA-CCA-CDA |
| 29 | A | 4001 | BCR | C1-C6-C7-C8 |
| 29 | B | 4003 | BCR | C23-C24-C25-C30 |
| 29 | G | 4001 | BCR | C5-C6-C7-C8 |
| 29 | K | 4002 | BCR | C1-C6-C7-C8 |
| 43 | 4 | 501 | LUT | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | 5 | 502 | LUT | C1-C6-C7-C8 |
| 43 | 5 | 505 | LUT | C5-C6-C7-C8 |
| 43 | 6 | 502 | LUT | C1-C6-C7-C8 |
| 43 | 8 | 502 | LUT | C1-C6-C7-C8 |
| 43 | 9 | 501 | LUT | C1-C6-C7-C8 |
| 43 | 9 | 501 | LUT | C5-C6-C7-C8 |
| 33 | G | 5003 | PTY | C11-C12-C13-C14 |
| 47 | 4 | 803 | PLM | C9-CA-CB-CC |
| 26 | 3 | 611 | CHL | CAA-CBA-CGA-O2A |
| 25 | B | 1219 | CLA | C5-C6-C7-C8 |
| 47 | 6 | 804 | PLM | CC-CD-CE-CF |
| 25 | A | 1101 | CLA | C16-C17-C18-C20 |
| 47 | 6 | 804 | PLM | C6-C7-C8-C9 |
| 25 | A | 1123 | CLA | C13-C15-C16-C17 |
| 41 | 9 | 804 | SPH | C4-C5-C6-C7 |
| 26 | 4 | 609 | CHL | C2A-CAA-CBA-CGA |
| 32 | H | 5001 | SQD | C2-C1-O6-C44 |
| 30 | F | 5001 | LHG | O7-C5-C6-O8 |
| 25 | B | 1210 | CLA | C8-C10-C11-C12 |
| 30 | A | 5003 | LHG | C3-O3-P-O6 |
| 30 | B | 5001 | LHG | C4-O6-P-O3 |
| 30 | F | 5002 | LHG | C3-O3-P-O6 |
| 30 | F | 5002 | LHG | C4-O6-P-O3 |
| 30 | 1 | 801 | LHG | C3-O3-P-O6 |
| 30 | a | 801 | LHG | C3-O3-P-O6 |
| 30 | 4 | 802 | LHG | C4-O6-P-O3 |
| 30 | 5 | 801 | LHG | C4-O6-P-O3 |
| 30 | 7 | 801 | LHG | C3-O3-P-O6 |
| 30 | 9 | 801 | LHG | C4-O6-P-O3 |
| 33 | B | 5005 | PTY | C3-O11-P1-O14 |
| 33 | 7 | 804 | PTY | C5-O14-P1-O11 |
| 37 | B | 5004 | PCW | C4-O4P-P-O3P |
| 37 | K | 5001 | PCW | C1-O3P-P-O4P |
| 26 | 3 | 603 | CHL | C10-C11-C12-C13 |
| 33 | B | 5005 | PTY | C24-C25-C26-C27 |
| 33 | 5 | 802 | PTY | C38-C39-C40-C41 |
| 52 | 8 | 805 | P5S | C41-C42-C43-C44 |
| 25 | B | 1215 | CLA | C8-C10-C11-C12 |
| 25 | B | 1236 | CLA | C5-C6-C7-C8 |
| 33 | a | 802 | PTY | C37-C38-C39-C40 |
| 25 | 1 | 606 | CLA | C5-C6-C7-C8 |
| 25 | A | 1126 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1133 | CLA | C11-C10-C8-C7 |
| 25 | A | 1101 | CLA | C11-C12-C13-C15 |
| 25 | B | 1219 | CLA | C6-C7-C8-C10 |
| 25 | B | 1220 | CLA | C6-C7-C8-C10 |
| 25 | B | 1220 | CLA | C11-C10-C8-C7 |
| 25 | B | 1228 | CLA | C11-C12-C13-C15 |
| 25 | 1 | 607 | CLA | C11-C10-C8-C7 |
| 25 | 3 | 607 | CLA | C12-C13-C15-C16 |
| 25 | 7 | 610 | CLA | C6-C7-C8-C10 |
| 25 | 9 | 605 | CLA | C6-C7-C8-C10 |
| 25 | 9 | 612 | CLA | C12-C13-C15-C16 |
| 25 | 5 | 614 | CLA | O1A-CGA-O2A-C1 |
| 35 | 2 | 804 | LMT | C11-C10-C9-C8 |
| 25 | B | 1206 | CLA | C6-C7-C8-C9 |
| 25 | B | 1229 | CLA | C11-C10-C8-C9 |
| 25 | B | 1240 | CLA | C6-C7-C8-C9 |
| 25 | B | 1207 | CLA | C6-C7-C8-C9 |
| 25 | 1 | 601 | CLA | C11-C10-C8-C9 |
| 25 | 1 | 608 | CLA | C6-C7-C8-C9 |
| 25 | 1 | 612 | CLA | C14-C13-C15-C16 |
| 25 | 3 | 606 | CLA | C6-C7-C8-C9 |
| 25 | 4 | 611 | CLA | C6-C7-C8-C9 |
| 25 | 7 | 601 | CLA | C6-C7-C8-C9 |
| 26 | 3 | 603 | CHL | C6-C7-C8-C9 |
| 29 | B | 4002 | BCR | C13-C14-C15-C16 |
| 29 | H | 4001 | BCR | C9-C10-C11-C12 |
| 29 | 7 | 503 | BCR | C9-C10-C11-C12 |
| 29 | 7 | 503 | BCR | C19-C20-C21-C22 |
| 43 | 1 | 503 | LUT | C29-C30-C31-C32 |
| 43 | 8 | 501 | LUT | C29-C30-C31-C32 |
| 25 | a | 603 | CLA | C16-C17-C18-C19 |
| 25 | 4 | 610 | CLA | C16-C17-C18-C19 |
| 25 | 2 | 607 | CLA | C16-C17-C18-C19 |
| 25 | 2 | 621 | CLA | C16-C17-C18-C20 |
| 26 | 7 | 613 | CHL | C11-C12-C13-C15 |
| 35 | B | 5006 | LMT | C4B-C5B-C6B-O6B |
| 33 | 7 | 804 | PTY | C13-C14-C15-C16 |
| 25 | B | 1227 | CLA | CAA-CBA-CGA-O1A |
| 25 | B | 1221 | CLA | C15-C16-C17-C18 |
| 25 | B | 1219 | CLA | C11-C12-C13-C14 |
| 35 | A | 5008 | LMT | C3-C4-C5-C6 |
| 29 | 6 | 504 | BCR | C7-C8-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 5 | 604 | CLA | C16-C17-C18-C19 |
| 25 | 7 | 603 | CLA | C16-C17-C18-C19 |
| 30 | 1 | 802 | LHG | C30-C31-C32-C33 |
| 37 | K | 5001 | PCW | C39-C40-C41-C42 |
| 30 | 4 | 801 | LHG | C16-C17-C18-C19 |
| 26 | 8 | 604 | CHL | C12-C13-C15-C16 |
| 25 | 2 | 602 | CLA | C2-C3-C5-C6 |
| 25 | A | 1136 | CLA | C16-C17-C18-C20 |
| 25 | B | 1240 | CLA | C16-C17-C18-C19 |
| 25 | B | 1238 | CLA | CBA-CGA-O2A-C1 |
| 30 | 4 | 802 | LHG | C24-C23-O8-C6 |
| 30 | 5 | 801 | LHG | C26-C27-C28-C29 |
| 33 | A | 5006 | PTY | C35-C36-C37-C38 |
| 30 | 6 | 801 | LHG | C35-C36-C37-C38 |
| 24 | A | 1011 | CL0 | C5-C6-C7-C8 |
| 25 | F | 1302 | CLA | C5-C6-C7-C8 |
| 36 | B | 5003 | DGD | O6D-C5D-C6D-O5D |
| 37 | B | 5004 | PCW | C37-C38-C39-C40 |
| 25 | B | 1022 | CLA | C2A-CAA-CBA-CGA |
| 29 | B | 4001 | BCR | C19-C20-C21-C22 |
| 29 | B | 4007 | BCR | C19-C20-C21-C22 |
| 29 | K | 4002 | BCR | C9-C10-C11-C12 |
| 29 | L | 4003 | BCR | C13-C14-C15-C16 |
| 29 | L | 4003 | BCR | C19-C20-C21-C22 |
| 29 | 5 | 503 | BCR | C19-C20-C21-C22 |
| 29 | 6 | 503 | BCR | C19-C20-C21-C22 |
| 29 | 8 | 503 | BCR | C9-C10-C11-C12 |
| 29 | 8 | 503 | BCR | C19-C20-C21-C22 |
| 43 | 9 | 501 | LUT | C29-C30-C31-C32 |
| 44 | 7 | 504 | AXT | C9-C10-C11-C12 |
| 44 | 7 | 504 | AXT | C29-C30-C31-C32 |
| 50 | 9 | 504 | XAT | C9-C10-C11-C12 |
| 25 | A | 1136 | CLA | C10-C11-C12-C13 |
| 30 | B | 5001 | LHG | C17-C18-C19-C20 |
| 25 | B | 1210 | CLA | C16-C17-C18-C20 |
| 25 | 6 | 606 | CLA | C16-C17-C18-C19 |
| 25 | 6 | 615 | CLA | C16-C17-C18-C19 |
| 25 | 3 | 602 | CLA | CAA-CBA-CGA-O2A |
| 25 | 1 | 603 | CLA | C3-C5-C6-C7 |
| 26 | 3 | 603 | CHL | C3-C5-C6-C7 |
| 30 | 5 | 801 | LHG | C9-C10-C11-C12 |
| 25 | A | 1102 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | A | 1134 | CLA | C4-C3-C5-C6 |
| 30 | A | 5001 | LHG | C34-C35-C36-C37 |
| 32 | I | 5001 | SQD | C15-C16-C17-C18 |
| 25 | 3 | 605 | CLA | C8-C10-C11-C12 |
| 30 | 1 | 802 | LHG | C18-C19-C20-C21 |
| 25 | A | 1102 | CLA | C2-C1-O2A-CGA |
| 25 | B | 1217 | CLA | C2-C1-O2A-CGA |
| 25 | 1 | 608 | CLA | C2-C1-O2A-CGA |
| 25 | 5 | 601 | CLA | C2-C1-O2A-CGA |
| 25 | 6 | 603 | CLA | C2-C1-O2A-CGA |
| 26 | 5 | 611 | CHL | C2-C1-O2A-CGA |
| 26 | 9 | 610 | CHL | C2-C1-O2A-CGA |
| 35 | 1 | 804 | LMT | O1'-C1-C2-C3 |
| 25 | 2 | 605 | CLA | C5-C6-C7-C8 |
| 25 | B | 1237 | CLA | C16-C17-C18-C20 |
| 26 | 9 | 603 | CHL | C4C-C3C-CAC-CBC |
| 25 | B | 1201 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 1202 | CLA | C2A-CAA-CBA-CGA |
| 25 | 1 | 603 | CLA | C2A-CAA-CBA-CGA |
| 25 | 6 | 603 | CLA | C2A-CAA-CBA-CGA |
| 25 | 9 | 612 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 608 | CLA | CBD-CGD-O2D-CED |
| 30 | 1 | 802 | LHG | O10-C23-C24-C25 |
| 30 | 3 | 801 | LHG | C30-C31-C32-C33 |
| 25 | A | 1140 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1212 | CLA | C3A-C2A-CAA-CBA |
| 25 | L | 1501 | CLA | C3A-C2A-CAA-CBA |
| 25 | 1 | 605 | CLA | C3A-C2A-CAA-CBA |
| 25 | 3 | 613 | CLA | C3A-C2A-CAA-CBA |
| 26 | 5 | 618 | CHL | C3A-C2A-CAA-CBA |
| 26 | 7 | 615 | CHL | C3A-C2A-CAA-CBA |
| 48 | 2 | 803 | DGA | CA4-CA5-CA6-CA7 |
| 25 | 3 | 613 | CLA | CAA-CBA-CGA-O2A |
| 25 | 4 | 607 | CLA | CAA-CBA-CGA-O2A |
| 41 | 4 | 805 | SPH | C6-C7-C8-C9 |
| 26 | 6 | 610 | CHL | CAA-CBA-CGA-O1A |
| 29 | A | 4004 | BCR | C19-C20-C21-C22 |
| 25 | B | 1210 | CLA | C13-C15-C16-C17 |
| 41 | 6 | 806 | SPH | C6-C7-C8-C9 |
| 41 | 6 | 806 | SPH | C7-C8-C9-C10 |
| 25 | A | 1107 | CLA | C4-C3-C5-C6 |
| 37 | B | 5004 | PCW | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1021 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1116 | CLA | C11-C10-C8-C9 |
| 25 | A | 1119 | CLA | C11-C10-C8-C9 |
| 25 | A | 1122 | CLA | C11-C10-C8-C9 |
| 25 | A | 1127 | CLA | C11-C12-C13-C14 |
| 25 | A | 1132 | CLA | C11-C10-C8-C9 |
| 25 | A | 1101 | CLA | C11-C10-C8-C9 |
| 25 | B | 1231 | CLA | C6-C7-C8-C9 |
| 25 | 6 | 603 | CLA | C6-C7-C8-C9 |
| 25 | 6 | 615 | CLA | C6-C7-C8-C9 |
| 26 | 8 | 604 | CHL | C6-C7-C8-C9 |
| 25 | A | 1115 | CLA | C11-C12-C13-C14 |
| 25 | A | 1116 | CLA | C11-C12-C13-C15 |
| 25 | A | 1132 | CLA | C16-C17-C18-C20 |
| 25 | A | 1110 | CLA | C6-C7-C8-C9 |
| 47 | 4 | 804 | PLM | O1-C1-C2-C3 |
| 51 | 7 | 807 | 4RF | C15-C16-O18-C19 |
| 30 | A | 5002 | LHG | C33-C34-C35-C36 |
| 30 | 9 | 802 | LHG | C10-C11-C12-C13 |
| 25 | B | 1214 | CLA | C10-C11-C12-C13 |
| 26 | A | 1114 | CHL | C10-C11-C12-C13 |
| 29 | A | 4005 | BCR | C16-C17-C18-C36 |
| 29 | B | 4003 | BCR | C11-C10-C9-C34 |
| 29 | B | 4003 | BCR | C20-C21-C22-C37 |
| 29 | H | 4001 | BCR | C20-C21-C22-C37 |
| 30 | A | 5002 | LHG | C1-C2-C3-O3 |
| 30 | A | 5002 | LHG | C4-C5-C6-O8 |
| 30 | 7 | 801 | LHG | C4-C5-C6-O8 |
| 36 | 8 | 802 | DGD | C1G-C2G-C3G-O3G |
| 40 | 3 | 506 | RRX | C16-C17-C18-C36 |
| 43 | 1 | 503 | LUT | C39-C29-C30-C31 |
| 43 | 3 | 502 | LUT | C21-C26-C27-C28 |
| 43 | 2 | 507 | LUT | C11-C10-C9-C19 |
| 43 | 2 | 507 | LUT | C21-C26-C27-C28 |
| 43 | 2 | 507 | LUT | C40-C33-C34-C35 |
| 44 | 7 | 504 | AXT | C40-C33-C34-C35 |
| 25 | 8 | 620 | CLA | C2C-C3C-CAC-CBC |
| 45 | 1 | 803 | OLA | O1-C1-C2-C3 |
| 25 | B | 1212 | CLA | C8-C10-C11-C12 |
| 25 | B | 1234 | CLA | C2A-CAA-CBA-CGA |
| 32 | I | 5001 | SQD | C24-C25-C26-C27 |
| 25 | B | 1202 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1215 | CLA | C11-C12-C13-C15 |
| 30 | 1 | 801 | LHG | C25-C26-C27-C28 |
| 30 | 6 | 801 | LHG | C26-C27-C28-C29 |
| 47 | 4 | 804 | PLM | C8-C9-CA-CB |
| 47 | 4 | 804 | PLM | O2-C1-C2-C3 |
| 25 | B | 1202 | CLA | C5-C6-C7-C8 |
| 25 | 7 | 610 | CLA | C10-C11-C12-C13 |
| 53 | 8 | 810 | LAP | O1-C13-C14-C15 |
| 43 | 8 | 502 | LUT | C7-C8-C9-C10 |
| 33 | 9 | 803 | PTY | C5-C6-O7-C8 |
| 36 | 8 | 803 | DGD | C1G-C2G-O2G-C1B |
| 25 | A | 1127 | CLA | C5-C6-C7-C8 |
| 25 | B | 1205 | CLA | C4-C3-C5-C6 |
| 25 | B | 1224 | CLA | C4-C3-C5-C6 |
| 25 | 3 | 605 | CLA | C4-C3-C5-C6 |
| 26 | A | 1114 | CHL | C4-C3-C5-C6 |
| 24 | A | 1011 | CL0 | C1A-C2A-CAA-CBA |
| 25 | A | 1105 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1140 | CLA | C1A-C2A-CAA-CBA |
| 25 | 3 | 613 | CLA | C1A-C2A-CAA-CBA |
| 25 | 6 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 6 | 618 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 608 | CLA | C1A-C2A-CAA-CBA |
| 25 | A | 1119 | CLA | C16-C17-C18-C20 |
| 25 | B | 1209 | CLA | C16-C17-C18-C19 |
| 25 | A | 1012 | CLA | C2-C3-C5-C6 |
| 25 | A | 1013 | CLA | C11-C10-C8-C7 |
| 25 | A | 1121 | CLA | C11-C10-C8-C7 |
| 25 | A | 1128 | CLA | C12-C13-C15-C16 |
| 25 | A | 1133 | CLA | C6-C7-C8-C10 |
| 25 | A | 1138 | CLA | C11-C12-C13-C15 |
| 25 | 1 | 605 | CLA | C12-C13-C15-C16 |
| 25 | 4 | 604 | CLA | C6-C7-C8-C10 |
| 25 | 6 | 606 | CLA | C11-C12-C13-C15 |
| 25 | 2 | 621 | CLA | C11-C12-C13-C15 |
| 26 | 5 | 610 | CHL | C11-C12-C13-C15 |
| 26 | 8 | 603 | CHL | C11-C10-C8-C7 |
| 26 | 8 | 603 | CHL | C11-C12-C13-C15 |
| 30 | B | 5001 | LHG | C29-C30-C31-C32 |
| 25 | A | 1101 | CLA | C10-C11-C12-C13 |
| 30 | 4 | 802 | LHG | O10-C23-O8-C6 |
| 25 | 1 | 602 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 602 | CLA | CAA-CBA-CGA-O2A |
| 29 | 3 | 505 | BCR | C19-C20-C21-C22 |
| 39 | F | 4001 | NEX | C33-C34-C35-C15 |
| 32 | I | 5001 | SQD | C30-C31-C32-C33 |
| 33 | 9 | 803 | PTY | C31-C32-C33-C34 |
| 25 | A | 1109 | CLA | C15-C16-C17-C18 |
| 25 | 3 | 605 | CLA | C15-C16-C17-C18 |
| 30 | 1 | 802 | LHG | C11-C10-C9-C8 |
| 34 | A | 5007 | 3PH | C25-C26-C27-C28 |
| 26 | 1 | 609 | CHL | C2C-C3C-CAC-CBC |
| 25 | B | 1209 | CLA | C3-C5-C6-C7 |
| 30 | A | 5002 | LHG | C2-C3-O3-P |
| 25 | B | 1223 | CLA | C10-C11-C12-C13 |
| 25 | B | 1240 | CLA | C13-C15-C16-C17 |
| 30 | A | 5002 | LHG | C29-C30-C31-C32 |
| 47 | 6 | 804 | PLM | CA-CB-CC-CD |
| 47 | 8 | 807 | PLM | C4-C5-C6-C7 |
| 25 | A | 1133 | CLA | C10-C11-C12-C13 |
| 25 | A | 1109 | CLA | CBA-CGA-O2A-C1 |
| 37 | 6 | 803 | PCW | C16-C17-C18-C19 |
| 30 | 5 | 801 | LHG | O6-C4-C5-C6 |
| 37 | K | 5002 | PCW | O3P-C1-C2-C3 |
| 30 | 2 | 802 | LHG | C29-C30-C31-C32 |
| 32 | G | 5001 | SQD | C15-C16-C17-C18 |
| 26 | 7 | 613 | CHL | C4-C3-C5-C6 |
| 25 | 3 | 605 | CLA | C2-C3-C5-C6 |
| 47 | 4 | 803 | PLM | CC-CD-CE-CF |
| 25 | A | 1126 | CLA | C13-C15-C16-C17 |
| 48 | 3 | 803 | DGA | OA1-CA1-CA2-CA3 |
| 29 | A | 4005 | BCR | C16-C17-C18-C19 |
| 29 | B | 4003 | BCR | C11-C10-C9-C8 |
| 29 | B | 4003 | BCR | C20-C21-C22-C23 |
| 40 | 3 | 506 | RRX | C16-C17-C18-C19 |
| 43 | 1 | 503 | LUT | C28-C29-C30-C31 |
| 43 | 2 | 507 | LUT | C11-C10-C9-C8 |
| 43 | 2 | 507 | LUT | C32-C33-C34-C35 |
| 44 | 7 | 504 | AXT | C32-C33-C34-C35 |
| 47 | 8 | 806 | PLM | C7-C8-C9-CA |
| 25 | B | 1222 | CLA | CBA-CGA-O2A-C1 |
| 26 | 4 | 609 | CHL | C15-C16-C17-C18 |
| 25 | 2 | 603 | CLA | CAA-CBA-CGA-O2A |
| 25 | a | 602 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | A | 4001 | BCR | C15-C16-C17-C18 |
| 29 | A | 4004 | BCR | C9-C10-C11-C12 |
| 29 | J | 4001 | BCR | C19-C20-C21-C22 |
| 29 | 3 | 503 | BCR | C9-C10-C11-C12 |
| 29 | 8 | 503 | BCR | C13-C14-C15-C16 |
| 39 | F | 4001 | NEX | C29-C30-C31-C32 |
| 40 | J | 4002 | RRX | C13-C14-C15-C16 |
| 43 | 1 | 501 | LUT | C29-C30-C31-C32 |
| 50 | 9 | 504 | XAT | C13-C14-C15-C35 |
| 45 | 1 | 803 | OLA | O2-C1-C2-C3 |
| 30 | 2 | 801 | LHG | C30-C31-C32-C33 |
| 48 | 3 | 803 | DGA | CG1-CG2-CG3-OXT |
| 47 | 6 | 804 | PLM | O1-C1-C2-C3 |
| 25 | B | 1237 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 610 | CLA | C4-C3-C5-C6 |
| 26 | 6 | 610 | CHL | C4-C3-C5-C6 |
| 32 | I | 5001 | SQD | C16-C17-C18-C19 |
| 25 | 4 | 601 | CLA | C2-C1-O2A-CGA |
| 25 | 5 | 604 | CLA | C2-C1-O2A-CGA |
| 25 | 6 | 608 | CLA | C2-C1-O2A-CGA |
| 25 | 7 | 603 | CLA | C2-C1-O2A-CGA |
| 25 | 9 | 604 | CLA | C2-C1-O2A-CGA |
| 26 | 7 | 617 | CHL | C2-C1-O2A-CGA |
| 25 | A | 1107 | CLA | C2-C3-C5-C6 |
| 25 | A | 1134 | CLA | C2-C3-C5-C6 |
| 33 | 9 | 803 | PTY | C39-C40-C41-C42 |
| 25 | A | 1113 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1117 | CLA | C11-C10-C8-C9 |
| 25 | B | 1206 | CLA | C14-C13-C15-C16 |
| 25 | B | 1216 | CLA | C11-C10-C8-C9 |
| 25 | B | 1235 | CLA | C11-C12-C13-C14 |
| 25 | B | 1239 | CLA | C11-C12-C13-C14 |
| 25 | a | 607 | CLA | C6-C7-C8-C9 |
| 25 | 5 | 601 | CLA | C8-C10-C11-C12 |
| 25 | B | 1238 | CLA | O1A-CGA-O2A-C1 |
| 51 | 7 | 807 | 4RF | O17-C16-O18-C19 |
| 30 | 7 | 802 | LHG | C9-C10-C11-C12 |
| 30 | 4 | 802 | LHG | C2-C3-O3-P |
| 30 | 1 | 802 | LHG | C17-C18-C19-C20 |
| 33 | 9 | 803 | PTY | C37-C38-C39-C40 |
| 37 | B | 5004 | PCW | C13-C14-C15-C16 |
| 47 | 6 | 804 | PLM | C7-C8-C9-CA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1226 | CLA | C13-C15-C16-C17 |
| 25 | B | 1219 | CLA | C2A-CAA-CBA-CGA |
| 25 | a | 605 | CLA | C2A-CAA-CBA-CGA |
| 26 | 5 | 610 | CHL | C2A-CAA-CBA-CGA |
| 25 | A | 1101 | CLA | C16-C17-C18-C19 |
| 25 | B | 1203 | CLA | C16-C17-C18-C19 |
| 25 | 5 | 614 | CLA | CAA-CBA-CGA-O1A |
| 25 | 2 | 604 | CLA | CAA-CBA-CGA-O1A |
| 25 | 6 | 612 | CLA | O1A-CGA-O2A-C1 |
| 29 | A | 4005 | BCR | C1-C6-C7-C8 |
| 29 | A | 4005 | BCR | C23-C24-C25-C30 |
| 29 | 6 | 504 | BCR | C1-C6-C7-C8 |
| 43 | 1 | 503 | LUT | C1-C6-C7-C8 |
| 43 | a | 503 | LUT | C1-C6-C7-C8 |
| 43 | 3 | 501 | LUT | C1-C6-C7-C8 |
| 43 | 3 | 501 | LUT | C5-C6-C7-C8 |
| 43 | 4 | 502 | LUT | C1-C6-C7-C8 |
| 43 | 4 | 502 | LUT | C5-C6-C7-C8 |
| 43 | 5 | 501 | LUT | C1-C6-C7-C8 |
| 43 | 8 | 501 | LUT | C1-C6-C7-C8 |
| 25 | 3 | 612 | CLA | CAA-CBA-CGA-O2A |
| 41 | J | 5002 | SPH | C15-C16-C17-C18 |
| 29 | A | 4001 | BCR | C9-C10-C11-C12 |
| 29 | B | 4002 | BCR | C15-C16-C17-C18 |
| 29 | 3 | 504 | BCR | C13-C14-C15-C16 |
| 25 | A | 1113 | CLA | C4-C3-C5-C6 |
| 25 | A | 1117 | CLA | C4-C3-C5-C6 |
| 25 | B | 1231 | CLA | C4-C3-C5-C6 |
| 25 | B | 1239 | CLA | C4-C3-C5-C6 |
| 25 | 4 | 602 | CLA | C4-C3-C5-C6 |
| 25 | 7 | 606 | CLA | C4-C3-C5-C6 |
| 26 | a | 609 | CHL | C4-C3-C5-C6 |
| 26 | 7 | 617 | CHL | C4-C3-C5-C6 |
| 26 | 9 | 601 | CHL | C4-C3-C5-C6 |
| 29 | 8 | 503 | BCR | C11-C12-C13-C14 |
| 25 | 2 | 607 | CLA | C16-C17-C18-C20 |
| 25 | B | 1214 | CLA | C11-C12-C13-C14 |
| 25 | A | 1102 | CLA | C2-C3-C5-C6 |
| 25 | A | 1122 | CLA | C2-C3-C5-C6 |
| 47 | 6 | 804 | PLM | O2-C1-C2-C3 |
| 36 | 7 | 806 | DGD | C2G-C3G-O3G-C1D |
| 25 | 6 | 603 | CLA | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | A | 5003 | LHG | C9-C10-C11-C12 |
| 33 | J | 5001 | PTY | C33-C34-C35-C36 |
| 25 | 7 | 607 | CLA | C2-C3-C5-C6 |
| 45 | 8 | 809 | OLA | C7-C8-C9-C10 |
| 30 | 6 | 801 | LHG | O6-C4-C5-O7 |
| 33 | a | 802 | PTY | O14-C5-C6-O7 |
| 26 | 7 | 609 | CHL | C14-C13-C15-C16 |
| 26 | 8 | 604 | CHL | C14-C13-C15-C16 |
| 25 | 4 | 608 | CLA | O1D-CGD-O2D-CED |
| 30 | 4 | 802 | LHG | C5-C6-O8-C23 |
| 25 | L | 1503 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1222 | CLA | C2A-CAA-CBA-CGA |
| 25 | 8 | 615 | CLA | C2A-CAA-CBA-CGA |
| 47 | 4 | 803 | PLM | CD-CE-CF-CG |
| 25 | B | 1232 | CLA | CAA-CBA-CGA-O2A |
| 36 | 8 | 802 | DGD | CCA-CDA-CEA-CFA |
| 30 | 7 | 801 | LHG | O6-C4-C5-C6 |
| 25 | a | 608 | CLA | CAA-CBA-CGA-O2A |
| 25 | G | 1602 | CLA | C4-C3-C5-C6 |
| 30 | A | 5001 | LHG | C17-C18-C19-C20 |
| 25 | A | 1111 | CLA | C11-C12-C13-C15 |
| 25 | A | 1113 | CLA | C6-C7-C8-C10 |
| 25 | A | 1116 | CLA | C2-C3-C5-C6 |
| 25 | A | 1117 | CLA | C11-C10-C8-C7 |
| 25 | A | 1127 | CLA | C11-C12-C13-C15 |
| 25 | A | 1133 | CLA | C12-C13-C15-C16 |
| 25 | B | 1216 | CLA | C6-C7-C8-C10 |
| 25 | B | 1224 | CLA | C2-C3-C5-C6 |
| 25 | 4 | 612 | CLA | C11-C10-C8-C7 |
| 25 | 5 | 607 | CLA | C2-C3-C5-C6 |
| 25 | 6 | 603 | CLA | C6-C7-C8-C10 |
| 26 | 7 | 613 | CHL | C2-C3-C5-C6 |
| 25 | 7 | 605 | CLA | CAA-CBA-CGA-O1A |
| 47 | 5 | 804 | PLM | O2-C1-C2-C3 |
| 25 | 6 | 612 | CLA | CBA-CGA-O2A-C1 |
| 41 | J | 5002 | SPH | C9-C10-C11-C12 |
| 30 | A | 5003 | LHG | O1-C1-C2-O2 |
| 25 | B | 1225 | CLA | C3-C5-C6-C7 |
| 30 | A | 5002 | LHG | C10-C11-C12-C13 |
| 25 | 6 | 618 | CLA | CAA-CBA-CGA-O1A |
| 29 | B | 4007 | BCR | C15-C16-C17-C18 |
| 29 | H | 4001 | BCR | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 29 | K | 4001 | BCR | C9-C10-C11-C12 |
| 29 | L | 4001 | BCR | C19-C20-C21-C22 |
| 25 | 7 | 602 | CLA | CAA-CBA-CGA-O2A |
| 30 | 9 | 801 | LHG | C2-C3-O3-P |
| 37 | K | 5002 | PCW | C16-C17-C18-C19 |
| 25 | B | 1206 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1206 | CLA | CBA-CGA-O2A-C1 |
| 33 | 3 | 802 | PTY | C13-C14-C15-C16 |
| 37 | K | 5001 | PCW | C14-C15-C16-C17 |
| 25 | K | 1404 | CLA | CAA-CBA-CGA-O2A |
| 25 | L | 1503 | CLA | CAA-CBA-CGA-O1A |
| 25 | 4 | 617 | CLA | CAA-CBA-CGA-O2A |
| 47 | 5 | 804 | PLM | O1-C1-C2-C3 |
| 25 | B | 1213 | CLA | CAA-CBA-CGA-O2A |
| 25 | 3 | 616 | CLA | CAA-CBA-CGA-O2A |
| 25 | 7 | 612 | CLA | CAA-CBA-CGA-O2A |
| 25 | 2 | 602 | CLA | CAA-CBA-CGA-O2A |
| 30 | 5 | 801 | LHG | O7-C7-C8-C9 |
| 48 | 8 | 804 | DGA | OG2-CB1-CB2-CB3 |
| 30 | F | 5001 | LHG | C17-C18-C19-C20 |
| 25 | H | 1702 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 605 | CLA | CAA-CBA-CGA-O2A |
| 50 | 9 | 507 | XAT | C40-C33-C34-C35 |
| 25 | A | 1121 | CLA | CAA-CBA-CGA-O2A |
| 37 | K | 5001 | PCW | O2-C31-C32-C33 |
| 33 | G | 5002 | PTY | C15-C16-C17-C18 |
| 25 | A | 1127 | CLA | C4-C3-C5-C6 |
| 25 | B | 1206 | CLA | C4-C3-C5-C6 |
| 25 | B | 1207 | CLA | C4-C3-C5-C6 |
| 25 | A | 1117 | CLA | C2-C3-C5-C6 |
| 26 | 6 | 610 | CHL | C2-C3-C5-C6 |
| 32 | I | 5001 | SQD | C17-C18-C19-C20 |
| 30 | A | 5002 | LHG | O7-C7-C8-C9 |
| 30 | 8 | 801 | LHG | O8-C23-C24-C25 |
| 37 | B | 5004 | PCW | O2-C31-C32-C33 |
| 25 | A | 1013 | CLA | C11-C10-C8-C9 |
| 25 | A | 1013 | CLA | C11-C12-C13-C14 |
| 25 | A | 1132 | CLA | C14-C13-C15-C16 |
| 25 | B | 1021 | CLA | C11-C12-C13-C14 |
| 25 | B | 1205 | CLA | C14-C13-C15-C16 |
| 25 | B | 1209 | CLA | C11-C10-C8-C9 |
| 25 | B | 1228 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1239 | CLA | C14-C13-C15-C16 |
| 25 | 4 | 604 | CLA | C6-C7-C8-C9 |
| 25 | 4 | 610 | CLA | C14-C13-C15-C16 |
| 25 | 6 | 606 | CLA | C11-C12-C13-C14 |
| 25 | 6 | 615 | CLA | C11-C10-C8-C9 |
| 25 | 2 | 605 | CLA | C6-C7-C8-C9 |
| 30 | 7 | 803 | LHG | C10-C11-C12-C13 |
| 25 | A | 1127 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1201 | CLA | C3A-C2A-CAA-CBA |
| 25 | B | 1231 | CLA | C3A-C2A-CAA-CBA |
| 26 | a | 613 | CHL | C3A-C2A-CAA-CBA |
| 26 | 7 | 617 | CHL | C3A-C2A-CAA-CBA |
| 25 | A | 1109 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 1222 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1110 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1126 | CLA | CAA-CBA-CGA-O2A |
| 26 | 9 | 601 | CHL | CAA-CBA-CGA-O2A |
| 26 | 9 | 608 | CHL | CAA-CBA-CGA-O2A |
| 30 | B | 5001 | LHG | O8-C23-C24-C25 |
| 30 | 6 | 802 | LHG | O8-C23-C24-C25 |
| 33 | A | 5006 | PTY | C12-C11-C8-O7 |
| 33 | 5 | 802 | PTY | O4-C30-C31-C32 |
| 37 | B | 5004 | PCW | C39-C40-C41-C42 |
| 45 | a | 805 | OLA | C7-C8-C9-C10 |
| 30 | 2 | 801 | LHG | C32-C33-C34-C35 |
| 25 | A | 1120 | CLA | CAD-CBD-CGD-O2D |
| 25 | A | 1134 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 1208 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 1235 | CLA | CAD-CBD-CGD-O2D |
| 25 | 1 | 606 | CLA | CAD-CBD-CGD-O2D |
| 25 | 6 | 604 | CLA | CAD-CBD-CGD-O2D |
| 25 | 8 | 607 | CLA | CAD-CBD-CGD-O2D |
| 25 | 9 | 606 | CLA | CAD-CBD-CGD-O2D |
| 26 | 1 | 610 | CHL | CAD-CBD-CGD-O2D |
| 26 | 3 | 608 | CHL | CAD-CBD-CGD-O2D |
| 26 | 5 | 617 | CHL | CAD-CBD-CGD-O2D |
| 26 | 6 | 613 | CHL | CAD-CBD-CGD-O2D |
| 26 | 6 | 617 | CHL | CAD-CBD-CGD-O2D |
| 26 | 7 | 611 | CHL | CAD-CBD-CGD-O2D |
| 33 | 9 | 803 | PTY | C1-C6-O7-C8 |
| 36 | 8 | 803 | DGD | C3G-C2G-O2G-C1B |
| 25 | 1 | 601 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 8 | 618 | CLA | C8-C10-C11-C12 |
| 25 | B | 1232 | CLA | CAA-CBA-CGA-O1A |
| 25 | 6 | 603 | CLA | CAA-CBA-CGA-O2A |
| 25 | 7 | 608 | CLA | CAA-CBA-CGA-O2A |
| 25 | 8 | 609 | CLA | CAA-CBA-CGA-O2A |
| 26 | 7 | 611 | CHL | CAA-CBA-CGA-O2A |
| 26 | 7 | 615 | CHL | CAA-CBA-CGA-O2A |
| 30 | 6 | 801 | LHG | O8-C23-C24-C25 |
| 33 | a | 803 | PTY | O4-C30-C31-C32 |
| 25 | 5 | 607 | CLA | C8-C10-C11-C12 |
| 33 | G | 5002 | PTY | C18-C19-C20-C21 |
| 36 | B | 5003 | DGD | CCA-CDA-CEA-CFA |
| 25 | B | 1210 | CLA | C4-C3-C5-C6 |
| 25 | L | 1502 | CLA | C4-C3-C5-C6 |
| 25 | B | 1204 | CLA | C16-C17-C18-C20 |
| 30 | 6 | 802 | LHG | C26-C27-C28-C29 |
| 25 | B | 1205 | CLA | C2-C3-C5-C6 |
| 25 | 4 | 610 | CLA | C2-C3-C5-C6 |
| 26 | 7 | 617 | CHL | C2-C3-C5-C6 |
| 25 | A | 1112 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1204 | CLA | CAA-CBA-CGA-O2A |
| 25 | 6 | 601 | CLA | CAA-CBA-CGA-O2A |
| 33 | G | 5003 | PTY | C12-C11-C8-O7 |
| 33 | J | 5001 | PTY | C12-C11-C8-O7 |
| 30 | 6 | 801 | LHG | C29-C30-C31-C32 |
| 29 | B | 4006 | BCR | C21-C22-C23-C24 |
| 29 | I | 4001 | BCR | C11-C12-C13-C14 |
| 29 | 6 | 504 | BCR | C7-C8-C9-C10 |
| 29 | 6 | 504 | BCR | C17-C18-C19-C20 |
| 41 | 6 | 806 | SPH | C4-C5-C6-C7 |
| 45 | 8 | 809 | OLA | C9-C10-C11-C12 |
| 30 | 1 | 802 | LHG | C19-C20-C21-C22 |
| 30 | 5 | 801 | LHG | O6-C4-C5-O7 |
| 25 | A | 1122 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1211 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1238 | CLA | CAA-CBA-CGA-O2A |
| 25 | L | 1504 | CLA | CAA-CBA-CGA-O2A |
| 25 | a | 603 | CLA | CAA-CBA-CGA-O2A |
| 30 | A | 5002 | LHG | O8-C23-C24-C25 |
| 30 | 2 | 802 | LHG | O8-C23-C24-C25 |
| 33 | 7 | 804 | PTY | O4-C30-C31-C32 |
| 32 | H | 5001 | SQD | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 5 | 608 | CLA | CAA-CBA-CGA-O1A |
| 25 | 5 | 608 | CLA | CAA-CBA-CGA-O2A |
| 45 | 8 | 809 | OLA | O2-C1-C2-C3 |
| 25 | B | 1214 | CLA | O2A-C1-C2-C3 |
| 26 | 3 | 603 | CHL | O2A-C1-C2-C3 |
| 26 | 6 | 611 | CHL | O2A-C1-C2-C3 |
| 25 | 1 | 606 | CLA | O1A-CGA-O2A-C1 |
| 47 | 8 | 806 | PLM | C3-C4-C5-C6 |
| 25 | 5 | 602 | CLA | CBA-CGA-O2A-C1 |
| 25 | 7 | 601 | CLA | C2A-CAA-CBA-CGA |
| 33 | 9 | 803 | PTY | C41-C42-C43-C44 |
| 36 | B | 5003 | DGD | CFA-CGA-CHA-CIA |
| 26 | 6 | 619 | CHL | CAA-CBA-CGA-O2A |
| 25 | 5 | 602 | CLA | O1A-CGA-O2A-C1 |
| 47 | 8 | 807 | PLM | O1-C1-C2-C3 |
| 25 | 1 | 603 | CLA | C8-C10-C11-C12 |
| 25 | 6 | 615 | CLA | C16-C17-C18-C20 |
| 25 | A | 1127 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1012 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1012 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1013 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1013 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1112 | CLA | CHA-CBD-CGD-O2D |
| 25 | A | 1127 | CLA | CHA-CBD-CGD-O1D |
| 25 | A | 1127 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1237 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1237 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1022 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1022 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1206 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1206 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1212 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1212 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1219 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1221 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1221 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1223 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1227 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1228 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1228 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1230 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1230 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1234 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1234 | CLA | CHA-CBD-CGD-O2D |
| 25 | B | 1236 | CLA | CHA-CBD-CGD-O1D |
| 25 | B | 1236 | CLA | CHA-CBD-CGD-O2D |
| 25 | G | 1601 | CLA | CHA-CBD-CGD-O1D |
| 25 | G | 1601 | CLA | CHA-CBD-CGD-O2D |
| 25 | L | 1502 | CLA | CHA-CBD-CGD-O1D |
| 25 | L | 1502 | CLA | CHA-CBD-CGD-O2D |
| 25 | O | 1803 | CLA | CHA-CBD-CGD-O1D |
| 25 | O | 1803 | CLA | CHA-CBD-CGD-O2D |
| 25 | 1 | 601 | CLA | CHA-CBD-CGD-O1D |
| 25 | 1 | 601 | CLA | CHA-CBD-CGD-O2D |
| 25 | 1 | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | 1 | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | 1 | 615 | CLA | CHA-CBD-CGD-O1D |
| 25 | 1 | 615 | CLA | CHA-CBD-CGD-O2D |
| 25 | a | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | a | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | a | 605 | CLA | CHA-CBD-CGD-O1D |
| 25 | a | 605 | CLA | CHA-CBD-CGD-O2D |
| 25 | 3 | 601 | CLA | CHA-CBD-CGD-O2D |
| 25 | 3 | 602 | CLA | CHA-CBD-CGD-O1D |
| 25 | 3 | 602 | CLA | CHA-CBD-CGD-O2D |
| 25 | 3 | 616 | CLA | CHA-CBD-CGD-O2D |
| 25 | 4 | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 607 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 5 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 5 | 615 | CLA | CHA-CBD-CGD-O2D |
| 25 | 6 | 601 | CLA | CHA-CBD-CGD-O2D |
| 25 | 6 | 605 | CLA | CHA-CBD-CGD-O1D |
| 25 | 6 | 606 | CLA | CHA-CBD-CGD-O1D |
| 25 | 6 | 606 | CLA | CHA-CBD-CGD-O2D |
| 25 | 6 | 612 | CLA | CHA-CBD-CGD-O1D |
| 25 | 6 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 7 | 601 | CLA | CHA-CBD-CGD-O1D |
| 25 | 7 | 601 | CLA | CHA-CBD-CGD-O2D |
| 25 | 7 | 604 | CLA | CHA-CBD-CGD-O2D |
| 25 | 7 | 610 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 607 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 612 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 8 | 612 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 615 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 615 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 618 | CLA | CHA-CBD-CGD-O1D |
| 25 | 8 | 618 | CLA | CHA-CBD-CGD-O2D |
| 25 | 2 | 603 | CLA | CHA-CBD-CGD-O1D |
| 25 | 2 | 603 | CLA | CHA-CBD-CGD-O2D |
| 25 | 2 | 604 | CLA | CHA-CBD-CGD-O1D |
| 25 | 2 | 604 | CLA | CHA-CBD-CGD-O2D |
| 25 | 9 | 604 | CLA | CHA-CBD-CGD-O2D |
| 26 | 1 | 604 | CHL | CHA-CBD-CGD-O1D |
| 26 | 3 | 604 | CHL | CHA-CBD-CGD-O1D |
| 26 | 3 | 604 | CHL | CHA-CBD-CGD-O2D |
| 26 | 6 | 609 | CHL | CHA-CBD-CGD-O1D |
| 26 | 7 | 609 | CHL | CHA-CBD-CGD-O2D |
| 26 | 8 | 604 | CHL | CHA-CBD-CGD-O1D |
| 26 | 8 | 604 | CHL | CHA-CBD-CGD-O2D |
| 26 | 8 | 613 | CHL | CHA-CBD-CGD-O1D |
| 26 | 2 | 609 | CHL | CHA-CBD-CGD-O2D |
| 26 | 9 | 608 | CHL | CHA-CBD-CGD-O2D |
| 29 | A | 4005 | BCR | C9-C10-C11-C12 |
| 25 | 7 | 602 | CLA | CAA-CBA-CGA-O1A |
| 25 | A | 1108 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1130 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1210 | CLA | CAA-CBA-CGA-O2A |
| 25 | 1 | 603 | CLA | CAA-CBA-CGA-O2A |
| 30 | 4 | 801 | LHG | O8-C23-C24-C25 |
| 25 | B | 1023 | CLA | C2C-C3C-CAC-CBC |
| 25 | B | 1231 | CLA | C2-C3-C5-C6 |
| 25 | B | 1207 | CLA | C2-C3-C5-C6 |
| 25 | 7 | 606 | CLA | C2-C3-C5-C6 |
| 36 | B | 5003 | DGD | CAA-CBA-CCA-CDA |
| 30 | 6 | 801 | LHG | C15-C16-C17-C18 |
| 47 | 4 | 803 | PLM | C8-C9-CA-CB |
| 25 | K | 1404 | CLA | CAA-CBA-CGA-O1A |
| 25 | 5 | 606 | CLA | CAA-CBA-CGA-O2A |
| 26 | a | 604 | CHL | CAA-CBA-CGA-O2A |
| 30 | 7 | 801 | LHG | O8-C23-C24-C25 |
| 32 | A | 5005 | SQD | O48-C23-C24-C25 |
| 26 | 9 | 608 | CHL | C2-C1-O2A-CGA |
| 30 | 6 | 802 | LHG | C29-C30-C31-C32 |
| 33 | a | 802 | PTY | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 9 | 801 | LHG | O7-C5-C6-O8 |
| 30 | A | 5002 | LHG | C19-C20-C21-C22 |
| 45 | 8 | 809 | OLA | O1-C1-C2-C3 |
| 35 | 1 | 804 | LMT | C3'-C4'-O1B-C1B |
| 25 | B | 1209 | CLA | CAA-CBA-CGA-O2A |
| 25 | 1 | 605 | CLA | CAA-CBA-CGA-O2A |
| 25 | 4 | 603 | CLA | CAA-CBA-CGA-O2A |
| 25 | 5 | 603 | CLA | CAA-CBA-CGA-O2A |
| 25 | 7 | 603 | CLA | CAA-CBA-CGA-O2A |
| 25 | 2 | 601 | CLA | CAA-CBA-CGA-O2A |
| 26 | 1 | 613 | CHL | CAA-CBA-CGA-O2A |
| 33 | G | 5003 | PTY | C6-C1-O4-C30 |
| 25 | A | 1127 | CLA | CBA-CGA-O2A-C1 |
| 25 | 8 | 609 | CLA | C3-C5-C6-C7 |
| 26 | 8 | 610 | CHL | C4-C3-C5-C6 |
| 25 | 6 | 604 | CLA | C12-C13-C15-C16 |
| 25 | B | 1208 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1240 | CLA | CAA-CBA-CGA-O2A |
| 25 | a | 607 | CLA | CAA-CBA-CGA-O2A |
| 25 | 6 | 612 | CLA | CAA-CBA-CGA-O2A |
| 25 | 2 | 605 | CLA | CAA-CBA-CGA-O2A |
| 26 | 1 | 611 | CHL | CAA-CBA-CGA-O2A |
| 25 | A | 1125 | CLA | C6-C7-C8-C9 |
| 25 | A | 1133 | CLA | C6-C7-C8-C9 |
| 25 | A | 1138 | CLA | C11-C12-C13-C14 |
| 25 | B | 1234 | CLA | C14-C13-C15-C16 |
| 25 | 1 | 605 | CLA | C14-C13-C15-C16 |
| 25 | A | 1113 | CLA | C10-C11-C12-C13 |
| 25 | 1 | 606 | CLA | CBA-CGA-O2A-C1 |
| 30 | 8 | 801 | LHG | O7-C7-C8-C9 |
| 26 | 2 | 609 | CHL | CAA-CBA-CGA-O1A |
| 25 | A | 1119 | CLA | C16-C17-C18-C19 |
| 25 | B | 1210 | CLA | C16-C17-C18-C19 |
| 25 | 3 | 601 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 1109 | CLA | C5-C6-C7-C8 |
| 25 | 4 | 617 | CLA | CAA-CBA-CGA-O1A |
| 25 | 1 | 615 | CLA | C2A-CAA-CBA-CGA |
| 25 | 9 | 605 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1112 | CLA | CAA-CBA-CGA-O1A |
| 25 | A | 1121 | CLA | CAA-CBA-CGA-O1A |
| 25 | 3 | 616 | CLA | CAA-CBA-CGA-O1A |
| 26 | 9 | 608 | CHL | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 7 | 803 | LHG | C29-C30-C31-C32 |
| 33 | a | 802 | PTY | O4-C30-C31-C32 |
| 34 | A | 5007 | 3PH | C33-C34-C35-C36 |
| 29 | I | 4001 | BCR | C11-C12-C13-C35 |
| 25 | B | 1213 | CLA | CAA-CBA-CGA-O1A |
| 26 | 7 | 611 | CHL | CAA-CBA-CGA-O1A |
| 33 | A | 5006 | PTY | C12-C11-C8-O10 |
| 25 | B | 1237 | CLA | C16-C17-C18-C19 |
| 25 | B | 1023 | CLA | C10-C11-C12-C13 |
| 36 | 7 | 806 | DGD | C7A-C8A-C9A-CAA |
| 25 | B | 1211 | CLA | CAA-CBA-CGA-O1A |
| 25 | 2 | 602 | CLA | CAA-CBA-CGA-O1A |
| 26 | 4 | 609 | CHL | CAA-CBA-CGA-O1A |
| 26 | 6 | 619 | CHL | CAA-CBA-CGA-O1A |
| 30 | A | 5002 | LHG | O10-C23-C24-C25 |
| 25 | 3 | 601 | CLA | CBA-CGA-O2A-C1 |
| 47 | 4 | 804 | PLM | C3-C4-C5-C6 |
| 25 | B | 1206 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1212 | CLA | C1A-C2A-CAA-CBA |
| 25 | B | 1218 | CLA | C1A-C2A-CAA-CBA |
| 25 | G | 1601 | CLA | C1A-C2A-CAA-CBA |
| 25 | L | 1501 | CLA | C1A-C2A-CAA-CBA |
| 25 | 5 | 609 | CLA | C1A-C2A-CAA-CBA |
| 25 | 7 | 605 | CLA | CHA-CBD-CGD-O2D |
| 25 | 8 | 606 | CLA | C1A-C2A-CAA-CBA |
| 25 | 8 | 607 | CLA | C1A-C2A-CAA-CBA |
| 25 | 2 | 612 | CLA | C1A-C2A-CAA-CBA |
| 26 | 7 | 615 | CHL | C1A-C2A-CAA-CBA |
| 25 | A | 1122 | CLA | CAA-CBA-CGA-O1A |
| 25 | A | 1130 | CLA | CAA-CBA-CGA-O1A |
| 25 | 7 | 608 | CLA | CAA-CBA-CGA-O1A |
| 26 | 7 | 615 | CHL | CAA-CBA-CGA-O1A |
| 30 | A | 5002 | LHG | O9-C7-C8-C9 |
| 30 | 5 | 801 | LHG | O9-C7-C8-C9 |
| 30 | 8 | 801 | LHG | O9-C7-C8-C9 |
| 45 | 8 | 808 | OLA | C9-C10-C11-C12 |
| 25 | 4 | 604 | CLA | C2-C1-O2A-CGA |
| 26 | 9 | 603 | CHL | C2-C1-O2A-CGA |
| 25 | A | 1110 | CLA | CAA-CBA-CGA-O1A |
| 25 | a | 603 | CLA | CAA-CBA-CGA-O1A |
| 26 | 1 | 611 | CHL | CAA-CBA-CGA-O1A |
| 33 | J | 5001 | PTY | C12-C11-C8-O10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | K | 5001 | PCW | O31-C31-C32-C33 |
| 48 | 8 | 804 | DGA | OB1-CB1-CB2-CB3 |
| 30 | A | 5001 | LHG | C4-C5-C6-O8 |
| 30 | 2 | 802 | LHG | C4-C5-C6-O8 |
| 32 | A | 5005 | SQD | O6-C44-C45-C46 |
| 24 | A | 1011 | CL0 | CAA-CBA-CGA-O2A |
| 25 | H | 1702 | CLA | CAA-CBA-CGA-O2A |
| 30 | A | 5002 | LHG | C17-C18-C19-C20 |
| 25 | 4 | 607 | CLA | C5-C6-C7-C8 |
| 26 | 8 | 603 | CHL | C2A-CAA-CBA-CGA |
| 25 | 1 | 607 | CLA | C16-C17-C18-C20 |
| 26 | 4 | 609 | CHL | C16-C17-C18-C20 |
| 25 | A | 1108 | CLA | CAA-CBA-CGA-O1A |
| 25 | L | 1504 | CLA | CAA-CBA-CGA-O1A |
| 25 | 6 | 603 | CLA | CAA-CBA-CGA-O1A |
| 25 | 7 | 612 | CLA | CAA-CBA-CGA-O1A |
| 30 | B | 5001 | LHG | O10-C23-C24-C25 |
| 33 | a | 803 | PTY | O30-C30-C31-C32 |
| 25 | A | 1131 | CLA | C13-C15-C16-C17 |
| 25 | A | 1134 | CLA | C5-C6-C7-C8 |
| 30 | 5 | 801 | LHG | C16-C17-C18-C19 |
| 25 | F | 1301 | CLA | CAA-CBA-CGA-O2A |
| 25 | K | 1402 | CLA | CAA-CBA-CGA-O2A |
| 26 | 8 | 604 | CHL | CAA-CBA-CGA-O2A |
| 48 | 2 | 803 | DGA | OG2-CB1-CB2-CB3 |
| 25 | B | 1210 | CLA | CAA-CBA-CGA-O1A |
| 30 | 6 | 802 | LHG | O10-C23-C24-C25 |
| 30 | 8 | 801 | LHG | O10-C23-C24-C25 |
| 33 | 5 | 802 | PTY | O30-C30-C31-C32 |
| 33 | 7 | 804 | PTY | O30-C30-C31-C32 |
| 26 | a | 613 | CHL | CAA-CBA-CGA-O2A |
| 30 | A | 5003 | LHG | C3-O3-P-O5 |
| 30 | F | 5002 | LHG | C3-O3-P-O5 |
| 30 | 1 | 801 | LHG | C4-O6-P-O5 |
| 30 | a | 801 | LHG | C3-O3-P-O5 |
| 30 | 9 | 801 | LHG | C4-O6-P-O5 |
| 33 | a | 802 | PTY | C3-O11-P1-O13 |
| 33 | 5 | 802 | PTY | C3-O11-P1-O12 |
| 37 | B | 5004 | PCW | C4-O4P-P-O2P |
| 37 | K | 5001 | PCW | C4-O4P-P-O2P |
| 30 | 5 | 801 | LHG | C25-C26-C27-C28 |
| 33 | G | 5003 | PTY | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 603 | CLA | CAA-CBA-CGA-O1A |
| 25 | 5 | 606 | CLA | CAA-CBA-CGA-O1A |
| 25 | 6 | 601 | CLA | CAA-CBA-CGA-O1A |
| 25 | 6 | 612 | CLA | CAA-CBA-CGA-O1A |
| 26 | 9 | 601 | CHL | CAA-CBA-CGA-O1A |
| 30 | 4 | 801 | LHG | O10-C23-C24-C25 |
| 32 | A | 5005 | SQD | O10-C23-C24-C25 |
| 25 | G | 1602 | CLA | CAA-CBA-CGA-O2A |
| 33 | a | 802 | PTY | O14-C5-C6-C1 |
| 25 | 2 | 608 | CLA | CAA-CBA-CGA-O2A |
| 47 | 8 | 807 | PLM | O2-C1-C2-C3 |
| 29 | A | 4005 | BCR | C5-C6-C7-C8 |
| 43 | a | 503 | LUT | C5-C6-C7-C8 |
| 43 | 8 | 501 | LUT | C5-C6-C7-C8 |
| 30 | 7 | 801 | LHG | C24-C25-C26-C27 |
| 33 | A | 5006 | PTY | N1-C2-C3-O11 |
| 25 | 7 | 603 | CLA | CAA-CBA-CGA-O1A |
| 25 | 8 | 609 | CLA | CAA-CBA-CGA-O1A |
| 30 | 6 | 801 | LHG | O10-C23-C24-C25 |
| 36 | 8 | 802 | DGD | C6A-C7A-C8A-C9A |
| 25 | A | 1120 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1237 | CLA | CAA-CBA-CGA-O2A |
| 30 | 5 | 801 | LHG | O8-C23-C24-C25 |
| 25 | 6 | 606 | CLA | C5-C6-C7-C8 |
| 30 | 6 | 802 | LHG | C30-C31-C32-C33 |
| 26 | 2 | 613 | CHL | C2A-CAA-CBA-CGA |
| 25 | B | 1208 | CLA | CAA-CBA-CGA-O1A |
| 25 | B | 1215 | CLA | C10-C11-C12-C13 |
| 41 | 4 | 805 | SPH | C4-C5-C6-C7 |
| 25 | B | 1218 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1238 | CLA | CAA-CBA-CGA-O1A |
| 25 | 5 | 603 | CLA | CAA-CBA-CGA-O1A |
| 25 | 6 | 606 | CLA | C4-C3-C5-C6 |
| 33 | 5 | 802 | PTY | C16-C17-C18-C19 |
| 26 | 8 | 601 | CHL | C11-C12-C13-C14 |
| 30 | A | 5003 | LHG | C18-C19-C20-C21 |
| 47 | 5 | 804 | PLM | C9-CA-CB-CC |
| 25 | A | 1111 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1113 | CLA | CAD-CBD-CGD-O1D |
| 25 | A | 1135 | CLA | C2-C3-C5-C6 |
| 25 | B | 1022 | CLA | CAD-CBD-CGD-O1D |
| 25 | B | 1228 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | B | 1231 | CLA | CAD-CBD-CGD-O1D |
| 25 | O | 1803 | CLA | CAD-CBD-CGD-O1D |
| 25 | 1 | 615 | CLA | CAD-CBD-CGD-O1D |
| 25 | a | 607 | CLA | CAD-CBD-CGD-O1D |
| 25 | 3 | 616 | CLA | CAD-CBD-CGD-O1D |
| 25 | 5 | 607 | CLA | CAD-CBD-CGD-O1D |
| 25 | 5 | 609 | CLA | C2-C3-C5-C6 |
| 25 | 6 | 601 | CLA | CAD-CBD-CGD-O1D |
| 25 | 7 | 610 | CLA | CAD-CBD-CGD-O1D |
| 26 | 1 | 609 | CHL | CAD-CBD-CGD-O1D |
| 26 | 8 | 613 | CHL | CAD-CBD-CGD-O1D |
| 32 | G | 5001 | SQD | O5-C5-C6-S |
| 32 | I | 5001 | SQD | O5-C5-C6-S |
| 33 | J | 5001 | PTY | C2-C3-O11-P1 |
| 33 | a | 803 | PTY | C2-C3-O11-P1 |
| 25 | B | 1204 | CLA | CAA-CBA-CGA-O1A |
| 30 | 7 | 801 | LHG | O10-C23-C24-C25 |
| 33 | G | 5003 | PTY | C12-C11-C8-O10 |
| 37 | B | 5004 | PCW | O31-C31-C32-C33 |
| 30 | 1 | 801 | LHG | O8-C23-C24-C25 |
| 30 | 9 | 802 | LHG | O8-C23-C24-C25 |
| 48 | 2 | 803 | DGA | OG1-CA1-CA2-CA3 |
| 25 | 6 | 604 | CLA | C5-C6-C7-C8 |
| 25 | A | 1106 | CLA | C14-C13-C15-C16 |
| 25 | A | 1121 | CLA | C11-C10-C8-C9 |
| 25 | B | 1205 | CLA | C11-C12-C13-C14 |
| 25 | B | 1231 | CLA | C14-C13-C15-C16 |
| 25 | 4 | 601 | CLA | C11-C10-C8-C9 |
| 25 | 2 | 607 | CLA | C14-C13-C15-C16 |
| 27 | B | 2002 | PQN | C19-C18-C20-C21 |
| 30 | A | 5003 | LHG | C31-C32-C33-C34 |
| 30 | B | 5002 | LHG | C27-C28-C29-C30 |
| 35 | 1 | 804 | LMT | C3-C4-C5-C6 |
| 26 | a | 613 | CHL | CAA-CBA-CGA-O1A |
| 25 | A | 1113 | CLA | C8-C10-C11-C12 |
| 26 | 8 | 604 | CHL | CAA-CBA-CGA-O1A |
| 25 | B | 1023 | CLA | C16-C17-C18-C20 |
| 25 | A | 1118 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1128 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1228 | CLA | CAA-CBA-CGA-O2A |
| 25 | K | 1403 | CLA | CAA-CBA-CGA-O2A |
| 25 | 1 | 608 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 1 | 612 | CLA | CAA-CBA-CGA-O2A |
| 25 | 7 | 610 | CLA | CAA-CBA-CGA-O2A |
| 25 | 8 | 608 | CLA | CAA-CBA-CGA-O2A |
| 30 | F | 5001 | LHG | O8-C23-C24-C25 |
| 30 | 6 | 801 | LHG | O7-C7-C8-C9 |
| 33 | 7 | 804 | PTY | C12-C11-C8-O7 |
| 30 | B | 5002 | LHG | C34-C35-C36-C37 |
| 25 | A | 1133 | CLA | C15-C16-C17-C18 |
| 25 | 2 | 603 | CLA | C10-C11-C12-C13 |
| 25 | 5 | 601 | CLA | O1A-CGA-O2A-C1 |
| 30 | A | 5001 | LHG | C5-C6-O8-C23 |
| 33 | a | 803 | PTY | C13-C14-C15-C16 |
| 26 | 1 | 604 | CHL | C13-C15-C16-C17 |
| 25 | L | 1501 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1134 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1139 | CLA | CAA-CBA-CGA-O2A |
| 25 | G | 1601 | CLA | CAA-CBA-CGA-O2A |
| 25 | 1 | 615 | CLA | CAA-CBA-CGA-O2A |
| 25 | 5 | 602 | CLA | CAA-CBA-CGA-O2A |
| 25 | 5 | 607 | CLA | CAA-CBA-CGA-O2A |
| 25 | 5 | 609 | CLA | CAA-CBA-CGA-O2A |
| 25 | 7 | 607 | CLA | CAA-CBA-CGA-O2A |
| 25 | 8 | 605 | CLA | CAA-CBA-CGA-O2A |
| 25 | 8 | 618 | CLA | CAA-CBA-CGA-O2A |
| 30 | 3 | 801 | LHG | O8-C23-C24-C25 |
| 25 | 2 | 601 | CLA | CAA-CBA-CGA-O1A |
| 26 | a | 604 | CHL | CAA-CBA-CGA-O1A |
| 25 | A | 1106 | CLA | C4-C3-C5-C6 |
| 26 | 4 | 609 | CHL | C4-C3-C5-C6 |
| 30 | F | 5001 | LHG | C27-C28-C29-C30 |
| 35 | 2 | 804 | LMT | C5'-C4'-O1B-C1B |
| 25 | B | 1203 | CLA | C11-C10-C8-C7 |
| 25 | B | 1205 | CLA | C11-C12-C13-C15 |
| 25 | B | 1210 | CLA | C6-C7-C8-C10 |
| 25 | B | 1224 | CLA | C11-C12-C13-C15 |
| 25 | B | 1234 | CLA | C12-C13-C15-C16 |
| 25 | B | 1239 | CLA | C2-C3-C5-C6 |
| 25 | B | 1239 | CLA | C11-C12-C13-C15 |
| 25 | G | 1601 | CLA | C3A-C2A-CAA-CBA |
| 25 | 1 | 612 | CLA | C11-C12-C13-C15 |
| 25 | 5 | 612 | CLA | C12-C13-C15-C16 |
| 25 | 6 | 606 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 6 | 612 | CLA | C3A-C2A-CAA-CBA |
| 25 | 7 | 605 | CLA | CHA-CBD-CGD-O1D |
| 26 | A | 1114 | CHL | C11-C12-C13-C15 |
| 26 | 4 | 618 | CHL | C3A-C2A-CAA-CBA |
| 26 | 7 | 609 | CHL | C11-C12-C13-C15 |
| 26 | 7 | 617 | CHL | C11-C10-C8-C7 |
| 25 | H | 1702 | CLA | CAA-CBA-CGA-O1A |
| 25 | K | 1402 | CLA | CAA-CBA-CGA-O1A |
| 25 | 1 | 605 | CLA | CAA-CBA-CGA-O1A |
| 25 | a | 607 | CLA | CAA-CBA-CGA-O1A |
| 25 | 5 | 612 | CLA | CAA-CBA-CGA-O1A |
| 33 | 7 | 804 | PTY | C12-C11-C8-O10 |
| 48 | 2 | 803 | DGA | OA1-CA1-CA2-CA3 |
| 25 | A | 1116 | CLA | CAA-CBA-CGA-O2A |
| 25 | B | 1216 | CLA | CAA-CBA-CGA-O2A |
| 25 | 3 | 606 | CLA | CAA-CBA-CGA-O2A |
| 25 | 5 | 612 | CLA | CAA-CBA-CGA-O2A |
| 26 | 4 | 613 | CHL | CAA-CBA-CGA-O2A |
| 30 | a | 801 | LHG | O8-C23-C24-C25 |
| 33 | B | 5005 | PTY | C22-C23-C24-C25 |
| 29 | K | 4002 | BCR | C7-C8-C9-C10 |
| 39 | F | 4001 | NEX | C11-C12-C13-C14 |
| 40 | J | 4002 | RRX | C7-C8-C9-C10 |
| 40 | 3 | 506 | RRX | C21-C22-C23-C24 |
| 43 | 4 | 502 | LUT | C7-C8-C9-C10 |
| 50 | 9 | 507 | XAT | C31-C32-C33-C34 |
| 25 | B | 1237 | CLA | CAA-CBA-CGA-O1A |
| 25 | B | 1209 | CLA | CAA-CBA-CGA-O1A |
| 25 | 4 | 603 | CLA | CAA-CBA-CGA-O1A |
| 33 | a | 802 | PTY | O30-C30-C31-C32 |
| 48 | 2 | 803 | DGA | OB1-CB1-CB2-CB3 |
| 29 | L | 4002 | BCR | C15-C16-C17-C18 |
| 29 | L | 4002 | BCR | C19-C20-C21-C22 |
| 35 | 2 | 804 | LMT | C2-C1-O1'-C1' |
| 52 | 8 | 805 | P5S | O19-C17-C20-C21 |
| 30 | 6 | 801 | LHG | C18-C19-C20-C21 |
| 25 | 7 | 606 | CLA | C5-C6-C7-C8 |
| 30 | A | 5001 | LHG | C19-C20-C21-C22 |
| 25 | A | 1137 | CLA | CAA-CBA-CGA-O1A |
| 25 | A | 1139 | CLA | CAA-CBA-CGA-O1A |
| 25 | F | 1301 | CLA | CAA-CBA-CGA-O1A |
| 25 | G | 1601 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | 5 | 607 | CLA | CAA-CBA-CGA-O1A |
| 25 | 7 | 607 | CLA | CAA-CBA-CGA-O1A |
| 26 | 1 | 613 | CHL | CAA-CBA-CGA-O1A |
| 30 | 1 | 801 | LHG | O10-C23-C24-C25 |
| 30 | 5 | 801 | LHG | O10-C23-C24-C25 |
| 25 | 8 | 620 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1132 | CLA | C5-C6-C7-C8 |
| 30 | 2 | 802 | LHG | C26-C27-C28-C29 |
| 45 | a | 805 | OLA | C2-C3-C4-C5 |
| 25 | A | 1137 | CLA | CAA-CBA-CGA-O2A |
| 25 | 4 | 615 | CLA | CAA-CBA-CGA-O2A |
| 25 | 2 | 612 | CLA | CAA-CBA-CGA-O2A |
| 26 | 6 | 611 | CHL | CAA-CBA-CGA-O2A |
| 33 | B | 5005 | PTY | C12-C11-C8-O7 |
| 25 | 3 | 605 | CLA | C10-C11-C12-C13 |
| 25 | A | 1111 | CLA | CAA-CBA-CGA-O1A |
| 25 | A | 1118 | CLA | CAA-CBA-CGA-O1A |
| 25 | B | 1228 | CLA | CAA-CBA-CGA-O1A |
| 25 | K | 1403 | CLA | CAA-CBA-CGA-O1A |
| 25 | 1 | 615 | CLA | CAA-CBA-CGA-O1A |
| 25 | 7 | 610 | CLA | CAA-CBA-CGA-O1A |
| 30 | F | 5001 | LHG | O10-C23-C24-C25 |
| 30 | 6 | 801 | LHG | O9-C7-C8-C9 |
| 30 | 9 | 802 | LHG | O10-C23-C24-C25 |
| 25 | 4 | 617 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 1108 | CLA | C5-C6-C7-C8 |
| 25 | B | 1212 | CLA | CBA-CGA-O2A-C1 |
| 25 | A | 1128 | CLA | CAA-CBA-CGA-O1A |
| 25 | A | 1134 | CLA | CAA-CBA-CGA-O1A |
| 25 | 1 | 608 | CLA | CAA-CBA-CGA-O1A |
| 25 | 1 | 612 | CLA | CAA-CBA-CGA-O1A |
| 25 | 5 | 609 | CLA | CAA-CBA-CGA-O1A |
| 30 | 3 | 801 | LHG | O10-C23-C24-C25 |
| 32 | G | 5001 | SQD | C11-C12-C13-C14 |
| 25 | A | 1111 | CLA | CAA-CBA-CGA-O2A |
| 25 | A | 1129 | CLA | CAA-CBA-CGA-O2A |

There are no ring outliers.

362 monomers are involved in 1239 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | 9 | 802 | LHG | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 26 | 9 | 613 | CHL | 4 | 0 |
| 25 | B | 1232 | CLA | 2 | 0 |
| 52 | 8 | 805 | P5S | 2 | 0 |
| 29 | L | 4001 | BCR | 3 | 0 |
| 25 | 2 | 615 | CLA | 3 | 0 |
| 25 | H | 1703 | CLA | 5 | 0 |
| 25 | B | 1217 | CLA | 4 | 0 |
| 47 | 5 | 804 | PLM | 3 | 0 |
| 25 | 2 | 607 | CLA | 4 | 0 |
| 25 | 7 | 606 | CLA | 2 | 0 |
| 51 | 7 | 807 | 4RF | 6 | 0 |
| 48 | 3 | 803 | DGA | 3 | 0 |
| 25 | B | 1210 | CLA | 2 | 0 |
| 43 | 7 | 501 | LUT | 5 | 0 |
| 25 | 4 | 612 | CLA | 8 | 0 |
| 26 | 7 | 613 | CHL | 12 | 0 |
| 27 | A | 2001 | PQN | 7 | 0 |
| 29 | 5 | 504 | BCR | 4 | 0 |
| 25 | 8 | 612 | CLA | 6 | 0 |
| 25 | 8 | 605 | CLA | 3 | 0 |
| 25 | A | 1126 | CLA | 13 | 0 |
| 25 | 2 | 604 | CLA | 14 | 0 |
| 29 | O | 4001 | BCR | 1 | 0 |
| 25 | 2 | 603 | CLA | 5 | 0 |
| 29 | 5 | 503 | BCR | 6 | 0 |
| 25 | B | 1239 | CLA | 4 | 0 |
| 25 | 3 | 602 | CLA | 3 | 0 |
| 43 | 5 | 501 | LUT | 5 | 0 |
| 25 | L | 1504 | CLA | 4 | 0 |
| 25 | 5 | 601 | CLA | 4 | 0 |
| 25 | 7 | 610 | CLA | 7 | 0 |
| 25 | 1 | 603 | CLA | 6 | 0 |
| 38 | F | 5003 | LPX | 2 | 0 |
| 25 | 1 | 607 | CLA | 4 | 0 |
| 29 | J | 4001 | BCR | 5 | 0 |
| 50 | 9 | 507 | XAT | 5 | 0 |
| 24 | A | 1011 | CL0 | 6 | 0 |
| 25 | 4 | 601 | CLA | 6 | 0 |
| 25 | A | 1109 | CLA | 8 | 0 |
| 25 | A | 1110 | CLA | 4 | 0 |
| 25 | 7 | 605 | CLA | 5 | 0 |
| 37 | B | 5004 | PCW | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 43 | 5 | 502 | LUT | 4 | 0 |
| 25 | 1 | 602 | CLA | 2 | 0 |
| 25 | B | 1229 | CLA | 7 | 0 |
| 25 | 8 | 602 | CLA | 5 | 0 |
| 25 | B | 1237 | CLA | 3 | 0 |
| 25 | 4 | 615 | CLA | 3 | 0 |
| 43 | 4 | 501 | LUT | 4 | 0 |
| 25 | 3 | 606 | CLA | 5 | 0 |
| 26 | 6 | 611 | CHL | 3 | 0 |
| 43 | 5 | 505 | LUT | 4 | 0 |
| 50 | 9 | 504 | XAT | 4 | 0 |
| 26 | 1 | 604 | CHL | 7 | 0 |
| 25 | 2 | 608 | CLA | 1 | 0 |
| 25 | B | 1211 | CLA | 1 | 0 |
| 25 | K | 1402 | CLA | 3 | 0 |
| 30 | 1 | 802 | LHG | 4 | 0 |
| 25 | A | 1117 | CLA | 7 | 0 |
| 25 | B | 1238 | CLA | 2 | 0 |
| 25 | A | 1119 | CLA | 11 | 0 |
| 25 | 2 | 601 | CLA | 7 | 0 |
| 26 | 8 | 601 | CHL | 5 | 0 |
| 43 | 3 | 501 | LUT | 3 | 0 |
| 39 | F | 4001 | NEX | 5 | 0 |
| 25 | A | 1108 | CLA | 9 | 0 |
| 25 | F | 1301 | CLA | 3 | 0 |
| 29 | 8 | 503 | BCR | 3 | 0 |
| 26 | 4 | 609 | CHL | 6 | 0 |
| 29 | A | 4002 | BCR | 4 | 0 |
| 25 | F | 1302 | CLA | 5 | 0 |
| 25 | G | 1601 | CLA | 2 | 0 |
| 25 | L | 1502 | CLA | 7 | 0 |
| 25 | 7 | 602 | CLA | 2 | 0 |
| 25 | A | 1135 | CLA | 3 | 0 |
| 25 | B | 1240 | CLA | 6 | 0 |
| 32 | G | 5001 | SQD | 4 | 0 |
| 33 | G | 5002 | PTY | 1 | 0 |
| 25 | B | 1207 | CLA | 6 | 0 |
| 30 | F | 5001 | LHG | 2 | 0 |
| 43 | 2 | 507 | LUT | 7 | 0 |
| 25 | A | 1013 | CLA | 8 | 0 |
| 29 | A | 4005 | BCR | 9 | 0 |
| 26 | 6 | 609 | CHL | 7 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 36 | 8 | 803 | DGD | 5 | 0 |
| 25 | 2 | 612 | CLA | 4 | 0 |
| 30 | 2 | 801 | LHG | 5 | 0 |
| 25 | 8 | 615 | CLA | 2 | 0 |
| 25 | B | 1230 | CLA | 10 | 0 |
| 43 | 8 | 501 | LUT | 6 | 0 |
| 25 | 3 | 610 | CLA | 3 | 0 |
| 44 | 1 | 502 | AXT | 3 | 0 |
| 25 | A | 1125 | CLA | 8 | 0 |
| 25 | B | 1212 | CLA | 3 | 0 |
| 25 | 4 | 606 | CLA | 3 | 0 |
| 29 | 3 | 505 | BCR | 4 | 0 |
| 25 | B | 1213 | CLA | 3 | 0 |
| 47 | 8 | 806 | PLM | 1 | 0 |
| 25 | 8 | 608 | CLA | 2 | 0 |
| 29 | B | 4005 | BCR | 6 | 0 |
| 25 | 1 | 615 | CLA | 2 | 0 |
| 43 | 1 | 501 | LUT | 4 | 0 |
| 30 | F | 5002 | LHG | 2 | 0 |
| 25 | 1 | 608 | CLA | 9 | 0 |
| 30 | 4 | 801 | LHG | 4 | 0 |
| 25 | B | 1220 | CLA | 10 | 0 |
| 48 | 5 | 803 | DGA | 3 | 0 |
| 25 | A | 1128 | CLA | 8 | 0 |
| 25 | 4 | 611 | CLA | 3 | 0 |
| 25 | A | 1012 | CLA | 12 | 0 |
| 25 | A | 1101 | CLA | 7 | 0 |
| 26 | 2 | 609 | CHL | 4 | 0 |
| 26 | 9 | 610 | CHL | 5 | 0 |
| 25 | B | 1201 | CLA | 8 | 0 |
| 26 | 8 | 613 | CHL | 4 | 0 |
| 25 | 5 | 608 | CLA | 2 | 0 |
| 26 | 9 | 608 | CHL | 2 | 0 |
| 26 | 6 | 619 | CHL | 7 | 0 |
| 29 | A | 4001 | BCR | 4 | 0 |
| 25 | 5 | 614 | CLA | 1 | 0 |
| 29 | L | 4003 | BCR | 1 | 0 |
| 30 | 8 | 801 | LHG | 1 | 0 |
| 25 | B | 1215 | CLA | 4 | 0 |
| 37 | K | 5001 | PCW | 2 | 0 |
| 25 | B | 1231 | CLA | 7 | 0 |
| 25 | 6 | 612 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 26 | A | 1114 | CHL | 9 | 0 |
| 25 | 3 | 613 | CLA | 5 | 0 |
| 25 | A | 1121 | CLA | 1 | 0 |
| 29 | K | 4002 | BCR | 3 | 0 |
| 25 | 5 | 607 | CLA | 3 | 0 |
| 33 | A | 5006 | PTY | 4 | 0 |
| 25 | 6 | 603 | CLA | 5 | 0 |
| 32 | I | 5001 | SQD | 5 | 0 |
| 26 | 5 | 617 | CHL | 2 | 0 |
| 25 | 7 | 604 | CLA | 5 | 0 |
| 32 | A | 5005 | SQD | 8 | 0 |
| 27 | B | 2002 | PQN | 5 | 0 |
| 37 | K | 5002 | PCW | 1 | 0 |
| 25 | 8 | 618 | CLA | 6 | 0 |
| 25 | A | 1139 | CLA | 5 | 0 |
| 43 | 6 | 502 | LUT | 5 | 0 |
| 25 | A | 1137 | CLA | 6 | 0 |
| 26 | 1 | 613 | CHL | 6 | 0 |
| 25 | 1 | 612 | CLA | 16 | 0 |
| 30 | 9 | 801 | LHG | 3 | 0 |
| 25 | 5 | 604 | CLA | 5 | 0 |
| 25 | 5 | 603 | CLA | 3 | 0 |
| 47 | 4 | 804 | PLM | 3 | 0 |
| 26 | 9 | 603 | CHL | 7 | 0 |
| 25 | A | 1123 | CLA | 5 | 0 |
| 25 | 8 | 609 | CLA | 6 | 0 |
| 25 | G | 1603 | CLA | 4 | 0 |
| 26 | 3 | 604 | CHL | 6 | 0 |
| 29 | B | 4002 | BCR | 5 | 0 |
| 25 | B | 1221 | CLA | 5 | 0 |
| 26 | 4 | 613 | CHL | 4 | 0 |
| 25 | A | 1103 | CLA | 9 | 0 |
| 25 | 3 | 616 | CLA | 3 | 0 |
| 25 | 8 | 607 | CLA | 2 | 0 |
| 30 | B | 5002 | LHG | 1 | 0 |
| 30 | B | 5001 | LHG | 6 | 0 |
| 25 | B | 1214 | CLA | 6 | 0 |
| 41 | 9 | 804 | SPH | 2 | 0 |
| 43 | 4 | 502 | LUT | 6 | 0 |
| 29 | 3 | 504 | BCR | 5 | 0 |
| 29 | H | 4001 | BCR | 4 | 0 |
| 29 | G | 4001 | BCR | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 29 | 3 | 503 | BCR | 3 | 0 |
| 33 | G | 5003 | PTY | 1 | 0 |
| 29 | B | 4004 | BCR | 8 | 0 |
| 25 | A | 1133 | CLA | 7 | 0 |
| 25 | B | 1235 | CLA | 6 | 0 |
| 26 | 8 | 610 | CHL | 2 | 0 |
| 26 | 5 | 613 | CHL | 4 | 0 |
| 25 | B | 1206 | CLA | 7 | 0 |
| 30 | A | 5002 | LHG | 5 | 0 |
| 26 | 1 | 611 | CHL | 6 | 0 |
| 25 | 9 | 612 | CLA | 8 | 0 |
| 25 | 6 | 615 | CLA | 8 | 0 |
| 30 | 5 | 801 | LHG | 2 | 0 |
| 26 | 7 | 609 | CHL | 4 | 0 |
| 47 | 8 | 807 | PLM | 5 | 0 |
| 25 | 6 | 608 | CLA | 4 | 0 |
| 25 | B | 1236 | CLA | 7 | 0 |
| 25 | B | 1208 | CLA | 4 | 0 |
| 29 | 6 | 504 | BCR | 4 | 0 |
| 25 | B | 1023 | CLA | 7 | 0 |
| 26 | 5 | 611 | CHL | 3 | 0 |
| 33 | 3 | 802 | PTY | 3 | 0 |
| 25 | A | 1112 | CLA | 5 | 0 |
| 26 | 1 | 609 | CHL | 11 | 0 |
| 25 | B | 1202 | CLA | 5 | 0 |
| 25 | 2 | 605 | CLA | 4 | 0 |
| 25 | 3 | 601 | CLA | 8 | 0 |
| 29 | B | 4001 | BCR | 5 | 0 |
| 26 | 3 | 603 | CHL | 7 | 0 |
| 25 | B | 1205 | CLA | 6 | 0 |
| 25 | 4 | 605 | CLA | 3 | 0 |
| 25 | A | 1116 | CLA | 8 | 0 |
| 29 | 4 | 503 | BCR | 8 | 0 |
| 25 | B | 1218 | CLA | 4 | 0 |
| 25 | B | 1234 | CLA | 9 | 0 |
| 25 | A | 1111 | CLA | 8 | 0 |
| 25 | G | 1602 | CLA | 3 | 0 |
| 30 | A | 5001 | LHG | 3 | 0 |
| 25 | 4 | 602 | CLA | 2 | 0 |
| 29 | K | 4001 | BCR | 5 | 0 |
| 29 | B | 4007 | BCR | 4 | 0 |
| 25 | B | 1203 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 45 | 1 | 803 | OLA | 2 | 0 |
| 25 | B | 1216 | CLA | 7 | 0 |
| 25 | B | 1204 | CLA | 6 | 0 |
| 30 | 6 | 801 | LHG | 6 | 0 |
| 37 | 6 | 803 | PCW | 4 | 0 |
| 25 | 1 | 601 | CLA | 8 | 0 |
| 34 | A | 5007 | 3PH | 3 | 0 |
| 30 | 3 | 801 | LHG | 1 | 0 |
| 25 | K | 1401 | CLA | 5 | 0 |
| 26 | 7 | 615 | CHL | 1 | 0 |
| 25 | 2 | 602 | CLA | 2 | 0 |
| 25 | A | 1105 | CLA | 6 | 0 |
| 25 | A | 1122 | CLA | 5 | 0 |
| 33 | 5 | 802 | PTY | 3 | 0 |
| 25 | A | 1120 | CLA | 4 | 0 |
| 25 | 5 | 612 | CLA | 11 | 0 |
| 30 | 1 | 801 | LHG | 2 | 0 |
| 25 | 4 | 610 | CLA | 4 | 0 |
| 25 | 8 | 611 | CLA | 4 | 0 |
| 53 | 8 | 810 | LAP | 5 | 0 |
| 44 | 7 | 504 | AXT | 10 | 0 |
| 25 | L | 1503 | CLA | 6 | 0 |
| 25 | 7 | 612 | CLA | 9 | 0 |
| 25 | 4 | 617 | CLA | 1 | 0 |
| 25 | B | 1022 | CLA | 9 | 0 |
| 25 | A | 1115 | CLA | 9 | 0 |
| 30 | A | 5003 | LHG | 3 | 0 |
| 25 | K | 1403 | CLA | 3 | 0 |
| 25 | A | 1130 | CLA | 8 | 0 |
| 45 | 8 | 809 | OLA | 1 | 0 |
| 26 | 5 | 610 | CHL | 5 | 0 |
| 25 | 3 | 612 | CLA | 5 | 0 |
| 32 | 7 | 805 | SQD | 1 | 0 |
| 25 | 5 | 605 | CLA | 4 | 0 |
| 25 | 5 | 606 | CLA | 3 | 0 |
| 48 | 8 | 804 | DGA | 5 | 0 |
| 25 | O | 1802 | CLA | 4 | 0 |
| 26 | 6 | 610 | CHL | 2 | 0 |
| 25 | A | 1106 | CLA | 7 | 0 |
| 32 | H | 5001 | SQD | 3 | 0 |
| 26 | 4 | 618 | CHL | 5 | 0 |
| 25 | A | 1136 | CLA | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 26 | 3 | 608 | CHL | 2 | 0 |
| 25 | B | 1225 | CLA | 4 | 0 |
| 25 | 7 | 608 | CLA | 2 | 0 |
| 25 | 9 | 605 | CLA | 6 | 0 |
| 25 | 9 | 606 | CLA | 5 | 0 |
| 25 | A | 1104 | CLA | 3 | 0 |
| 25 | A | 1131 | CLA | 6 | 0 |
| 25 | A | 1118 | CLA | 3 | 0 |
| 48 | 2 | 803 | DGA | 6 | 0 |
| 35 | B | 5006 | LMT | 2 | 0 |
| 40 | 3 | 506 | RRX | 1 | 0 |
| 25 | 7 | 601 | CLA | 6 | 0 |
| 25 | B | 1223 | CLA | 2 | 0 |
| 25 | 6 | 602 | CLA | 2 | 0 |
| 33 | B | 5005 | PTY | 4 | 0 |
| 25 | A | 1113 | CLA | 7 | 0 |
| 25 | 4 | 603 | CLA | 3 | 0 |
| 25 | K | 1404 | CLA | 1 | 0 |
| 26 | 8 | 604 | CHL | 3 | 0 |
| 26 | 7 | 611 | CHL | 3 | 0 |
| 25 | 4 | 607 | CLA | 2 | 0 |
| 25 | 4 | 604 | CLA | 7 | 0 |
| 36 | 8 | 802 | DGD | 3 | 0 |
| 25 | B | 1222 | CLA | 6 | 0 |
| 29 | B | 4006 | BCR | 5 | 0 |
| 43 | 2 | 502 | LUT | 4 | 0 |
| 25 | B | 1021 | CLA | 9 | 0 |
| 26 | 3 | 611 | CHL | 7 | 0 |
| 47 | 6 | 804 | PLM | 1 | 0 |
| 25 | A | 1107 | CLA | 3 | 0 |
| 26 | 9 | 601 | CHL | 9 | 0 |
| 25 | A | 1134 | CLA | 4 | 0 |
| 43 | 1 | 503 | LUT | 3 | 0 |
| 25 | 9 | 602 | CLA | 2 | 0 |
| 25 | 3 | 618 | CLA | 1 | 0 |
| 30 | 2 | 802 | LHG | 6 | 0 |
| 26 | 7 | 617 | CHL | 5 | 0 |
| 26 | 2 | 613 | CHL | 1 | 0 |
| 25 | 5 | 615 | CLA | 1 | 0 |
| 25 | B | 1219 | CLA | 7 | 0 |
| 25 | 7 | 603 | CLA | 5 | 0 |
| 26 | 1 | 610 | CHL | 3 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 43 | 6 | 501 | LUT | 5 | 0 |
| 25 | B | 1226 | CLA | 6 | 0 |
| 25 | H | 1701 | CLA | 3 | 0 |
| 25 | L | 1501 | CLA | 1 | 0 |
| 25 | B | 1209 | CLA | 9 | 0 |
| 25 | 8 | 620 | CLA | 2 | 0 |
| 29 | A | 4004 | BCR | 4 | 0 |
| 25 | 3 | 605 | CLA | 6 | 0 |
| 29 | 6 | 503 | BCR | 4 | 0 |
| 29 | L | 4002 | BCR | 2 | 0 |
| 26 | 2 | 610 | CHL | 2 | 0 |
| 25 | 6 | 606 | CLA | 2 | 0 |
| 29 | A | 4003 | BCR | 4 | 0 |
| 25 | 6 | 601 | CLA | 7 | 0 |
| 25 | A | 1132 | CLA | 4 | 0 |
| 25 | 1 | 605 | CLA | 9 | 0 |
| 26 | 6 | 617 | CHL | 1 | 0 |
| 25 | A | 1102 | CLA | 4 | 0 |
| 25 | 6 | 604 | CLA | 5 | 0 |
| 25 | 6 | 605 | CLA | 2 | 0 |
| 25 | 9 | 609 | CLA | 3 | 0 |
| 35 | A | 5008 | LMT | 1 | 0 |
| 25 | 9 | 604 | CLA | 6 | 0 |
| 30 | 7 | 803 | LHG | 3 | 0 |
| 25 | 1 | 606 | CLA | 2 | 0 |
| 29 | B | 4003 | BCR | 1 | 0 |
| 26 | 5 | 618 | CHL | 4 | 0 |
| 43 | 9 | 501 | LUT | 9 | 0 |
| 25 | B | 1224 | CLA | 12 | 0 |
| 25 | 3 | 607 | CLA | 2 | 0 |
| 33 | 9 | 803 | PTY | 3 | 0 |
| 25 | 4 | 608 | CLA | 4 | 0 |
| 25 | 9 | 607 | CLA | 2 | 0 |
| 25 | 5 | 602 | CLA | 6 | 0 |
| 25 | J | 1901 | CLA | 1 | 0 |
| 25 | A | 1140 | CLA | 5 | 0 |
| 25 | 7 | 607 | CLA | 3 | 0 |
| 50 | 7 | 502 | XAT | 3 | 0 |
| 41 | 6 | 806 | SPH | 1 | 0 |
| 28 | C | 3003 | SF4 | 1 | 0 |
| 25 | 8 | 606 | CLA | 5 | 0 |
| 25 | 2 | 621 | CLA | 3 | 0 |

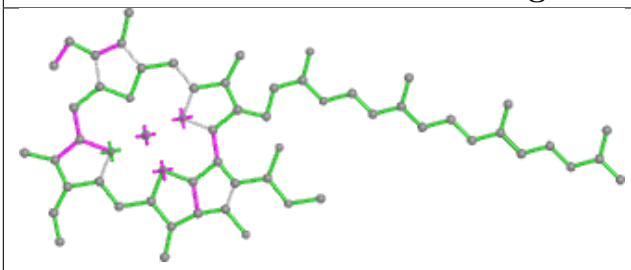
*Continued on next page...*

*Continued from previous page...*

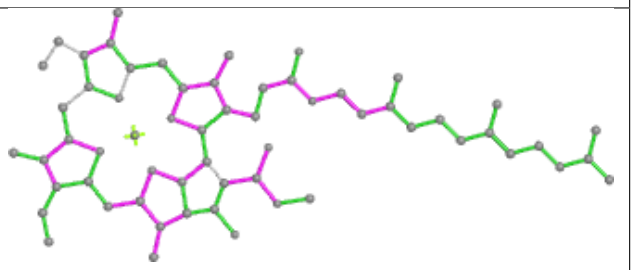
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 50 | 2 | 501 | XAT | 2 | 0 |
| 25 | A | 1129 | CLA | 5 | 0 |
| 25 | 5 | 609 | CLA | 2 | 0 |
| 25 | B | 1228 | CLA | 5 | 0 |
| 29 | 7 | 503 | BCR | 9 | 0 |
| 25 | A | 1124 | CLA | 4 | 0 |
| 25 | O | 1803 | CLA | 1 | 0 |
| 36 | B | 5003 | DGD | 4 | 0 |
| 43 | 8 | 502 | LUT | 5 | 0 |
| 43 | 9 | 502 | LUT | 8 | 0 |
| 40 | J | 4002 | RRX | 2 | 0 |
| 35 | 2 | 804 | LMT | 5 | 0 |
| 43 | 3 | 502 | LUT | 4 | 0 |
| 25 | B | 1227 | CLA | 5 | 0 |
| 35 | 1 | 804 | LMT | 5 | 0 |
| 42 | M | 4001 | ECH | 5 | 0 |
| 25 | A | 1127 | CLA | 10 | 0 |
| 26 | 8 | 603 | CHL | 5 | 0 |
| 33 | J | 5001 | PTY | 2 | 0 |
| 25 | A | 1138 | CLA | 8 | 0 |
| 29 | I | 4001 | BCR | 2 | 0 |
| 41 | J | 5002 | SPH | 1 | 0 |
| 36 | 7 | 806 | DGD | 3 | 0 |
| 25 | 4 | 616 | CLA | 3 | 0 |
| 26 | 6 | 613 | CHL | 5 | 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.

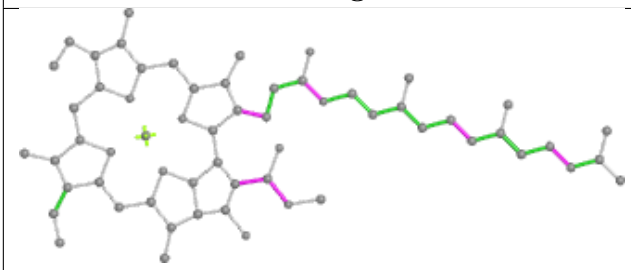
**Ligand CLA a 601**



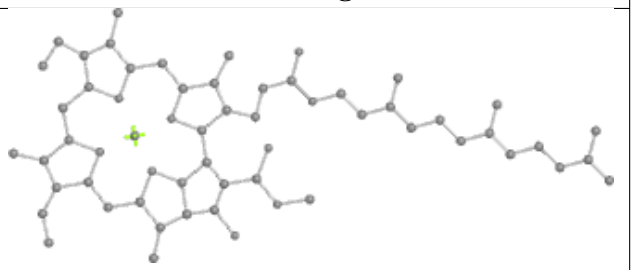
**Bond lengths**



**Bond angles**

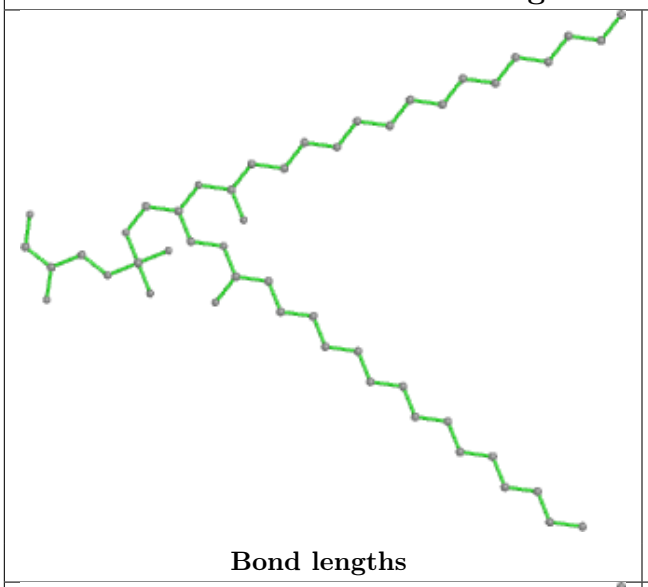


**Torsions**

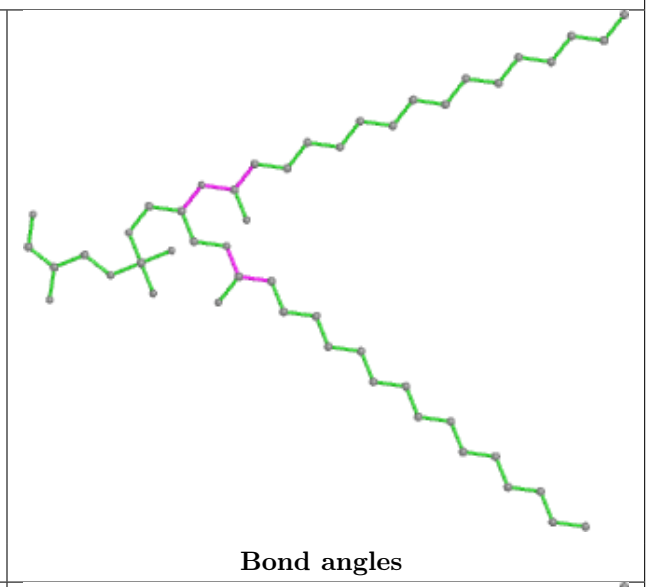


**Rings**

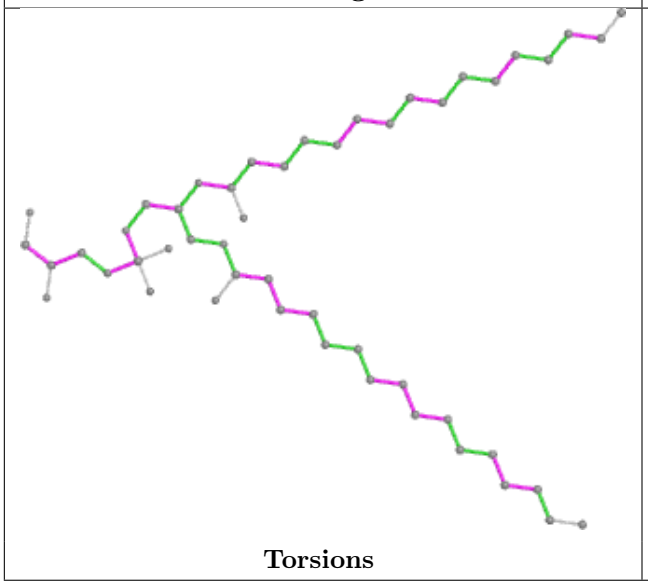
**Ligand LHG 9 802**



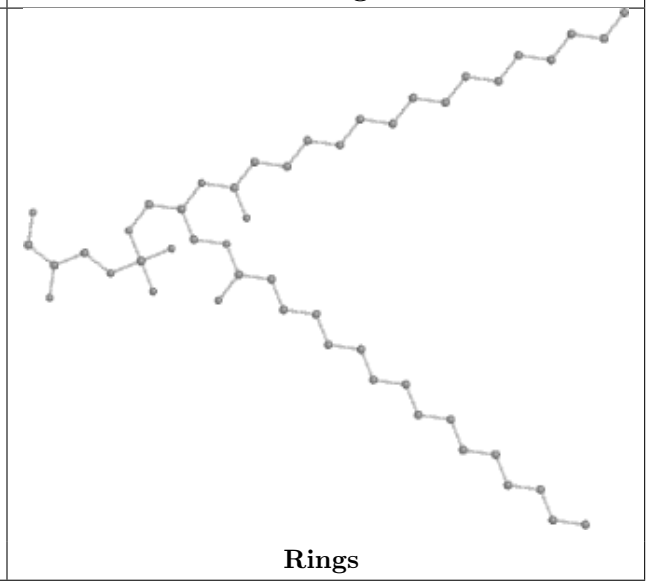
**Bond lengths**



**Bond angles**

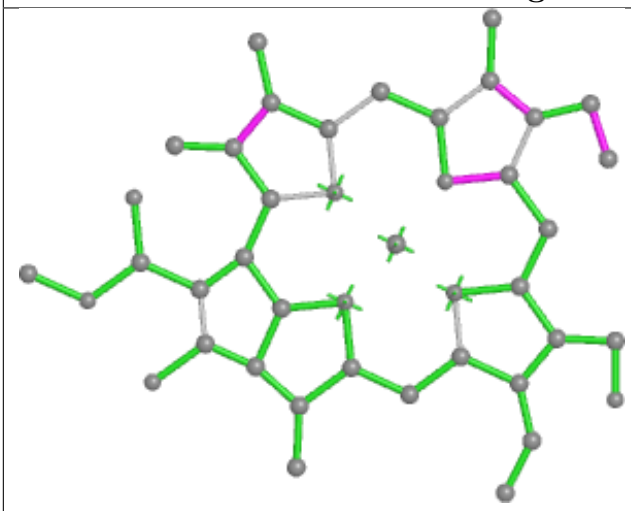


**Torsions**

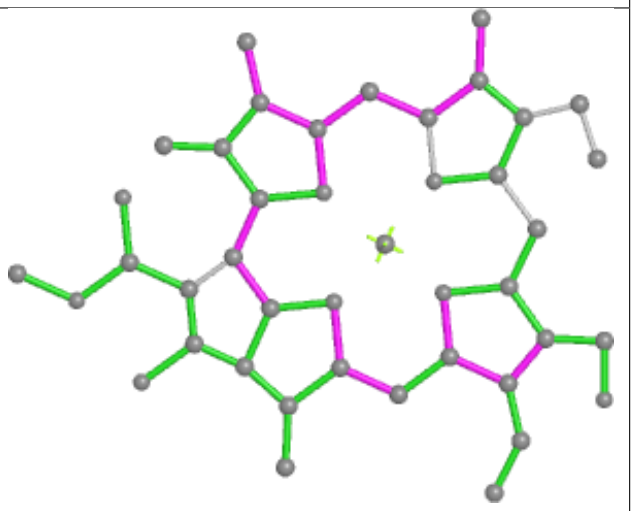


**Rings**

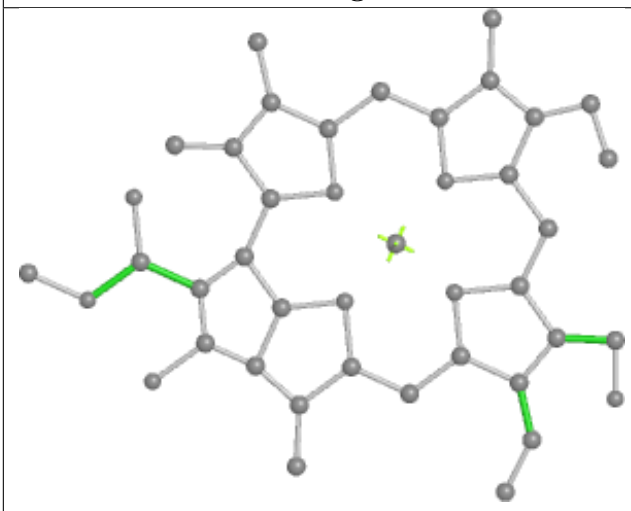
**Ligand CHL 9 613**



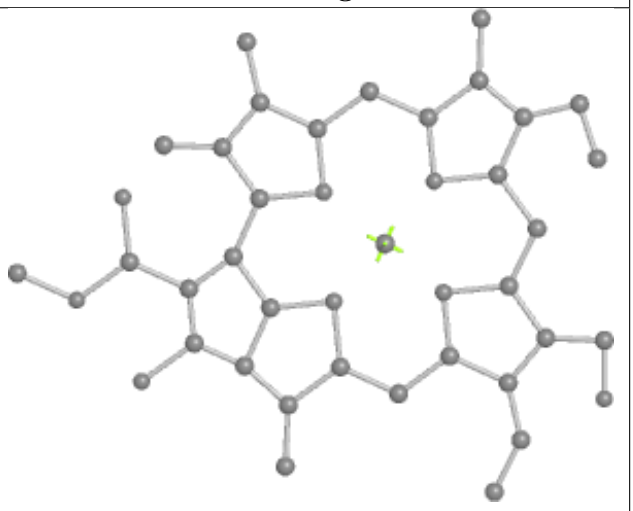
**Bond lengths**



**Bond angles**

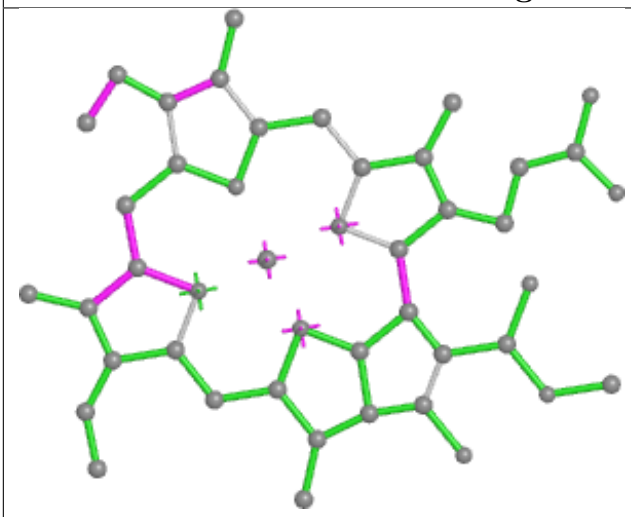


**Torsions**

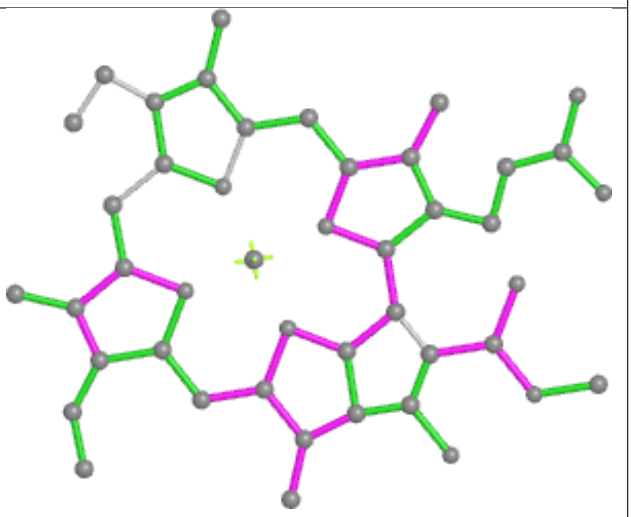


**Rings**

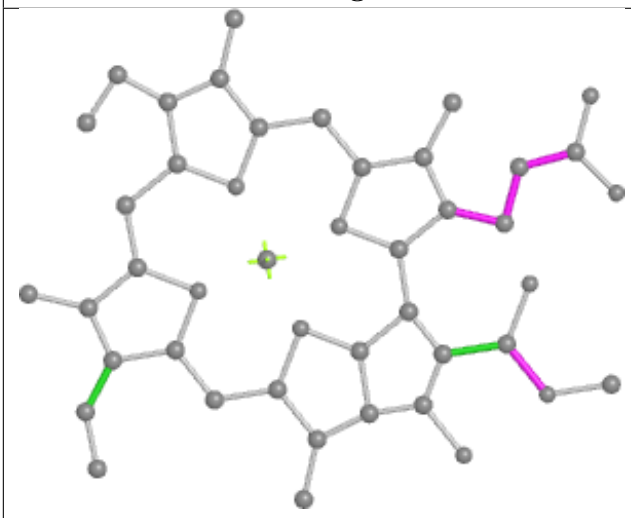
## Ligand CLA B 1232



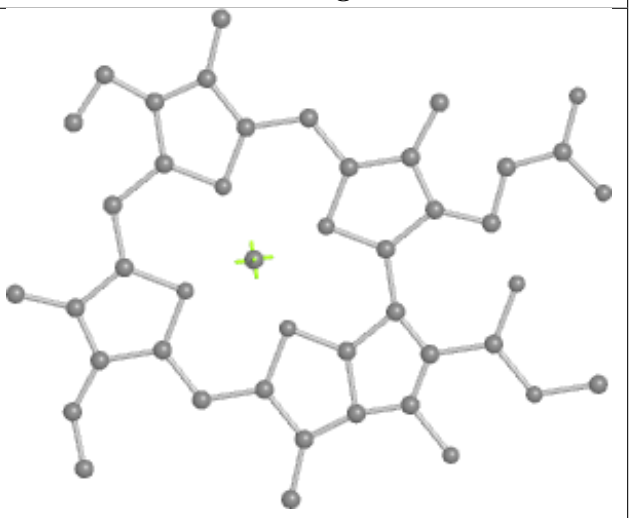
Bond lengths



Bond angles

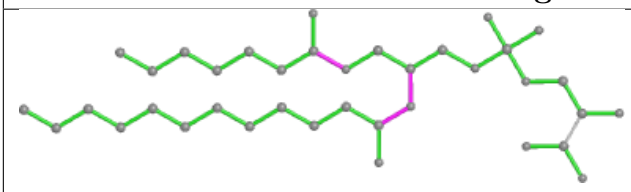


Torsions

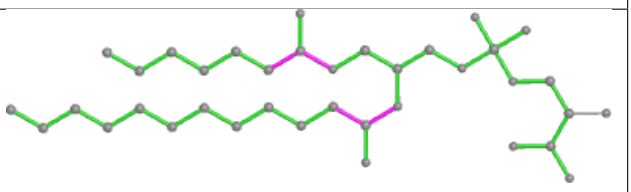


Rings

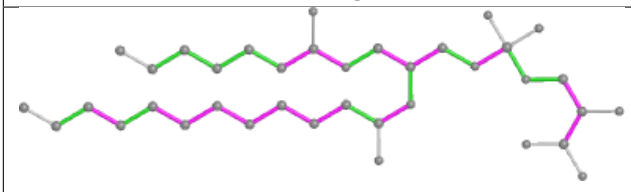
## Ligand P5S 8 805



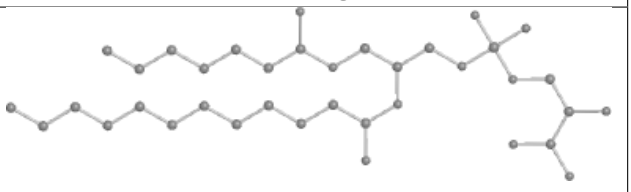
Bond lengths



Bond angles

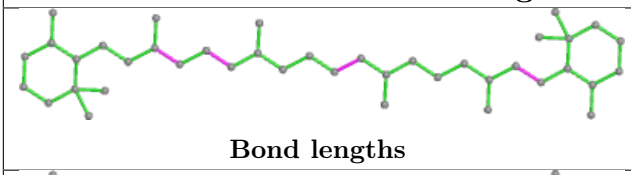


Torsions

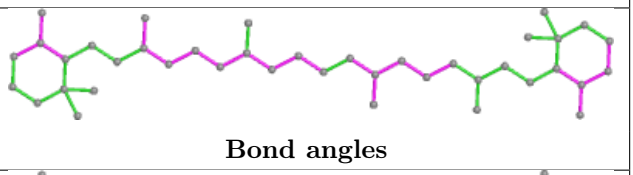


Rings

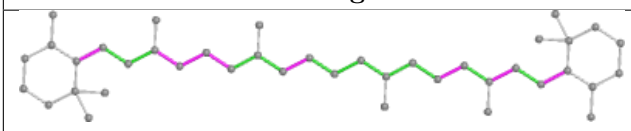
## Ligand BCR L 4001



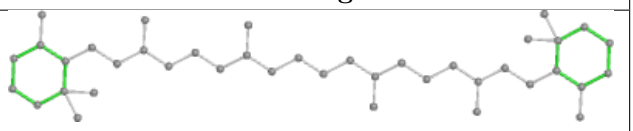
Bond lengths



Bond angles

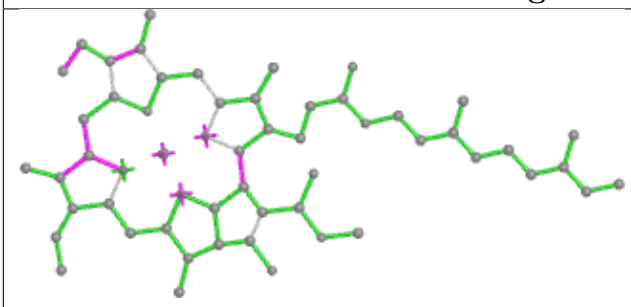


Torsions

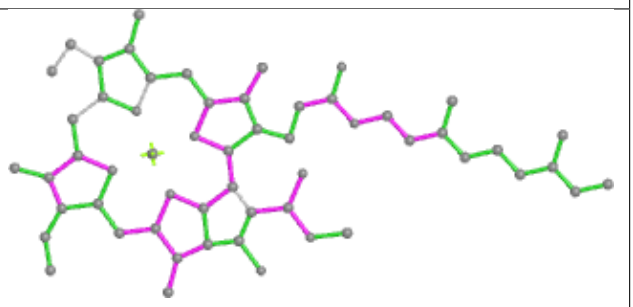


Rings

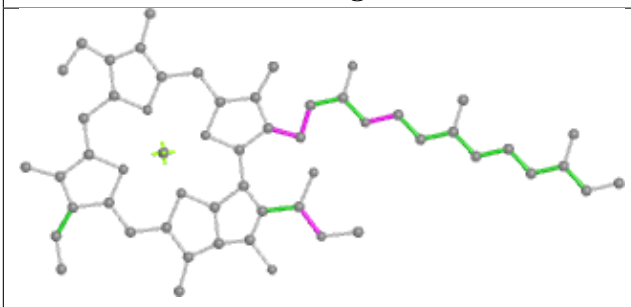
## Ligand CLA 2 615



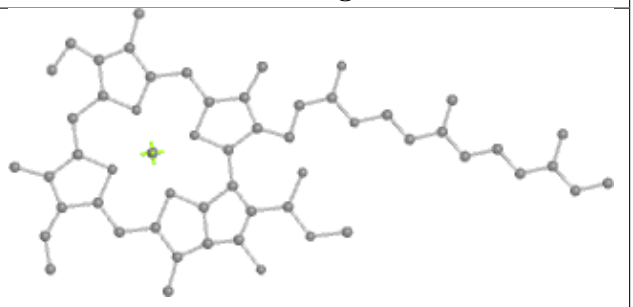
Bond lengths



Bond angles

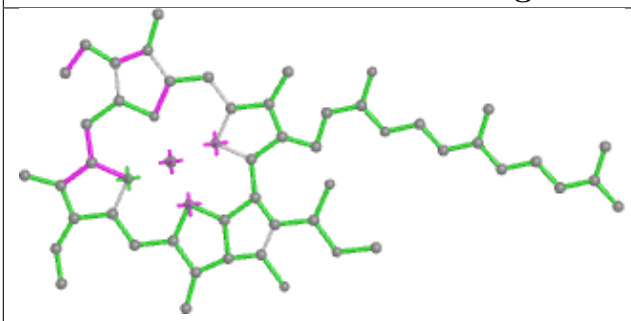


Torsions

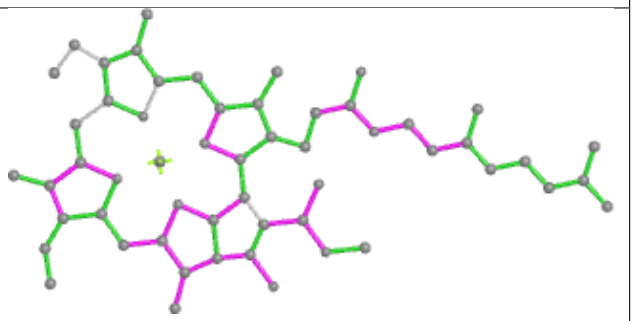


Rings

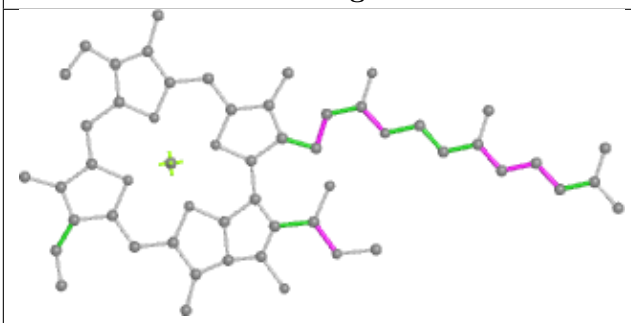
## Ligand CLA H 1703



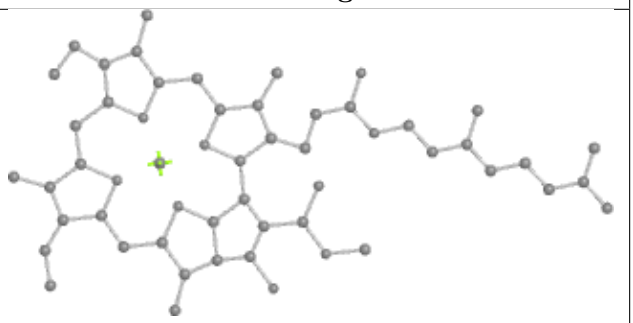
Bond lengths



Bond angles

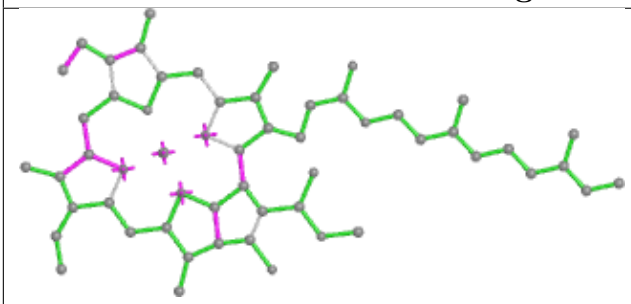


Torsions

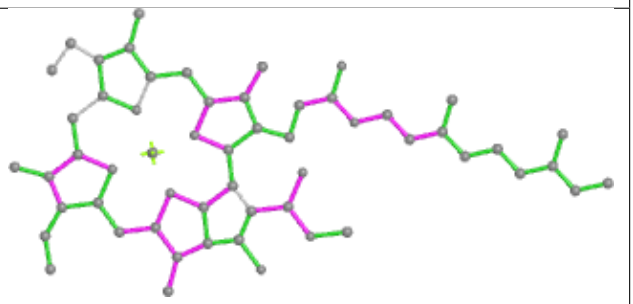


Rings

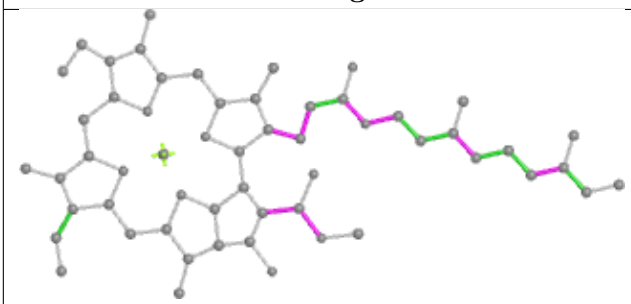
## Ligand CLA B 1217



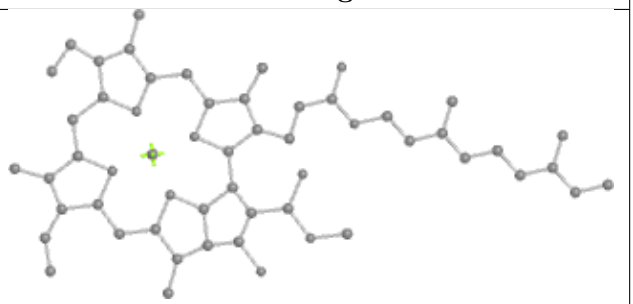
Bond lengths



Bond angles

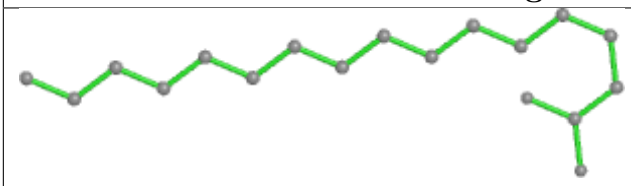


Torsions

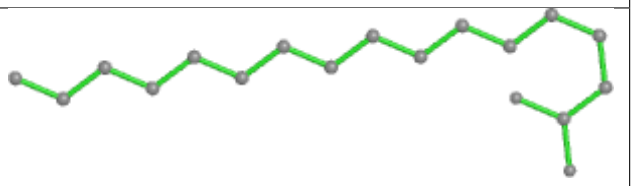


Rings

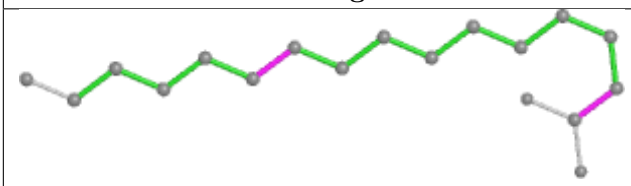
## Ligand PLM 5 804



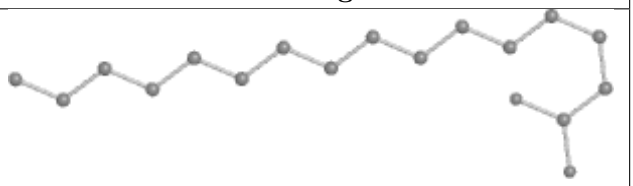
Bond lengths



Bond angles

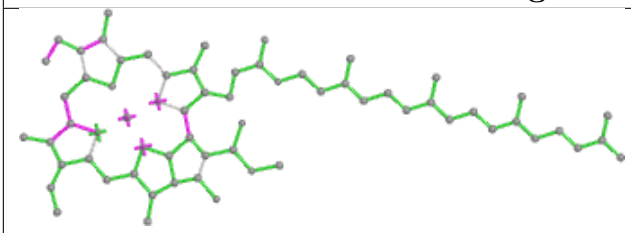


Torsions

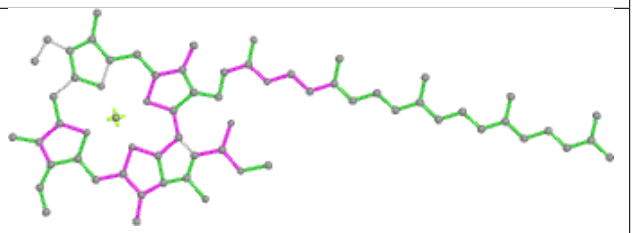


Rings

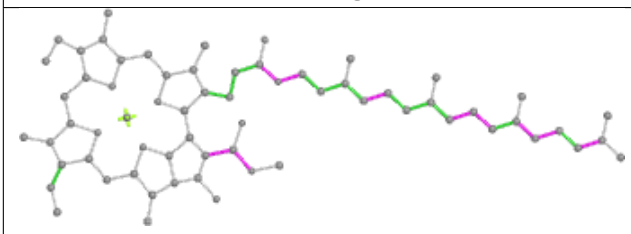
## Ligand CLA 2 607



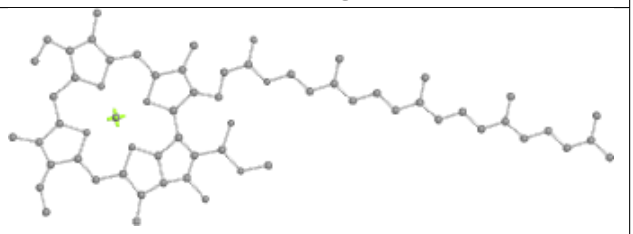
Bond lengths



Bond angles

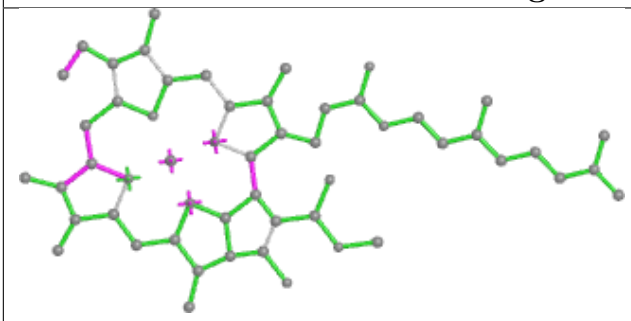


Torsions

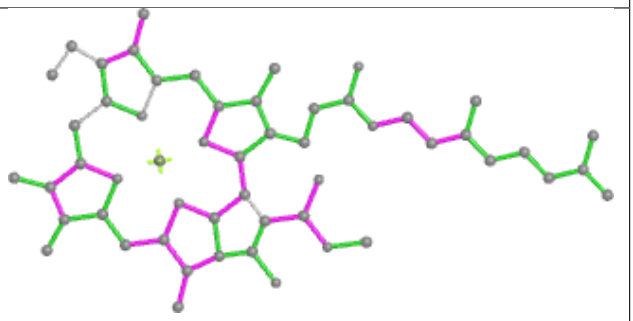


Rings

**Ligand CLA 7 606**



**Bond lengths**



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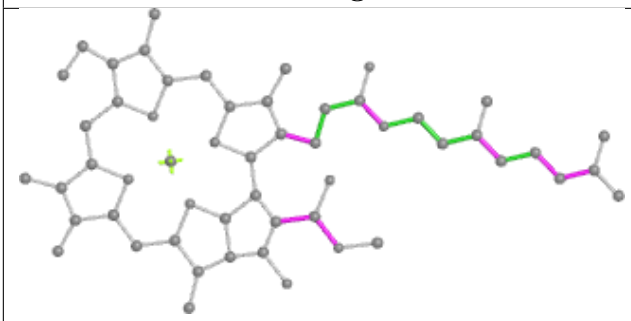
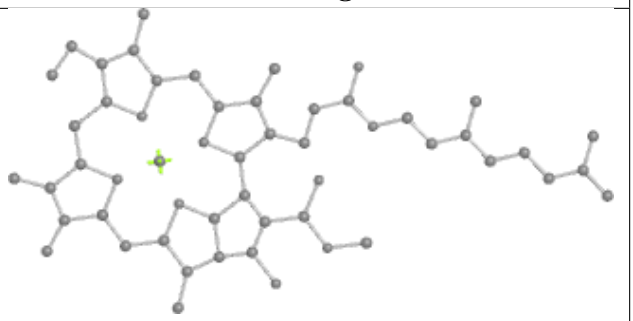
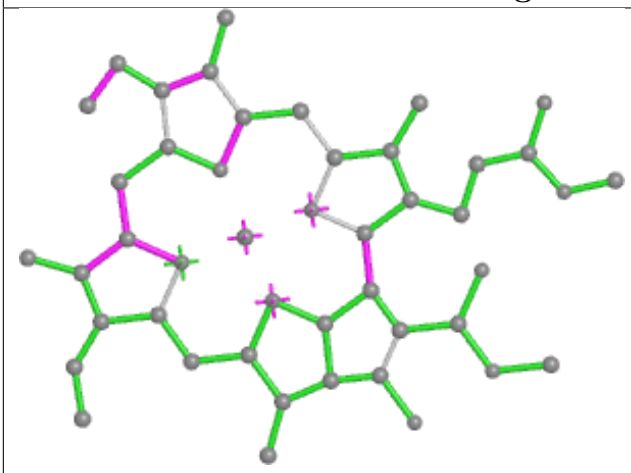


**Torsions**

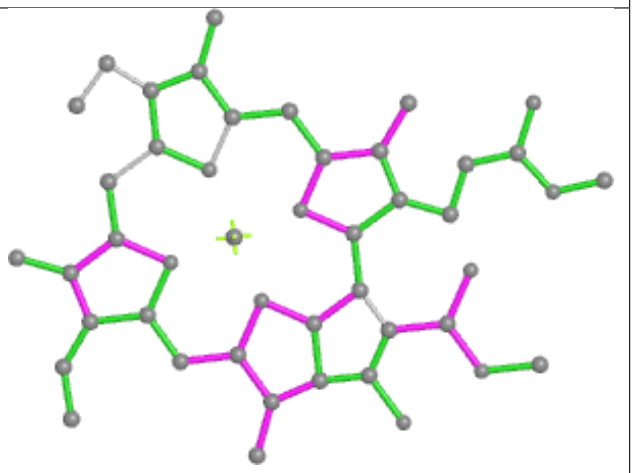


**Rings**

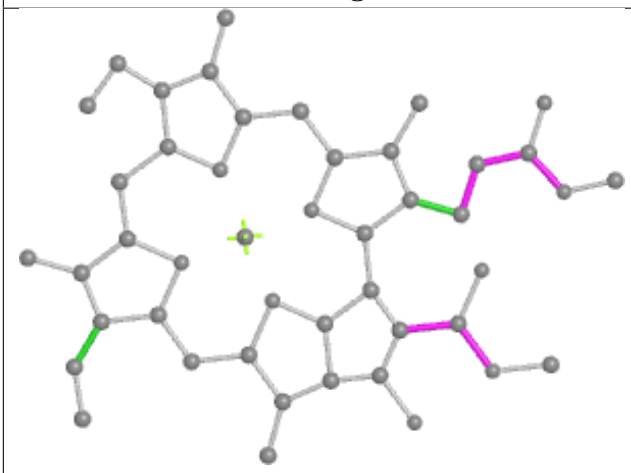
## Ligand CLA H 1702



Bond lengths



Bond angles



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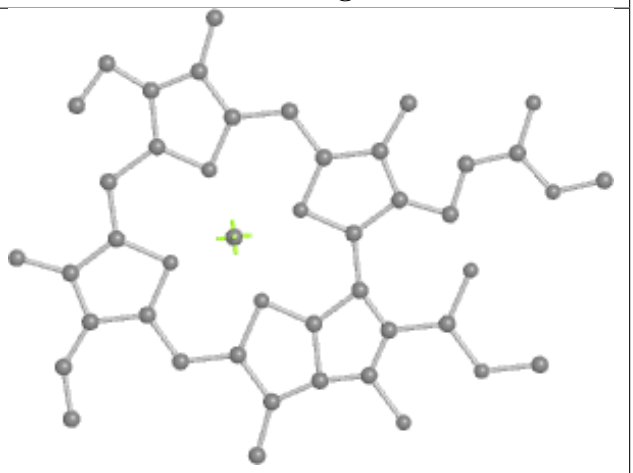
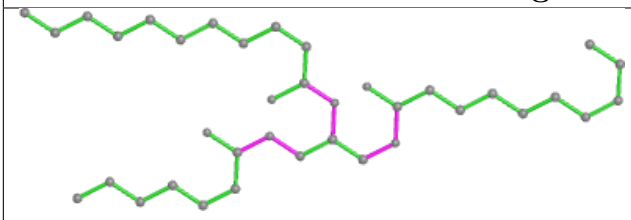


Rings

## Ligand 4RF 7 807



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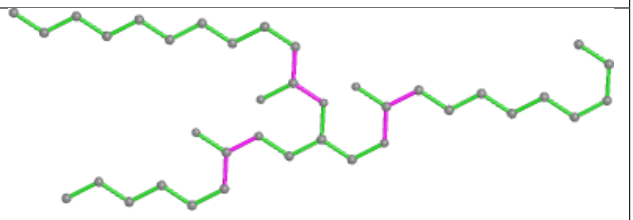
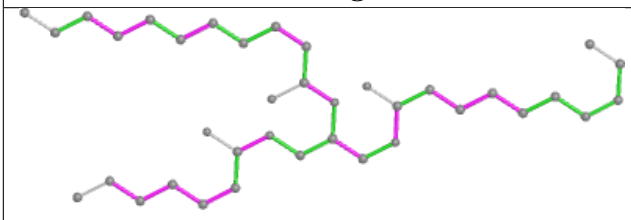
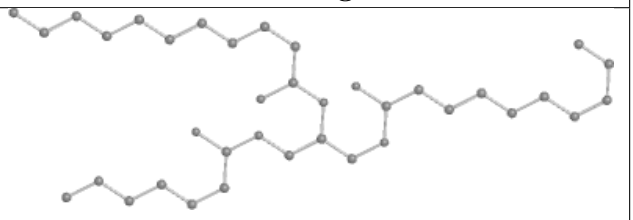


Bond angles

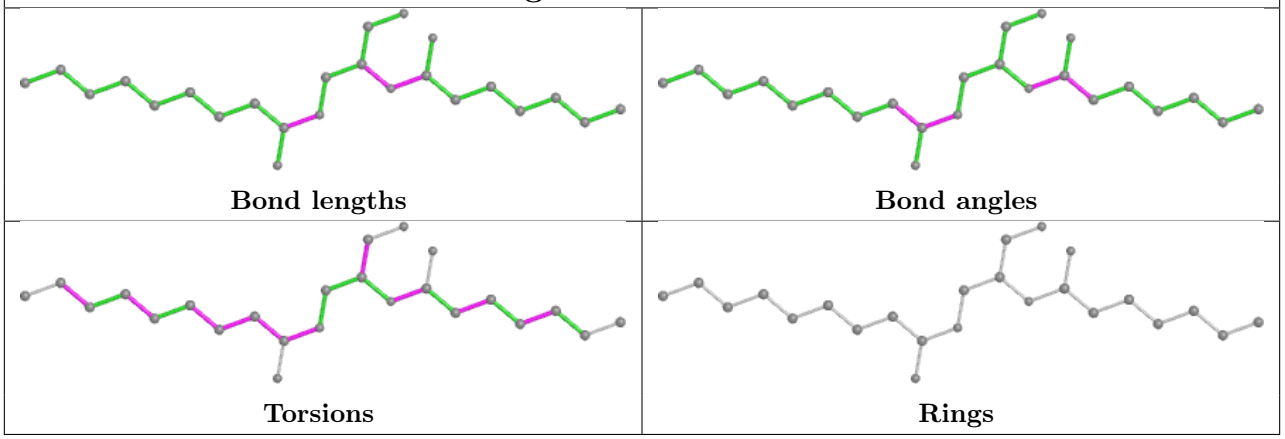


Torsions

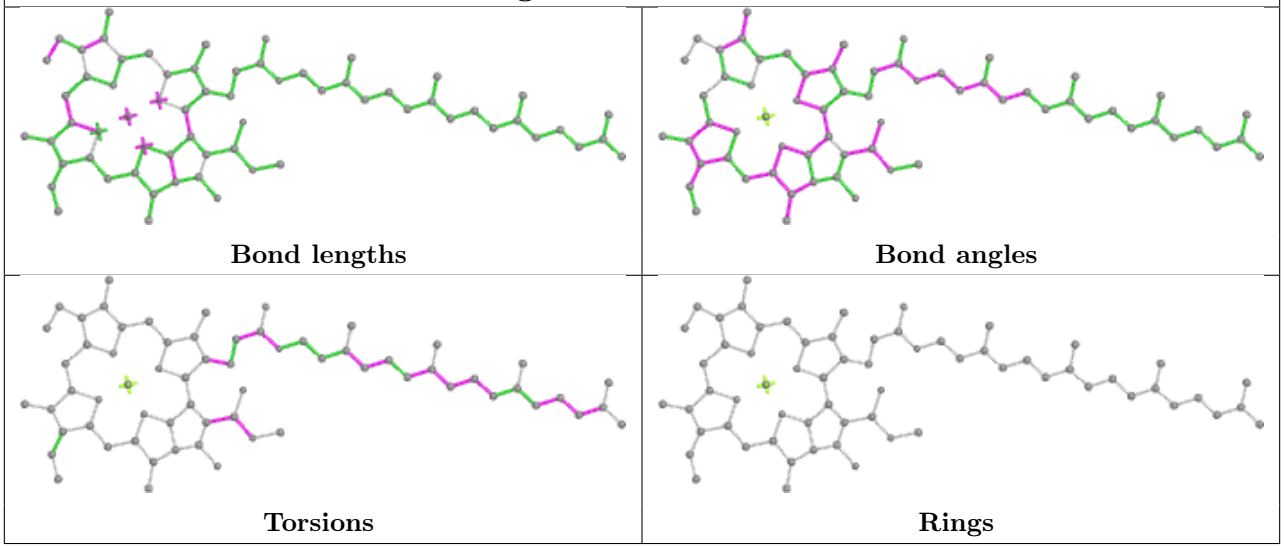


Rings

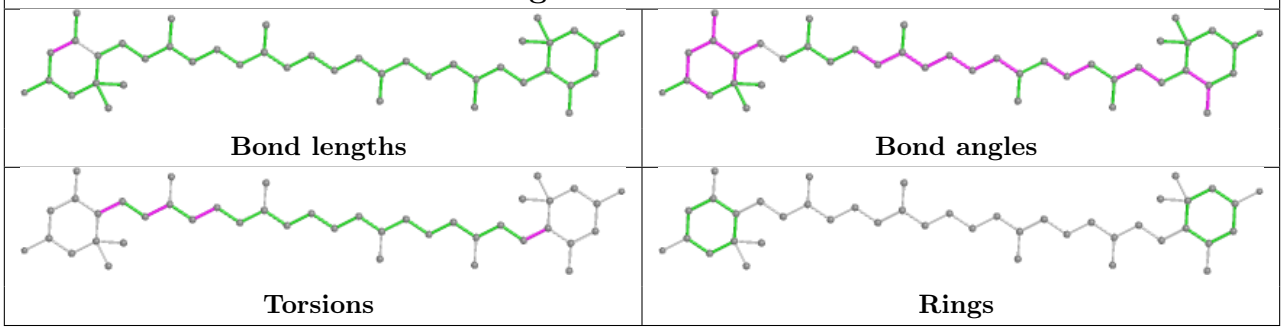
## Ligand DGA 3 803



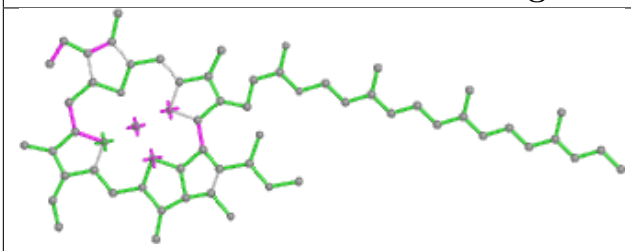

## Ligand CLA B 1210



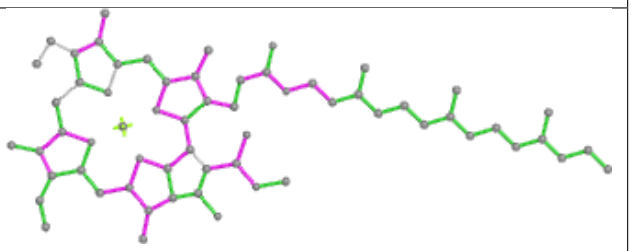

## Ligand LUT 7 501



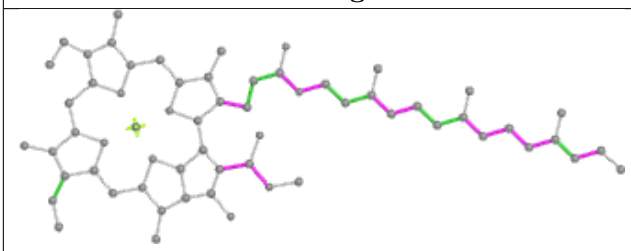
## Ligand CLA 4 612



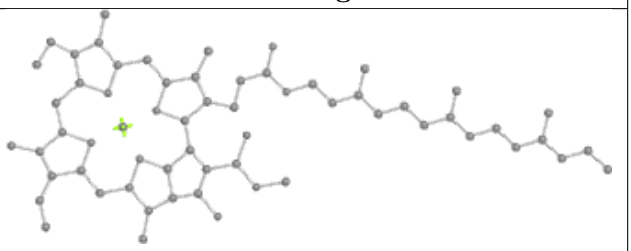
Bond lengths



Bond angles



Torsions



Rings

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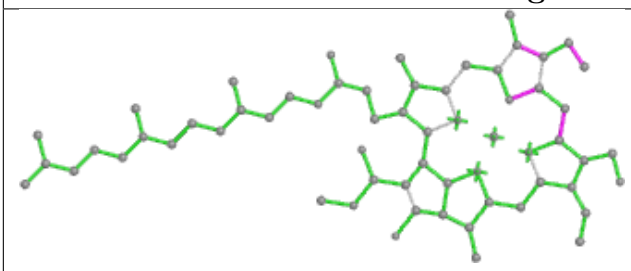

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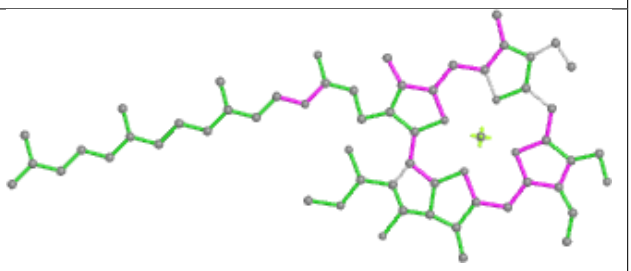
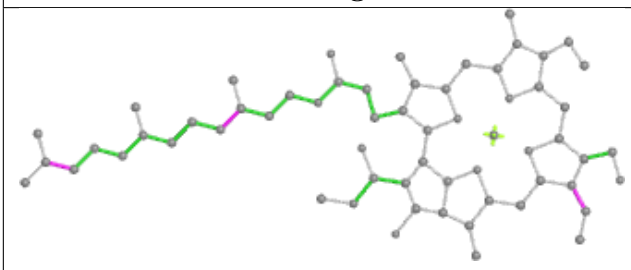


Bond angles



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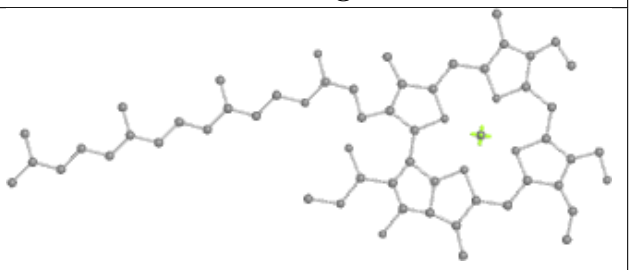
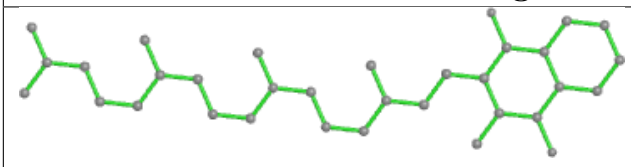


Rings

## Ligand PQN A 2001



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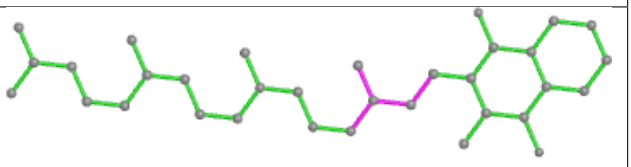
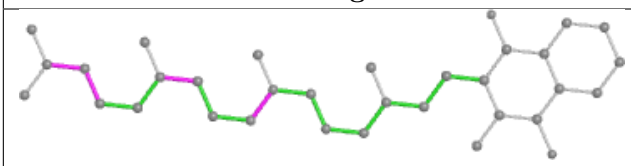


Bond angles



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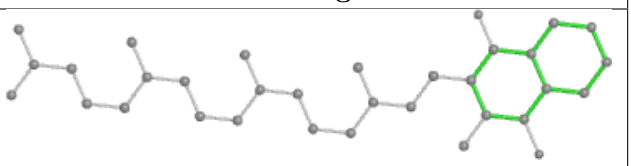
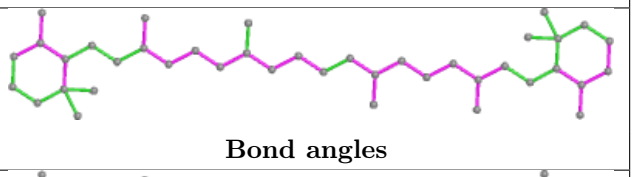


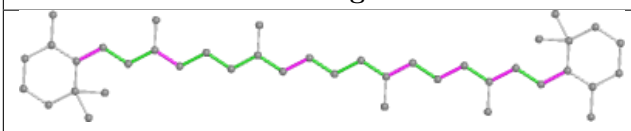
Rings

## Ligand BCR 5 504

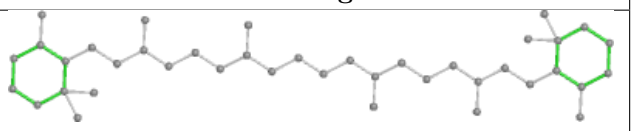
Bond lengths



Bond angles

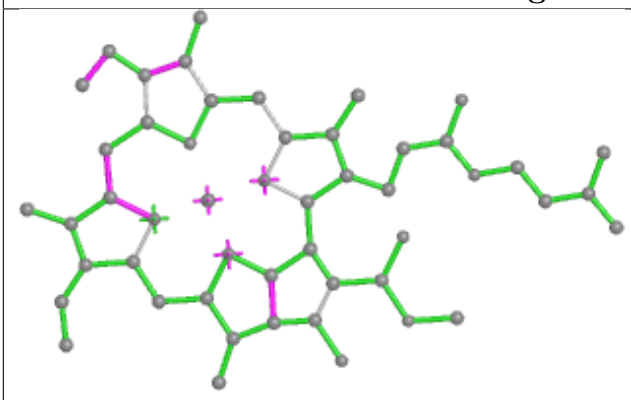


Torsions



Rings

## Ligand CLA 8 612



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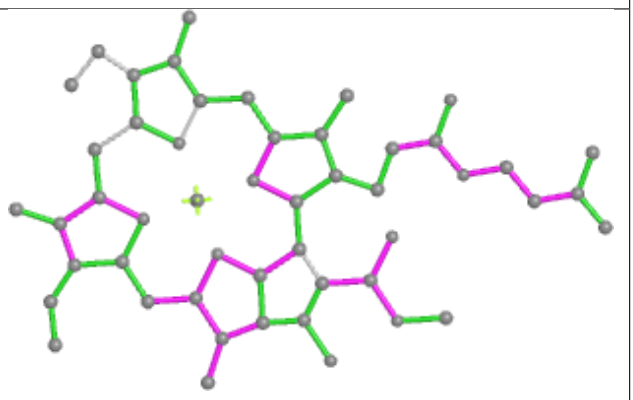
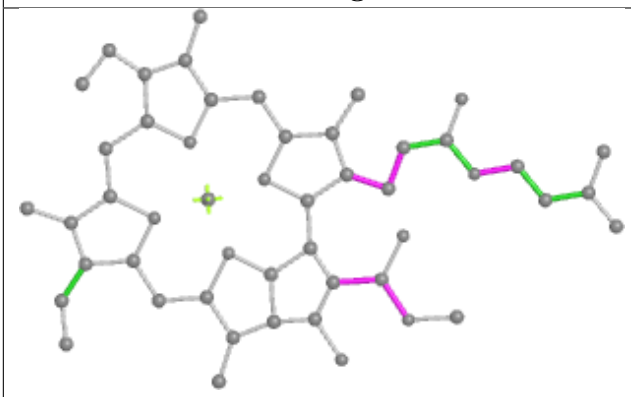


Bond angles



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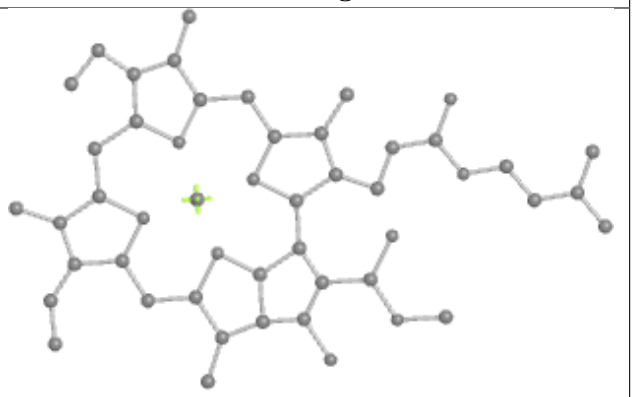
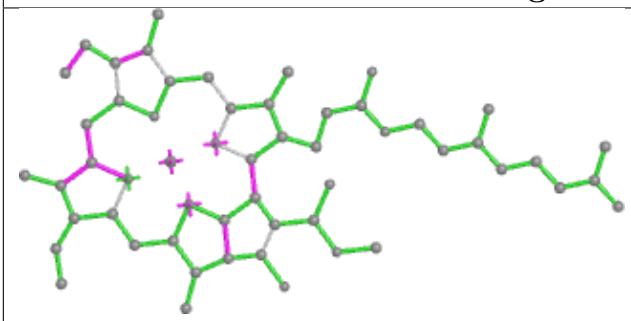


Rings

## Ligand CLA 8 605



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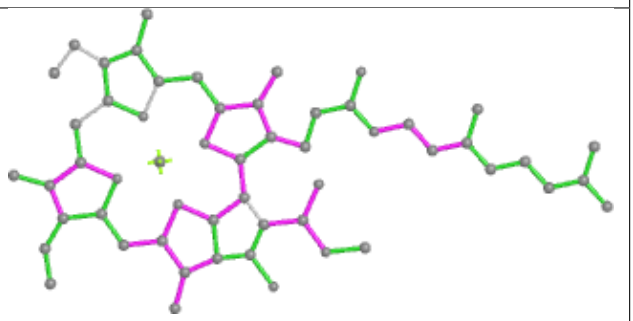
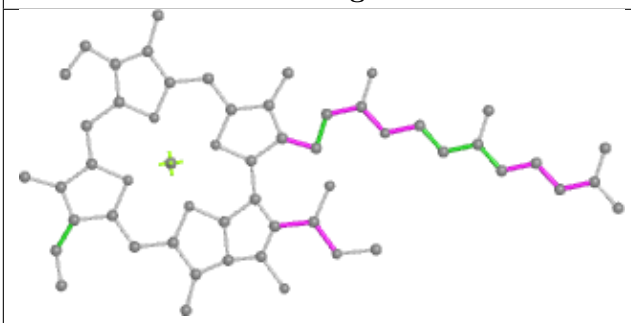
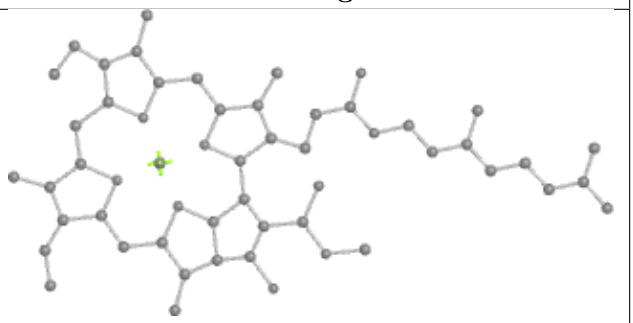


Bond angles

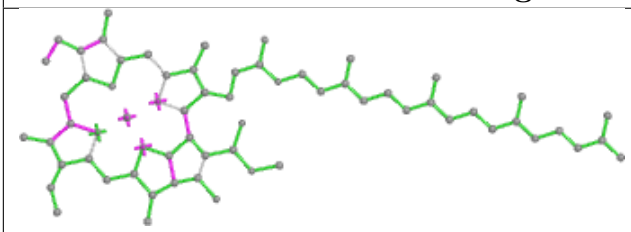


Torsions



Rings

## Ligand CLA A 1126



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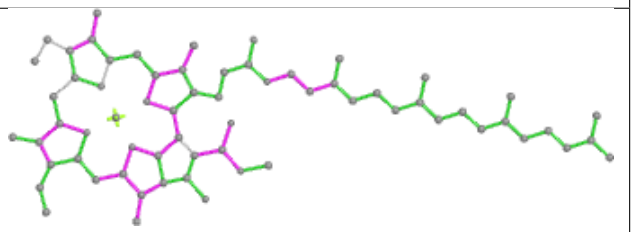
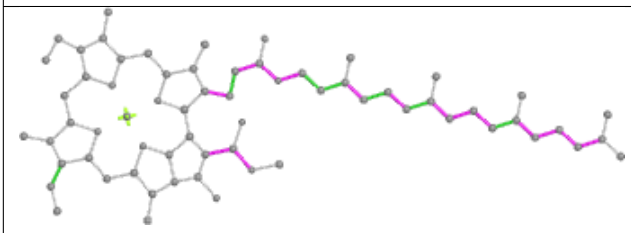
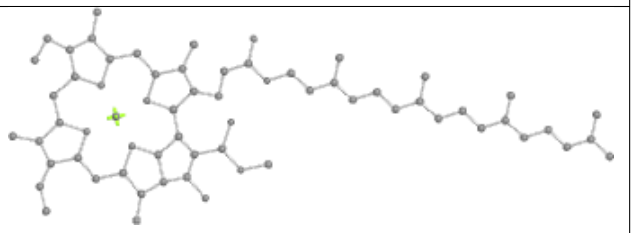


Bond angles

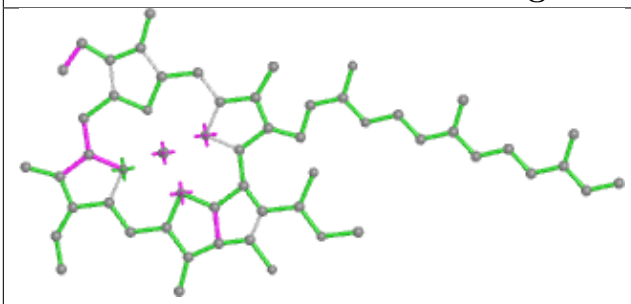


Torsions

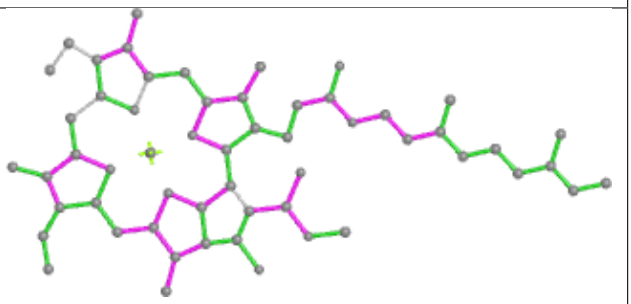


Rings

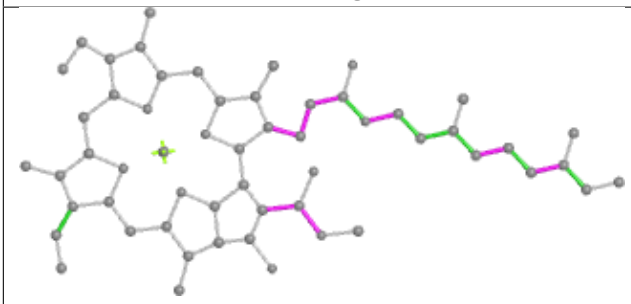
## Ligand CLA 2 604



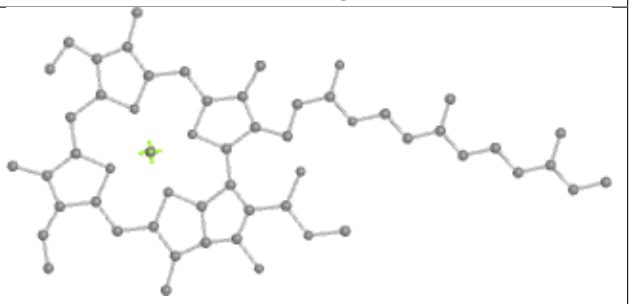
Bond lengths



Bond angles

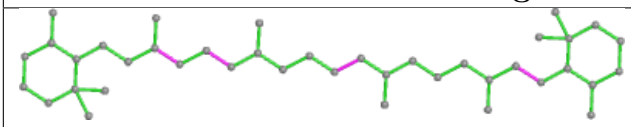


Torsions



Rings

## Ligand BCR O 4001



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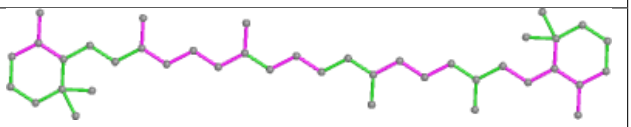
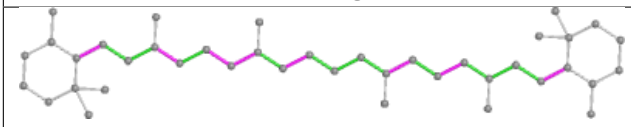


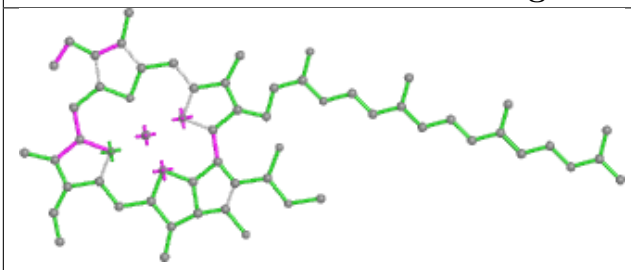
Bond angles



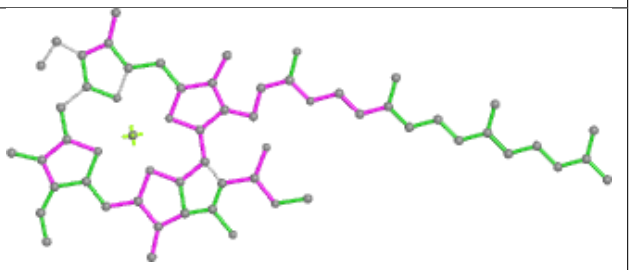
Torsions

Rings

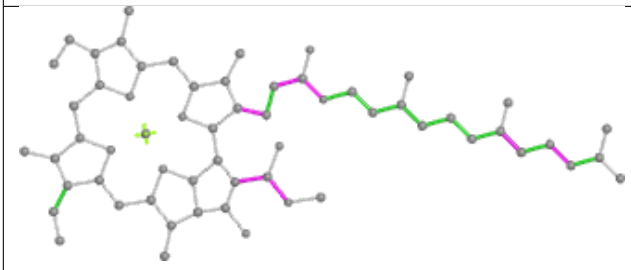
## Ligand CLA 2 603



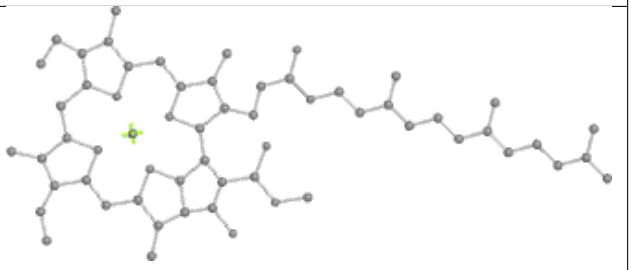
Bond lengths



Bond angles



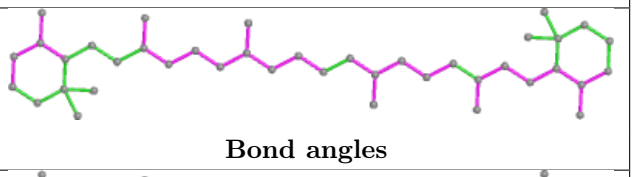
Torsions



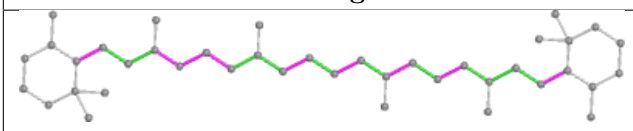
Rings

## Ligand BCR 5 503

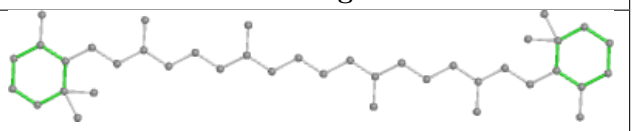
Bond lengths



Bond angles

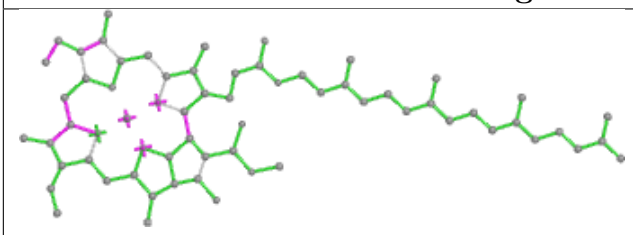


Torsions

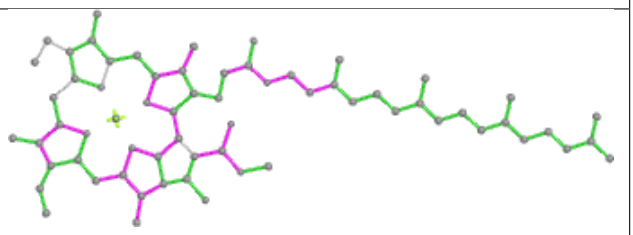


Rings

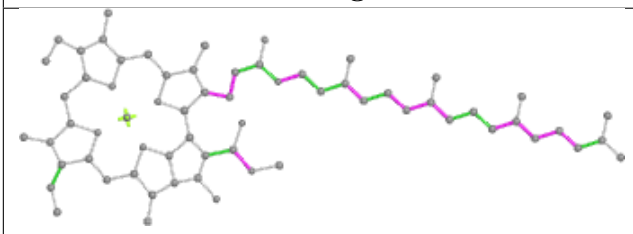
## Ligand CLA B 1239



Bond lengths



Bond angles



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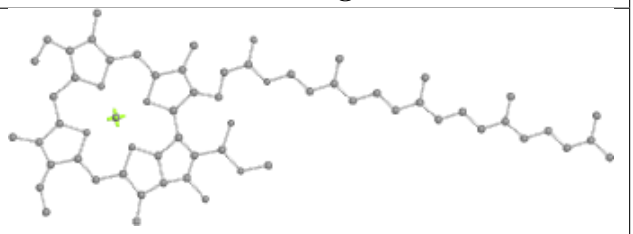
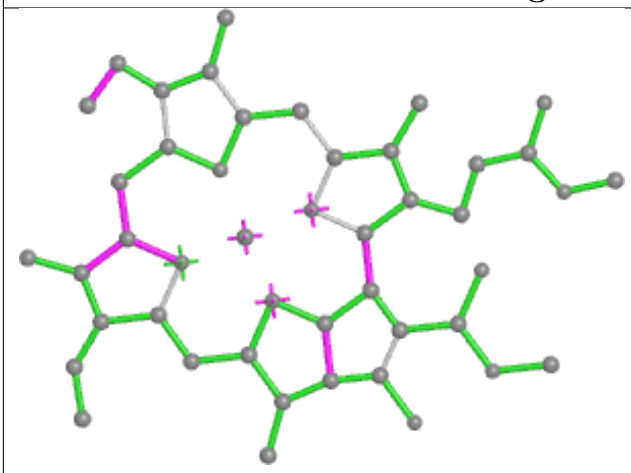
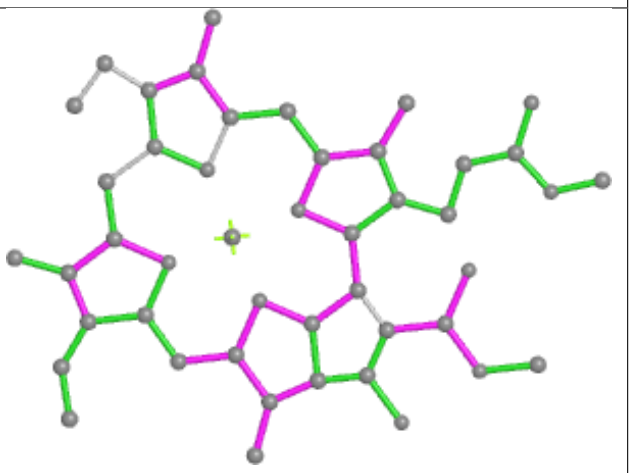


Rings

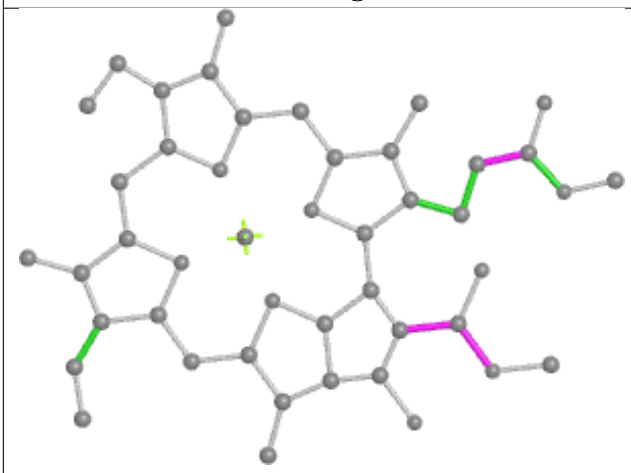
## Ligand CLA 3 602



Bond lengths



Bond angles



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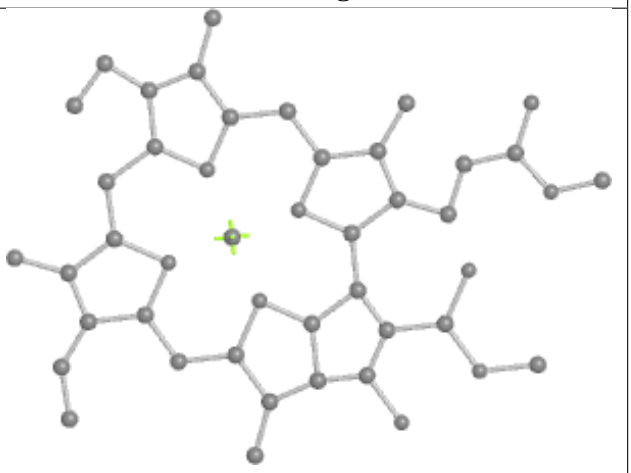
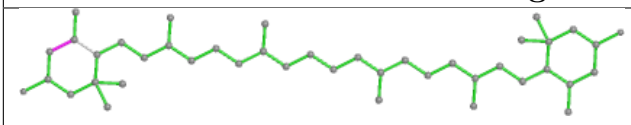


Rings

## Ligand LUT a 503



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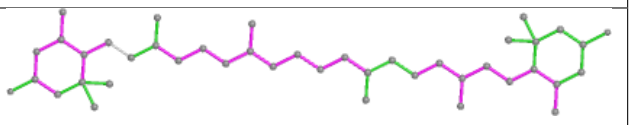
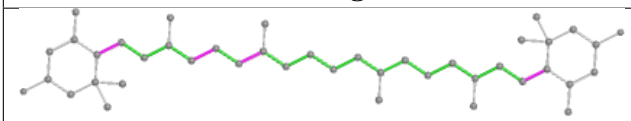


Bond angles



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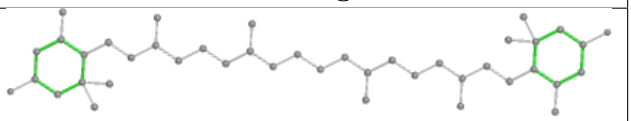
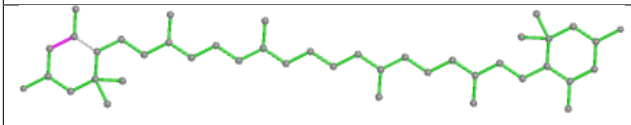


Rings

## Ligand LUT 5 501



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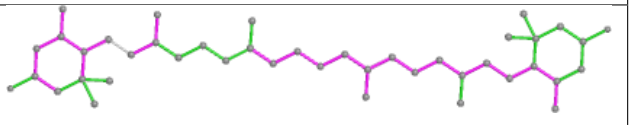

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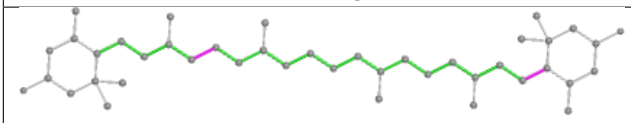

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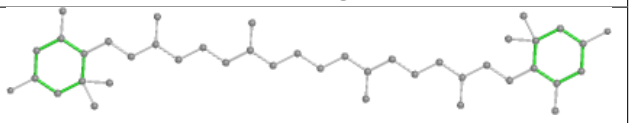
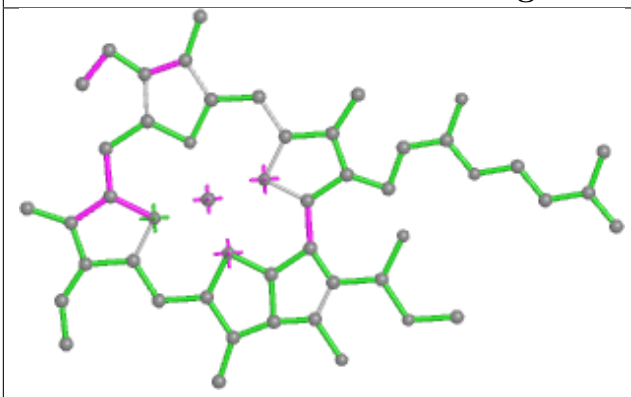


Rings

## Ligand CLA L 1504



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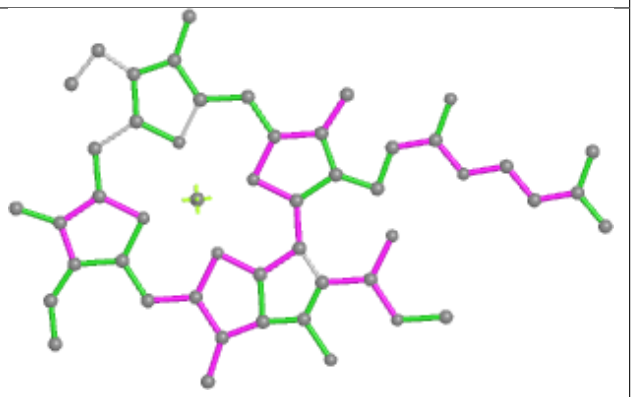
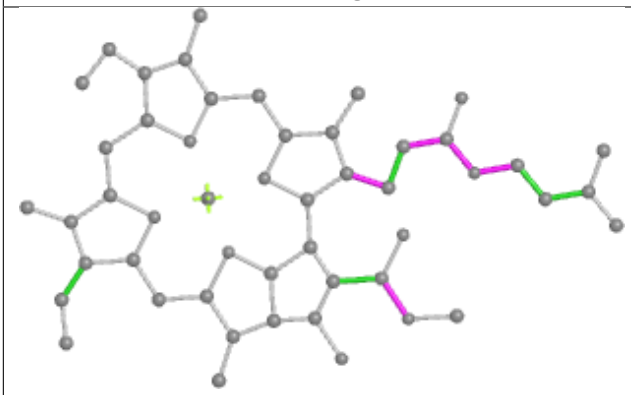


Bond angles



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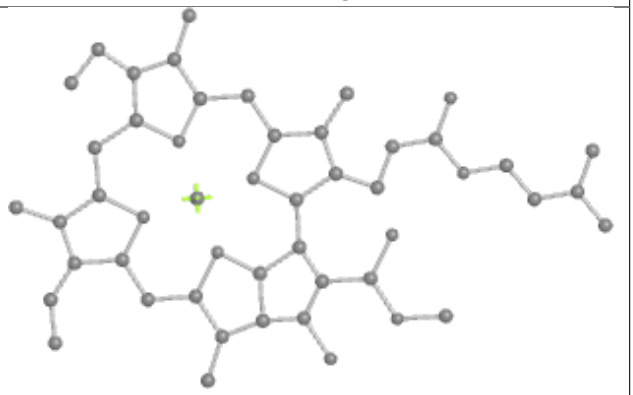
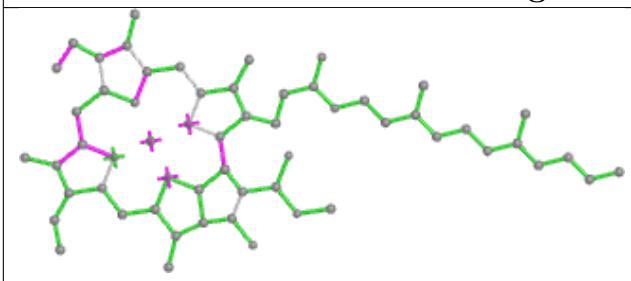


Rings

## Ligand CLA a 607



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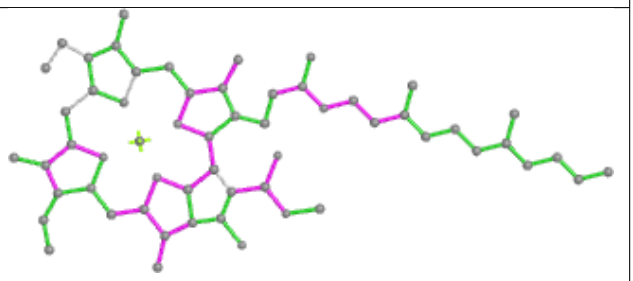
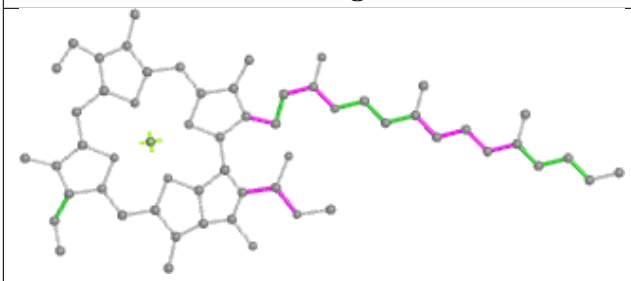


Bond angles



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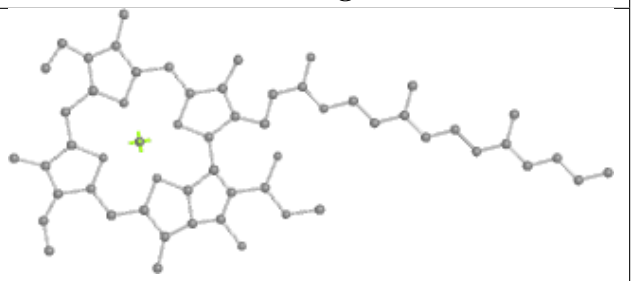
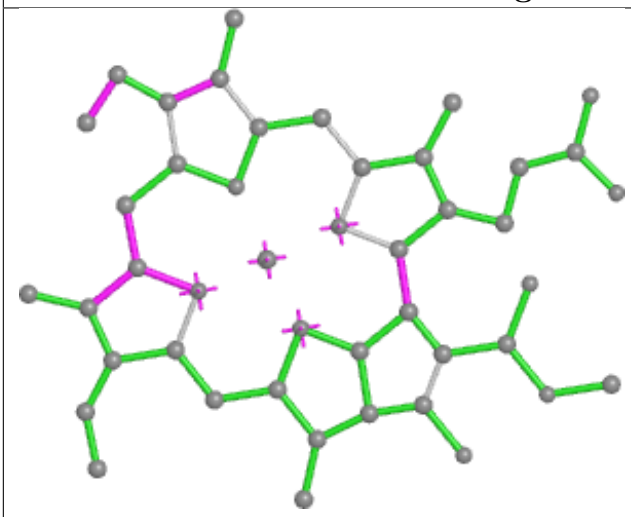
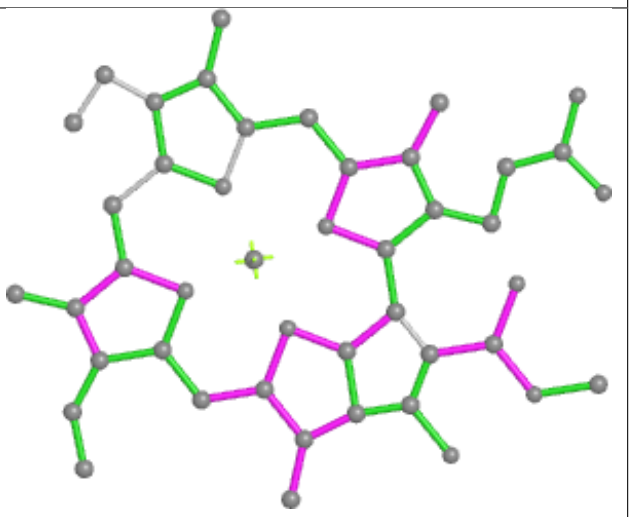


Rings

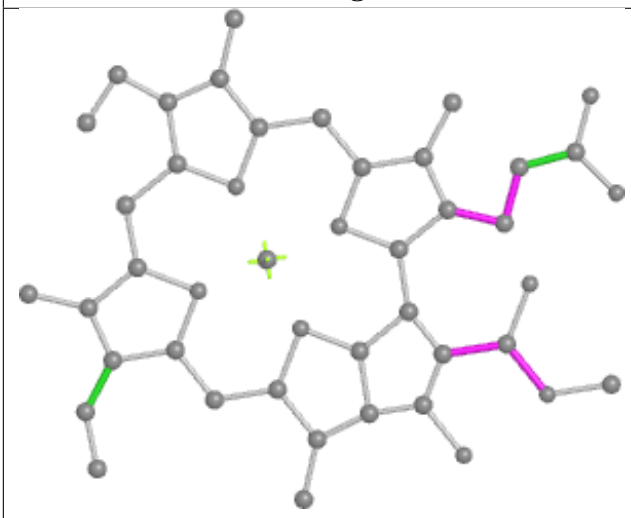
## Ligand CLA A 1141



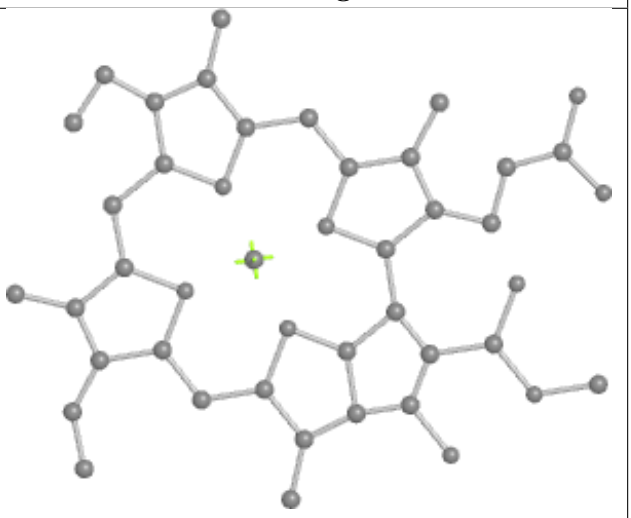
Bond lengths



Bond angles

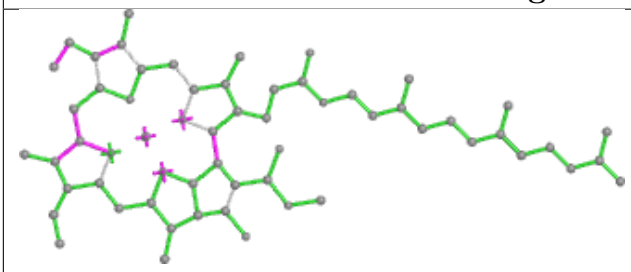


Torsions



Rings

## Ligand CLA 5 601



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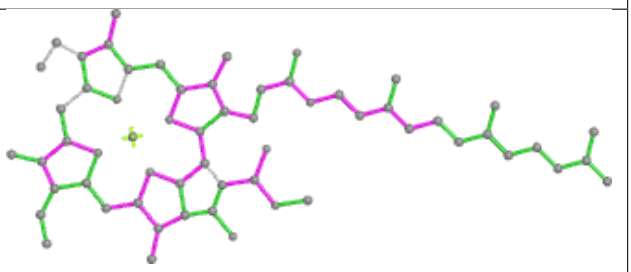
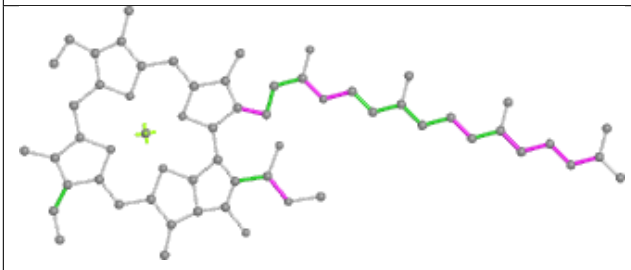


Bond angles



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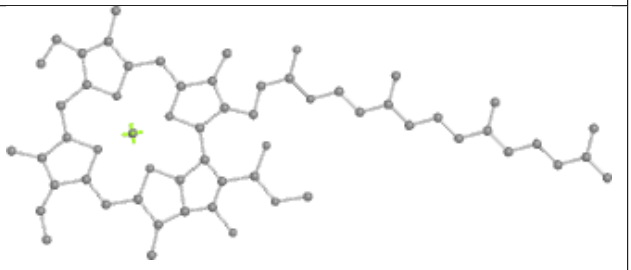
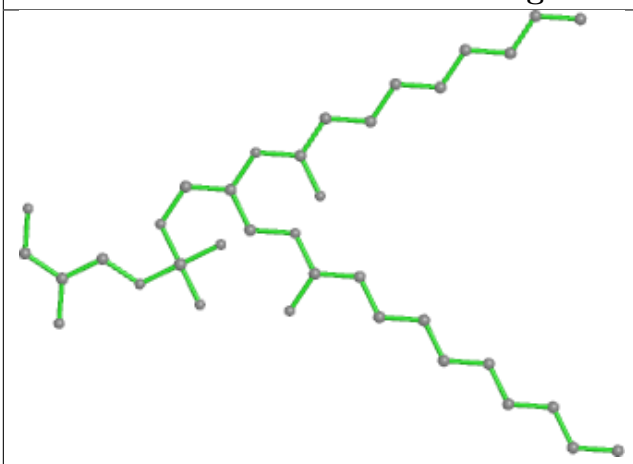


Rings

## Ligand LHG 7 802



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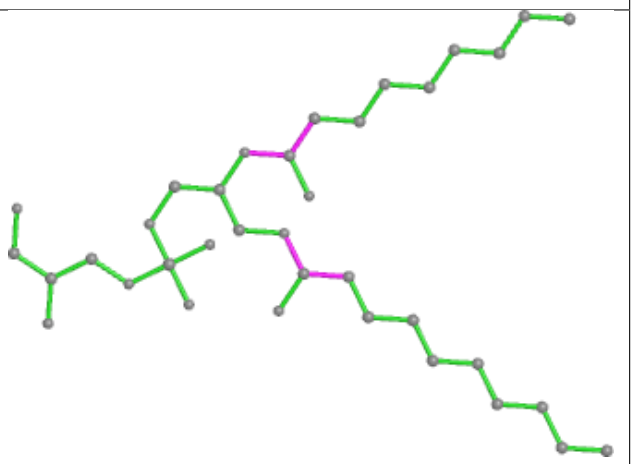
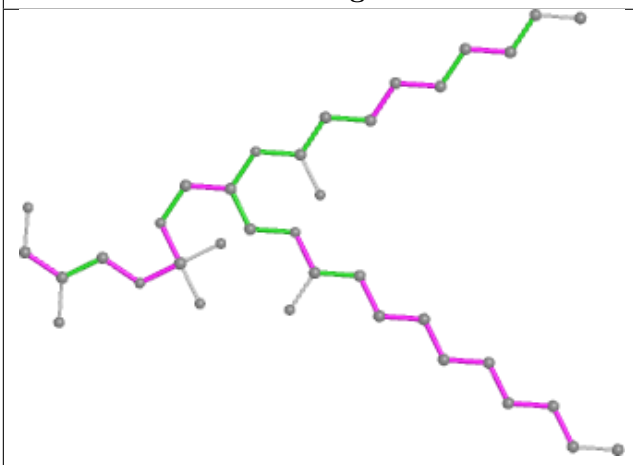


Bond angles



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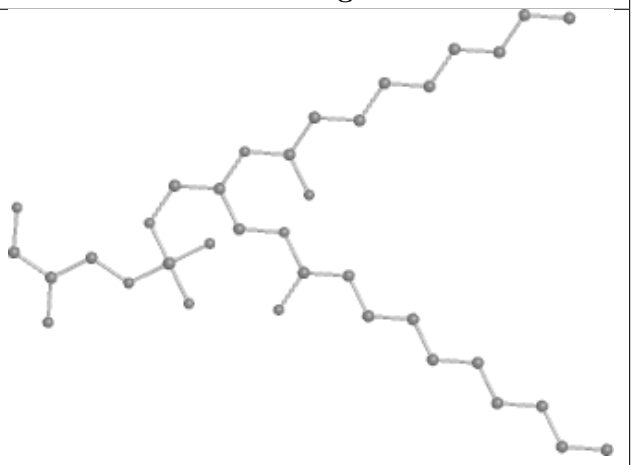
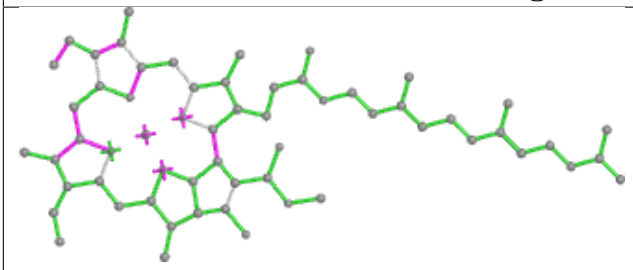


Rings

## Ligand CLA 7 610



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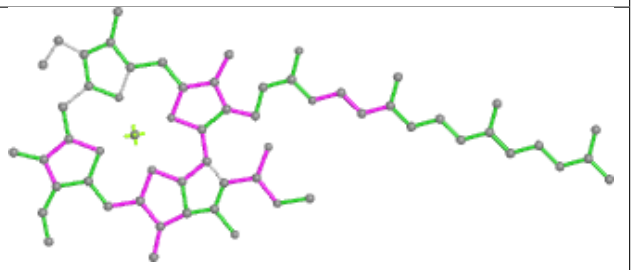
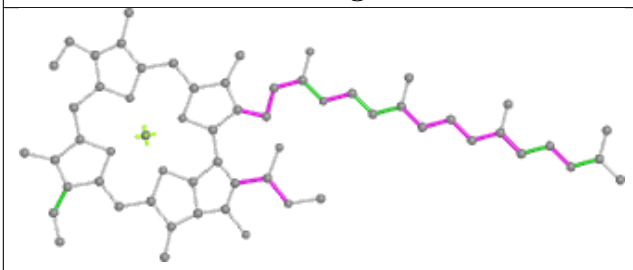
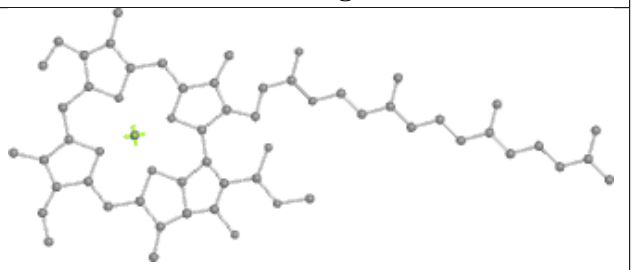


Bond angles

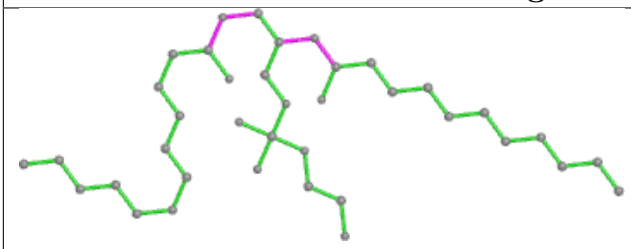


Torsions

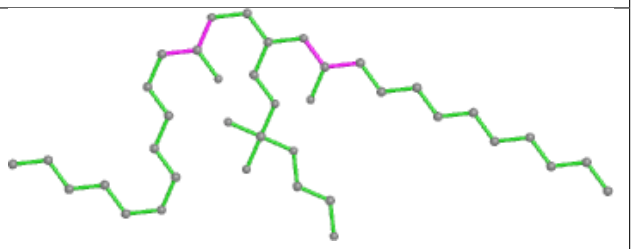


Rings

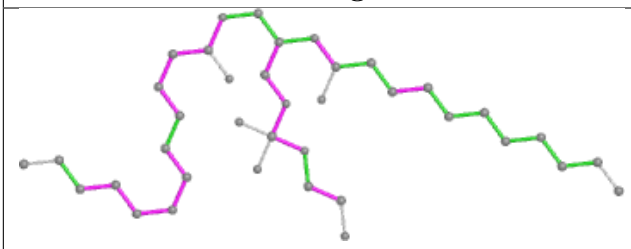
## Ligand PTY a 802



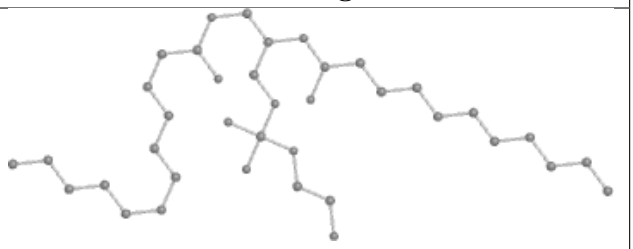
Bond lengths



Bond angles

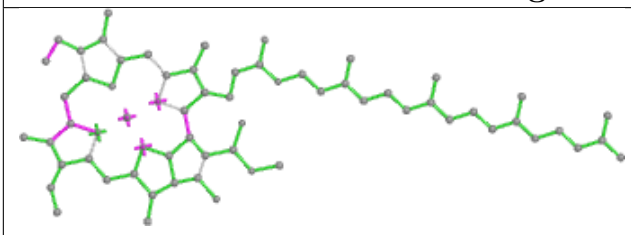


Torsions

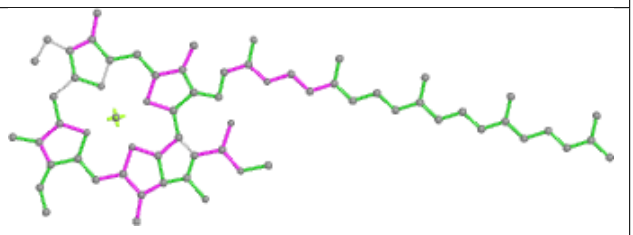


Rings

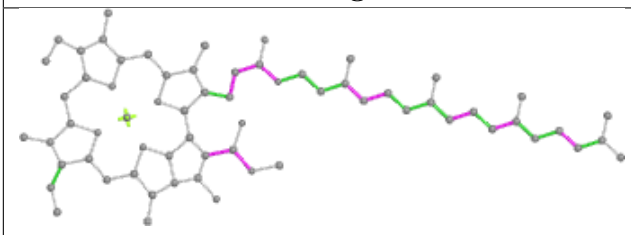
## Ligand CLA 1 603



Bond lengths



Bond angles



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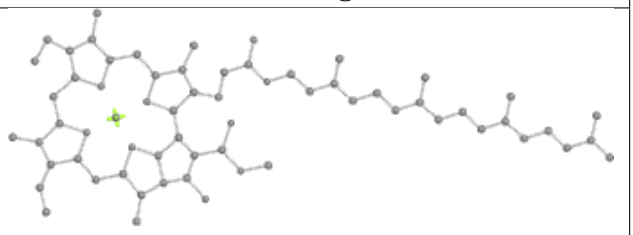
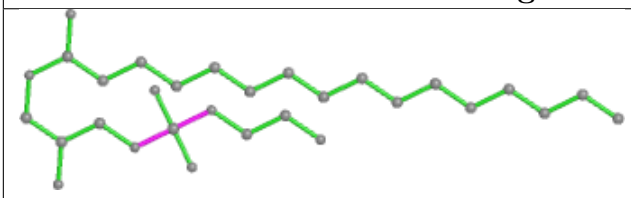
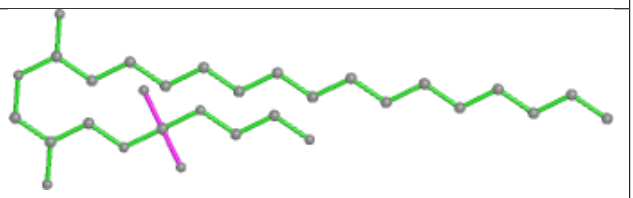


Rings

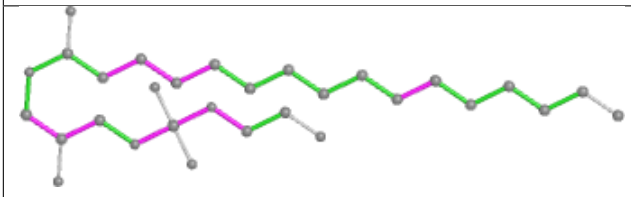
## Ligand LPX F 5003



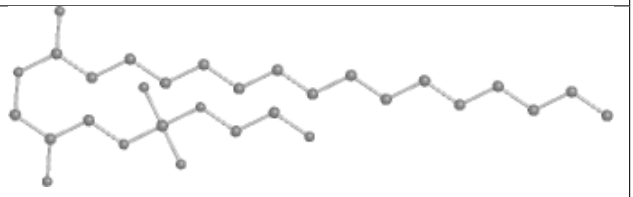
Bond lengths



Bond angles

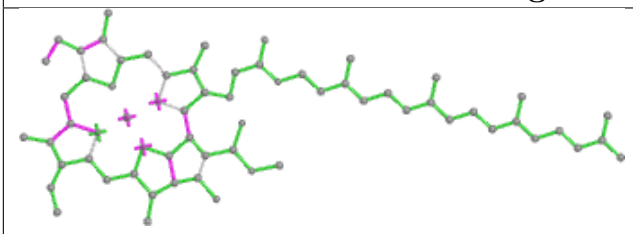


Torsions



Rings

## Ligand CLA 1 607



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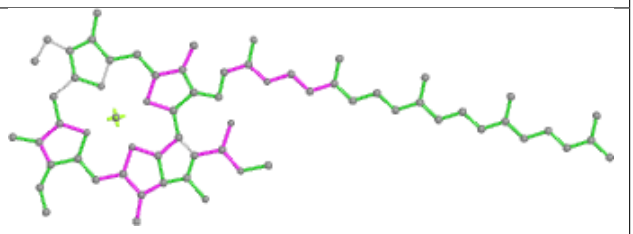

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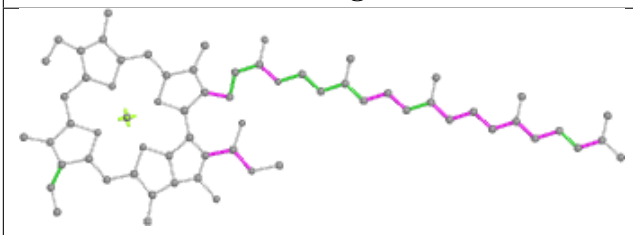

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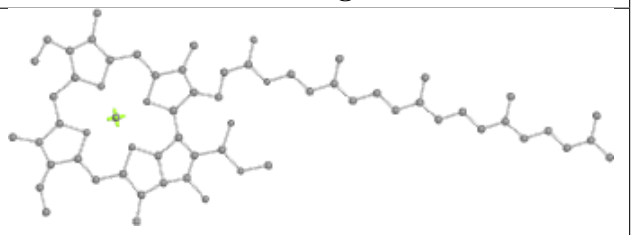

Rings

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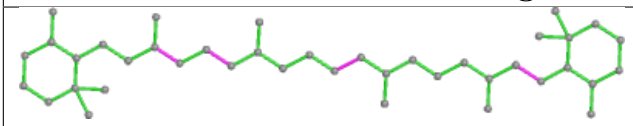

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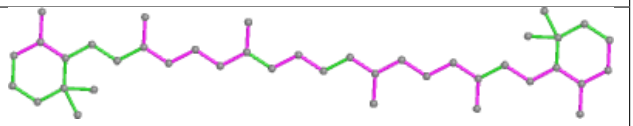
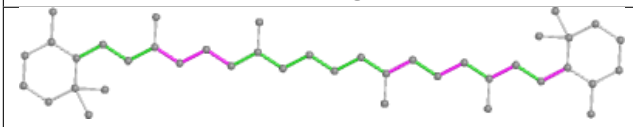


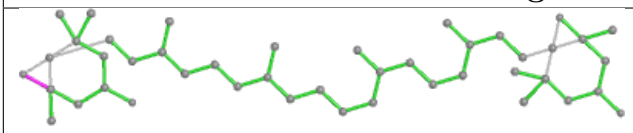
Bond angles



Torsions

Rings

## Ligand XAT 9 507



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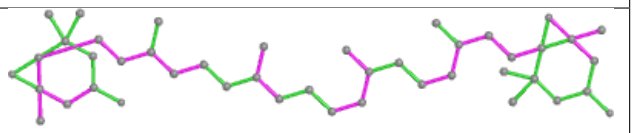
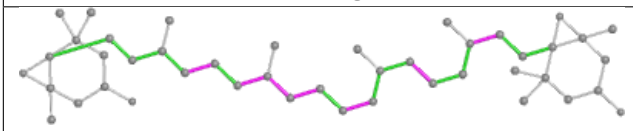
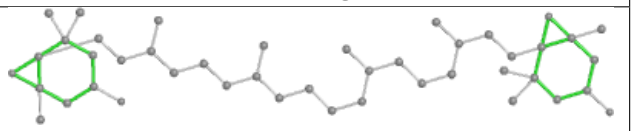


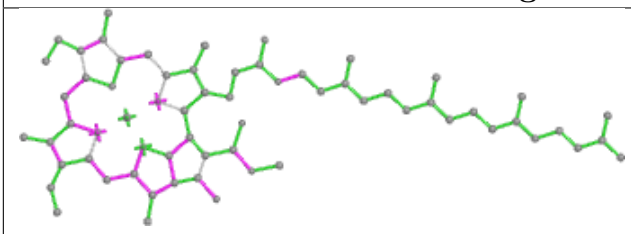
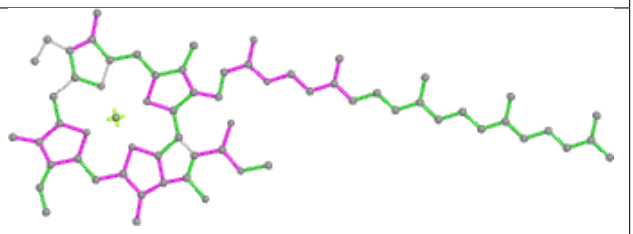
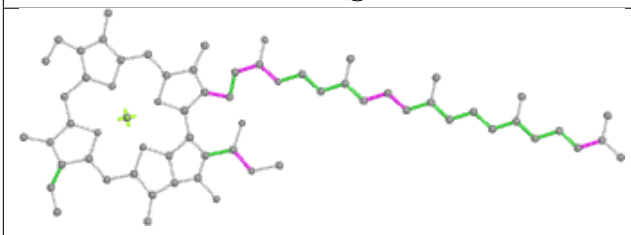
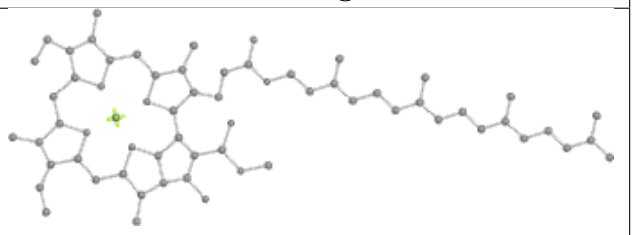
Bond angles



Torsions



Rings

| Ligand CL0 A 1011 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 4 601 | |
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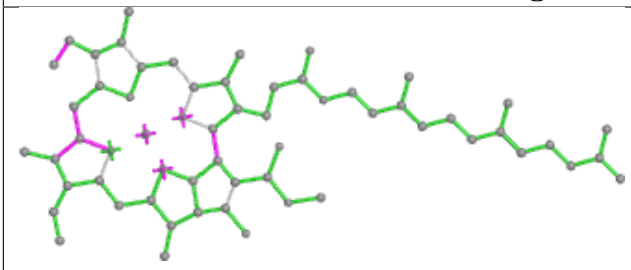
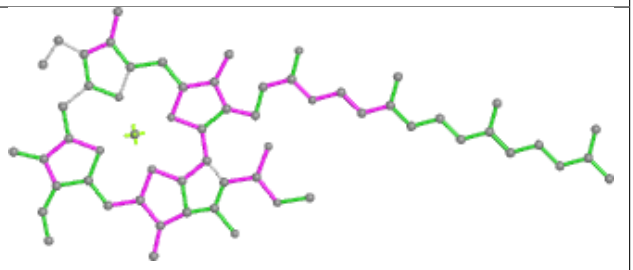
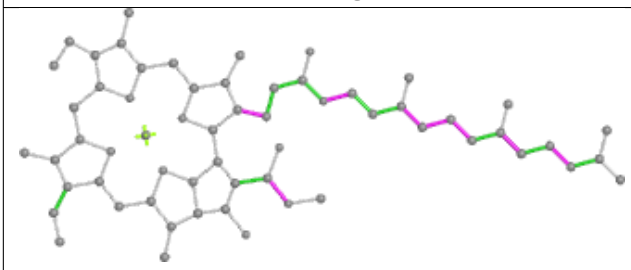
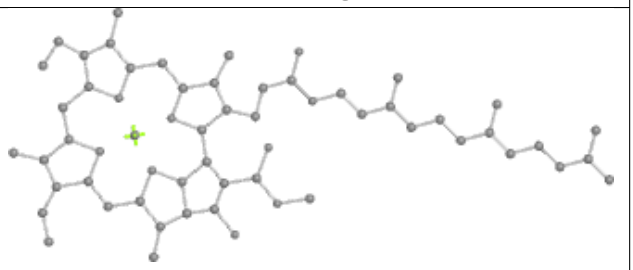
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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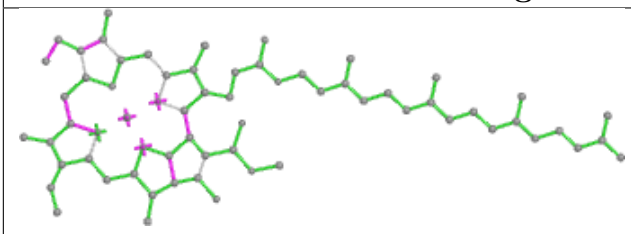
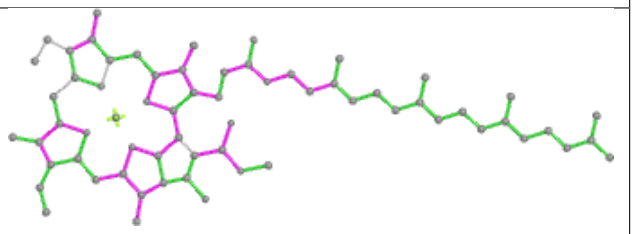
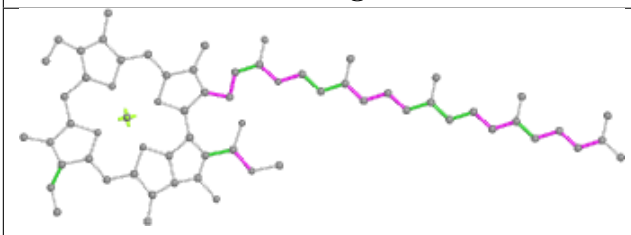


Bond lengths



Bond angles



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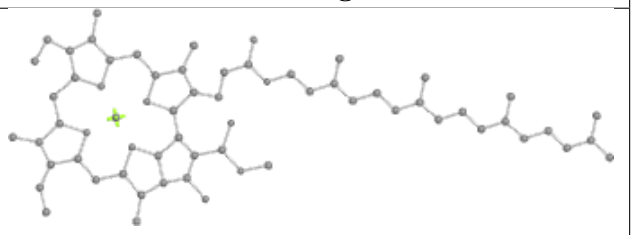
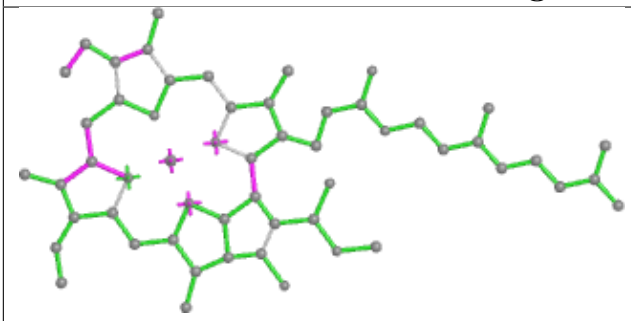


Rings

## Ligand CLA 6 607



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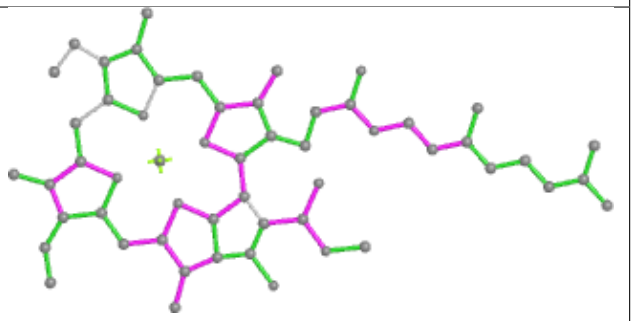
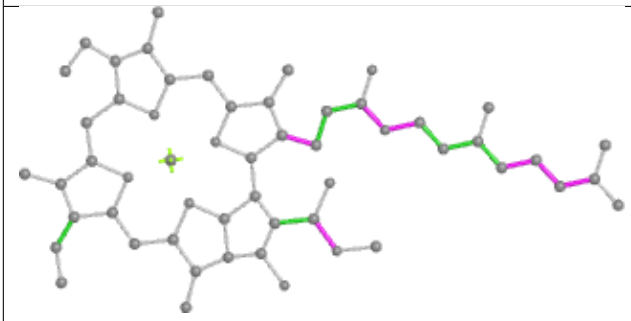


Bond angles



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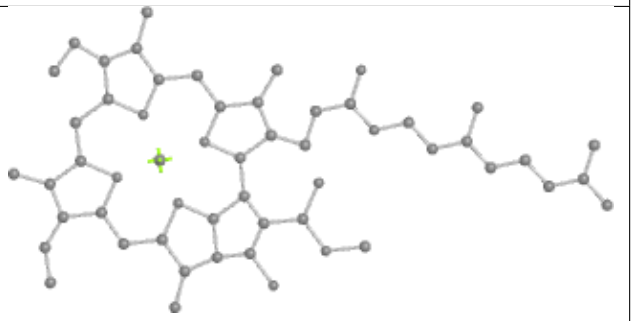
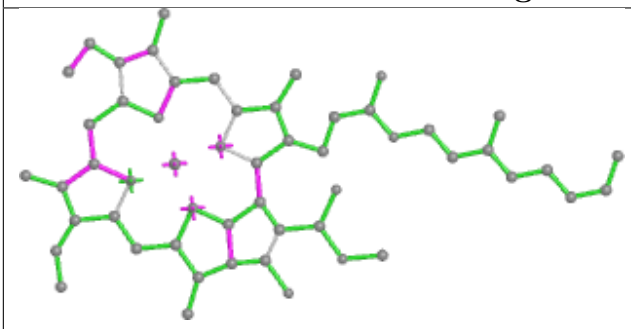


Rings

**Ligand CLA A 1110**



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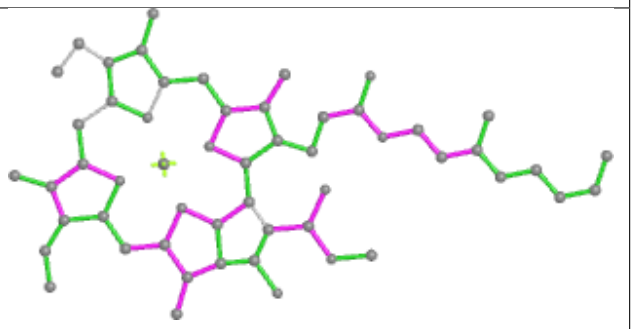

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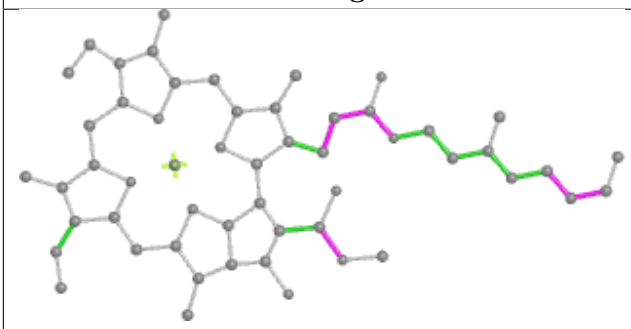

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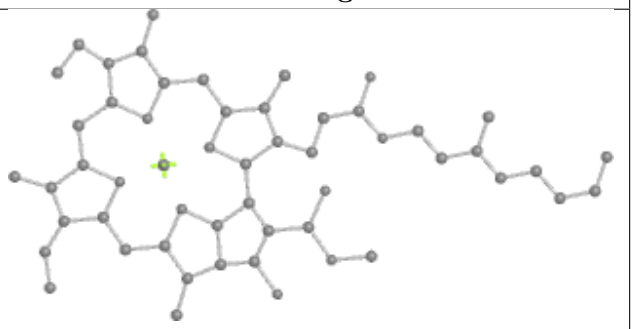
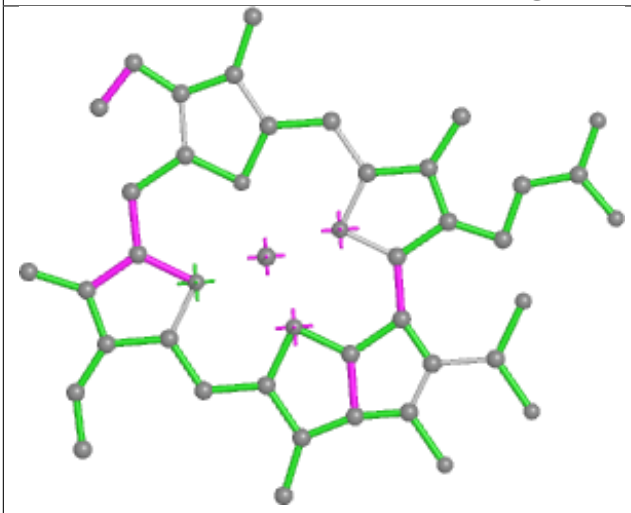


**Rings**

**Ligand CLA 7 605**



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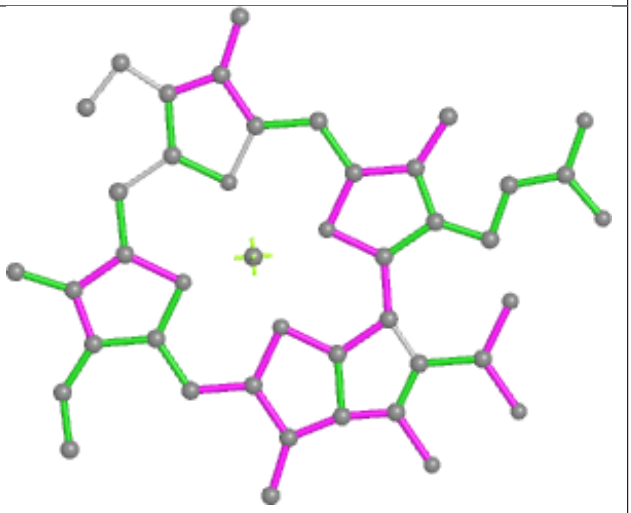

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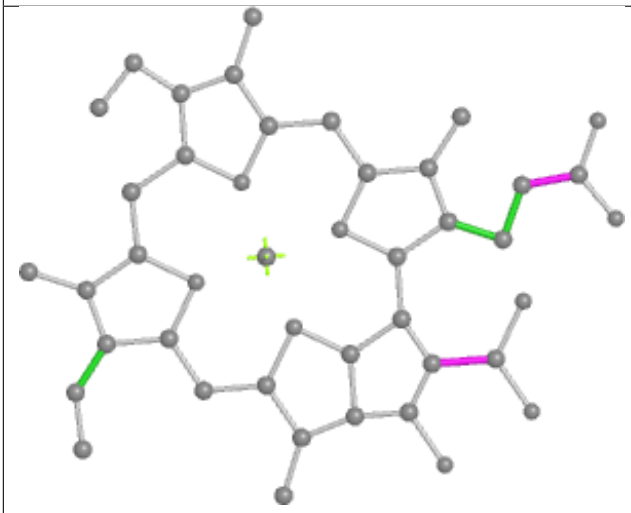

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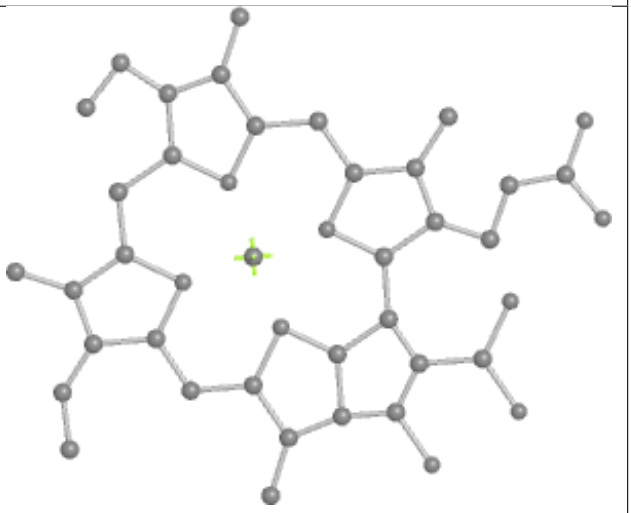
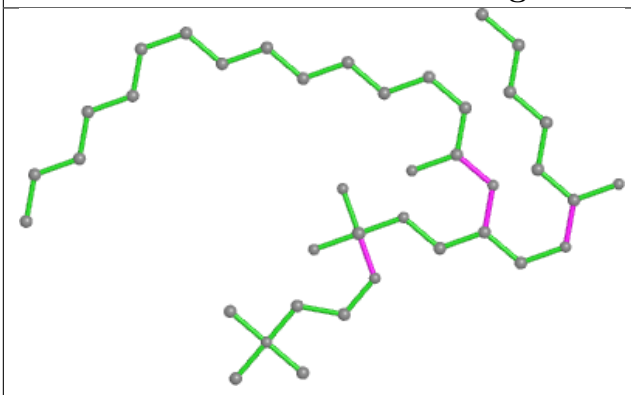


**Rings**

## Ligand PCW B 5004



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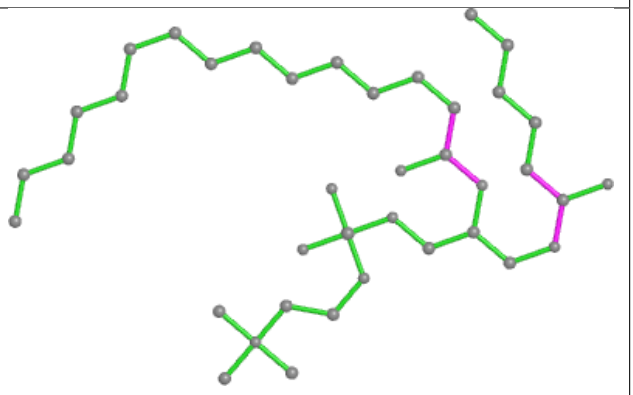

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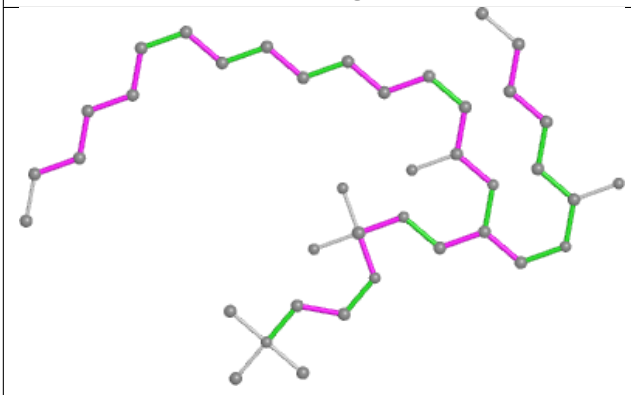

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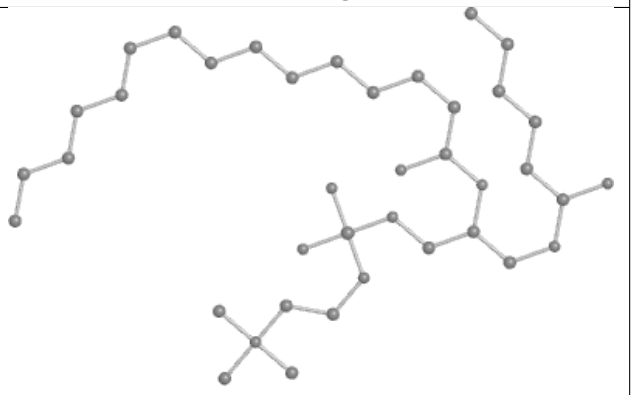
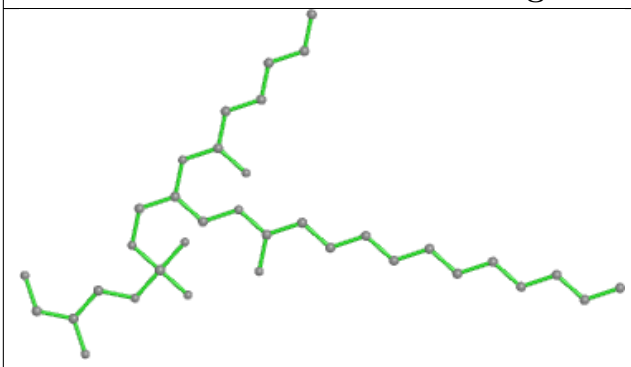


Rings

## Ligand LHG a 801



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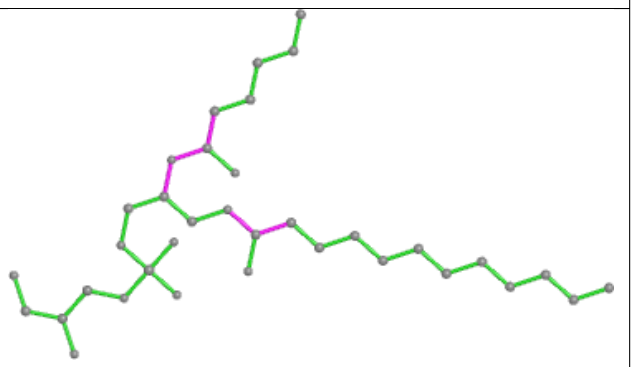
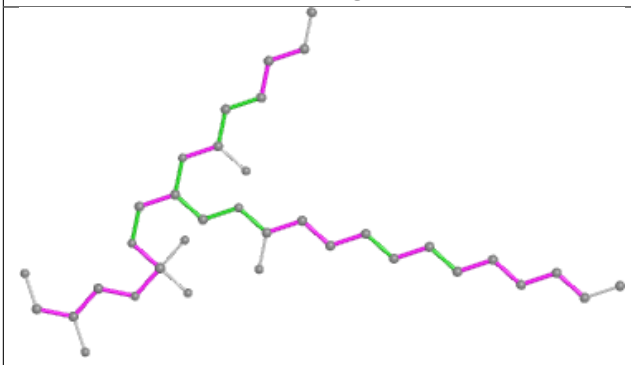


Bond angles



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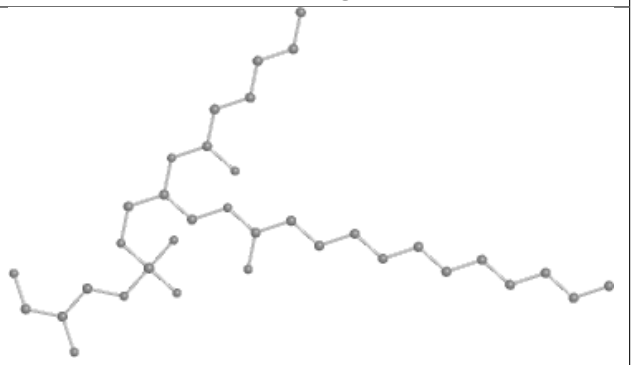

Rings

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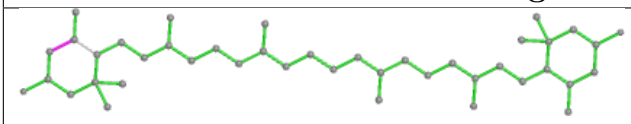

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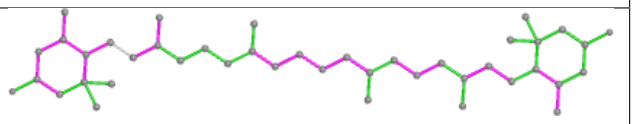
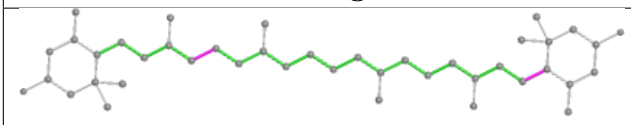


Bond angles



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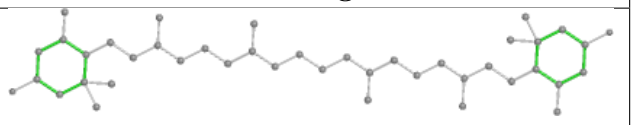
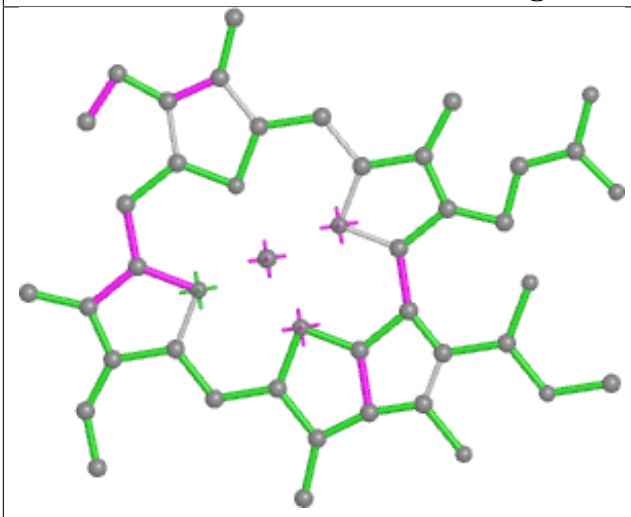


Rings

## Ligand CLA 1 602



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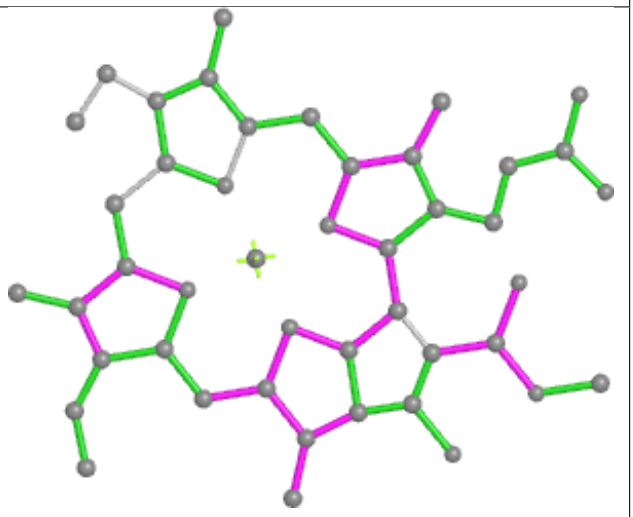
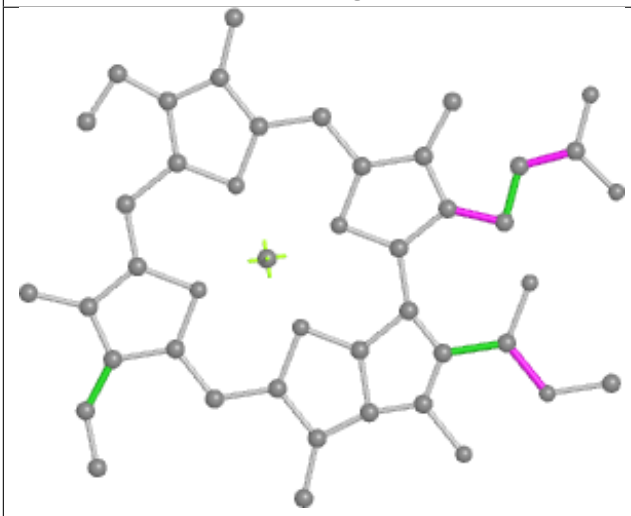
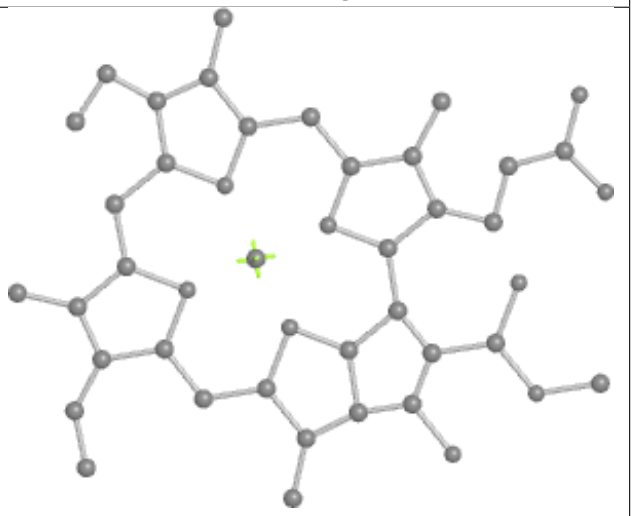


Bond angles

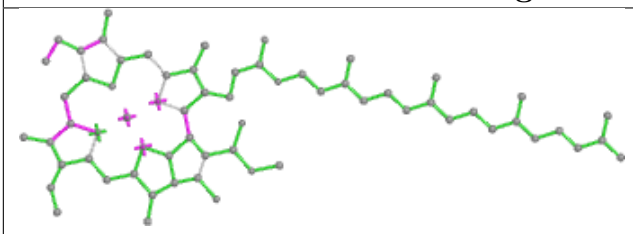


Torsions

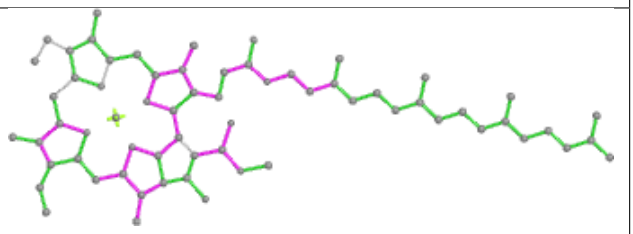


Rings

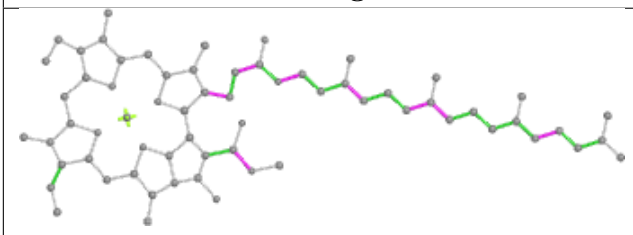
## Ligand CLA B 1229



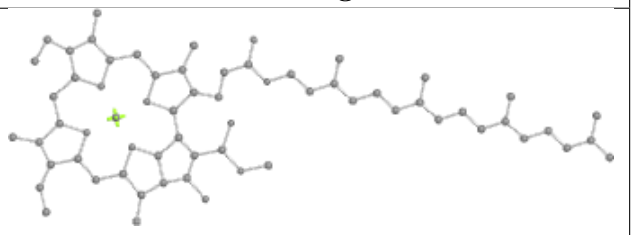
Bond lengths



Bond angles

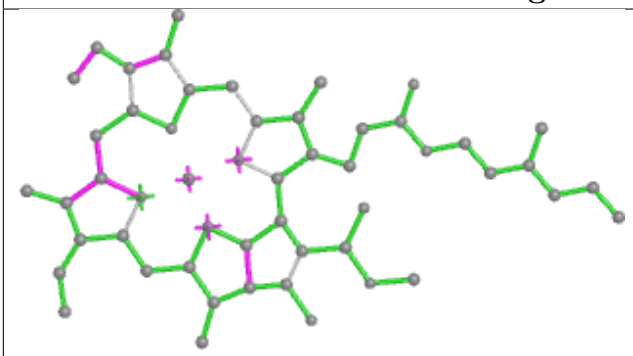


Torsions

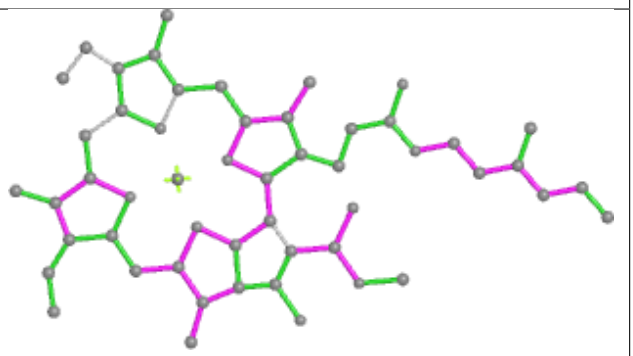


Rings

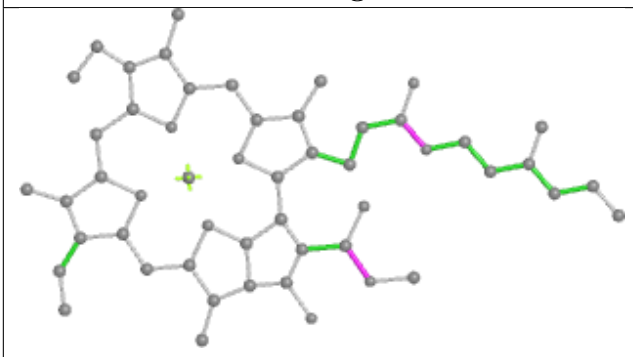
## Ligand CLA 8 602



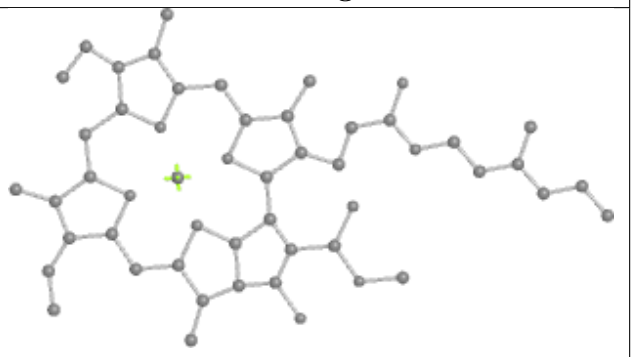
Bond lengths



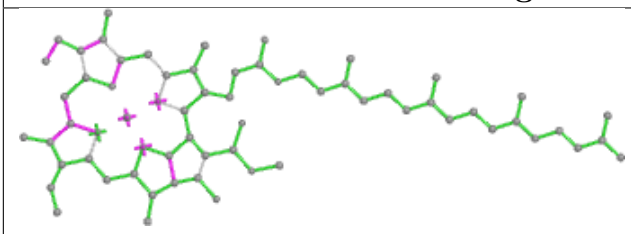
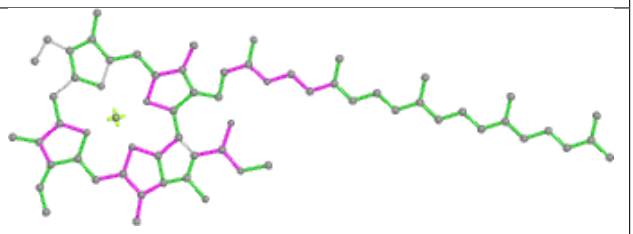
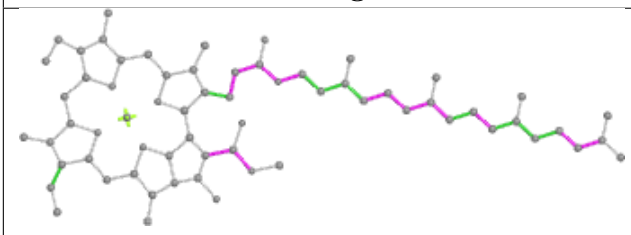
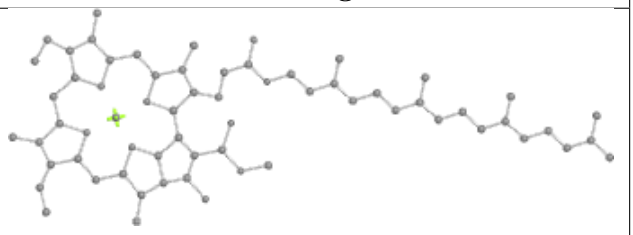
Bond angles

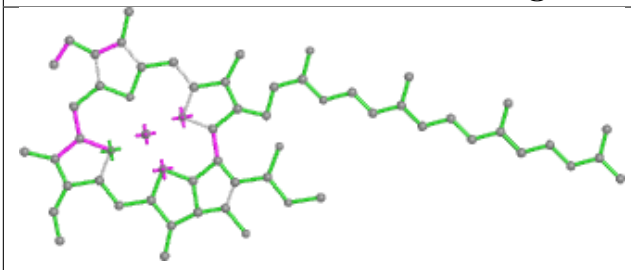
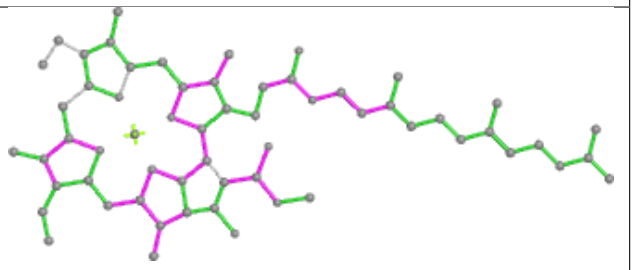
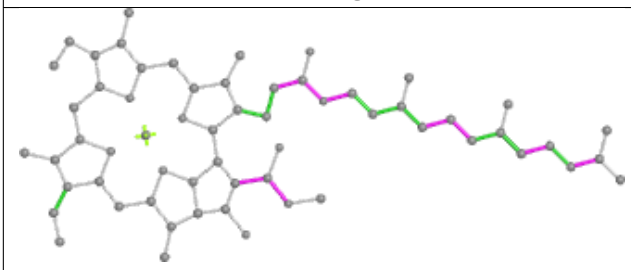
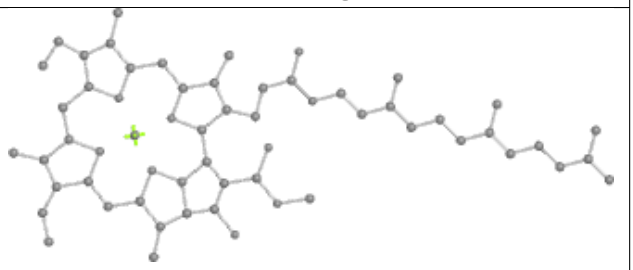


Torsions

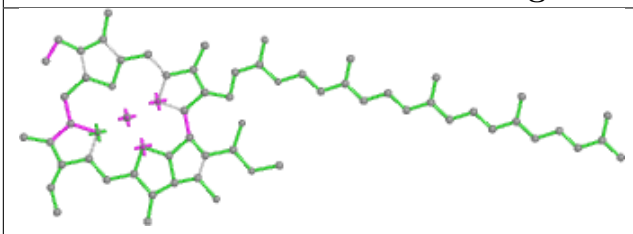


Rings

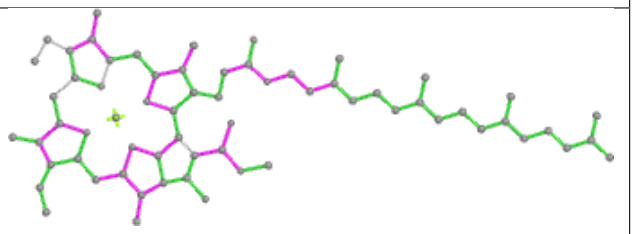
| Ligand CLA B 1237 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 4 615 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

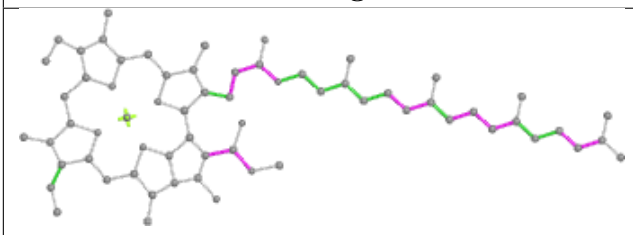
## Ligand CLA a 603



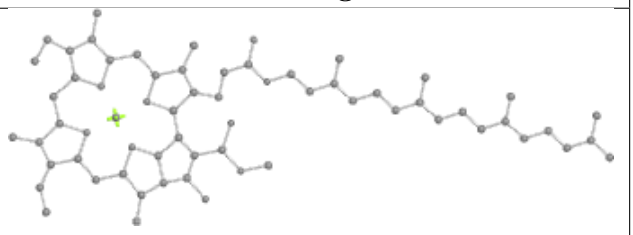
Bond lengths



Bond angles

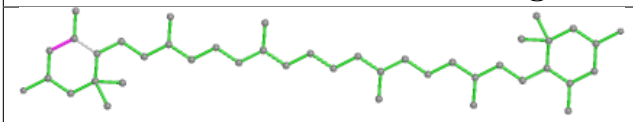


Torsions

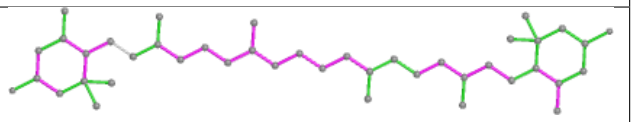


Rings

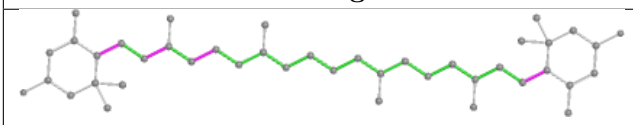
## Ligand LUT 4 501



Bond lengths



Bond angles



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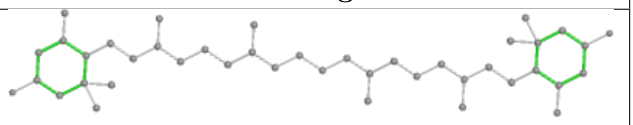
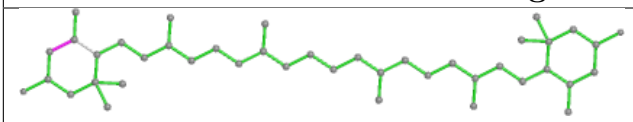
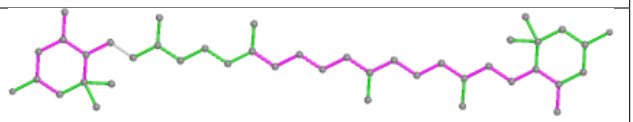


Rings

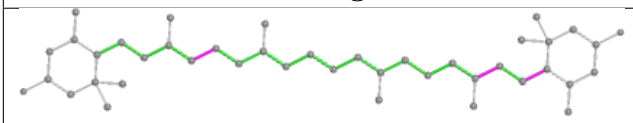
## Ligand LUT a 501



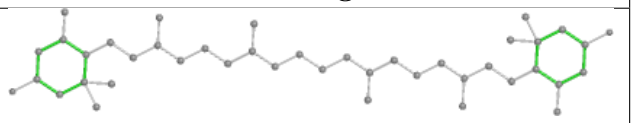
Bond lengths



Bond angles

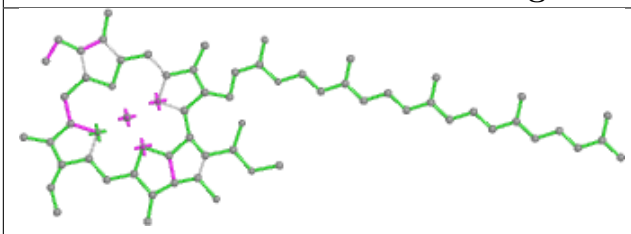


Torsions

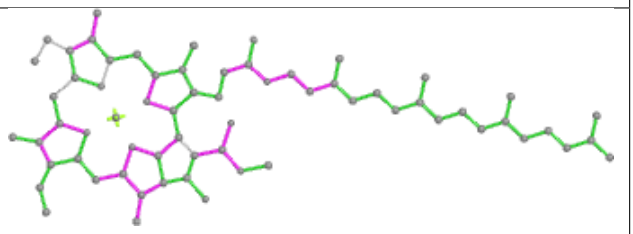


Rings

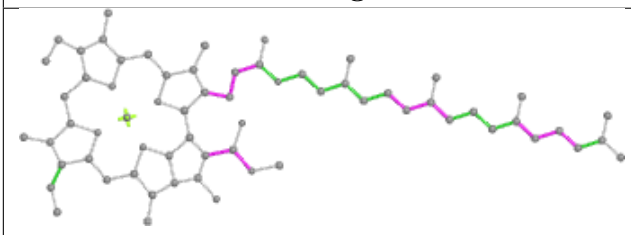
## Ligand CLA 3 606



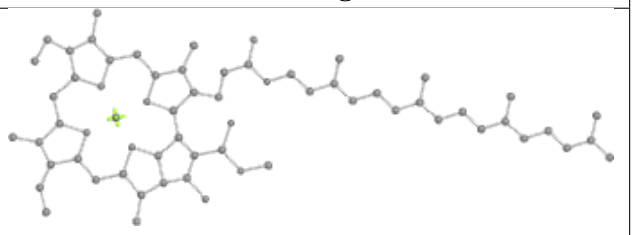
Bond lengths



Bond angles

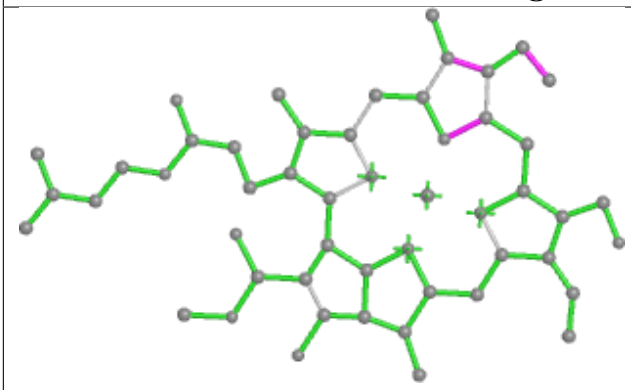


Torsions

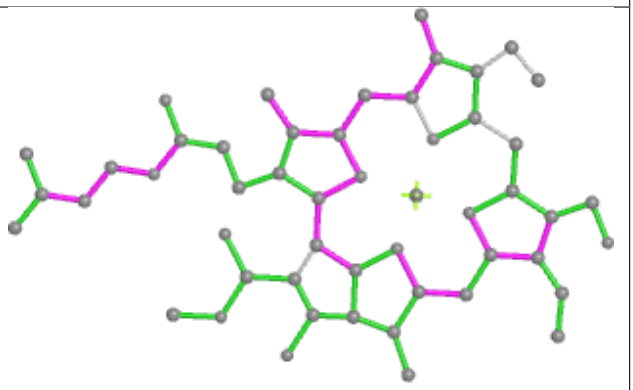


Rings

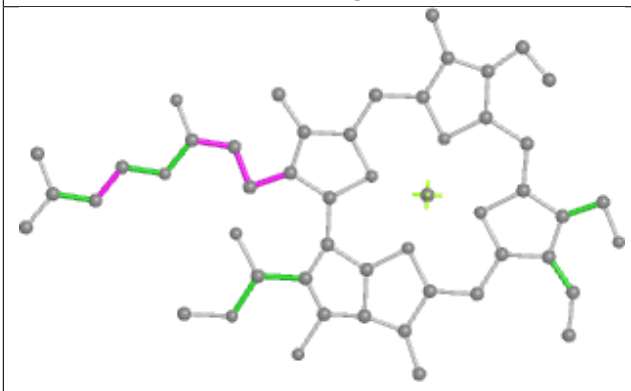
## Ligand CHL 6 611



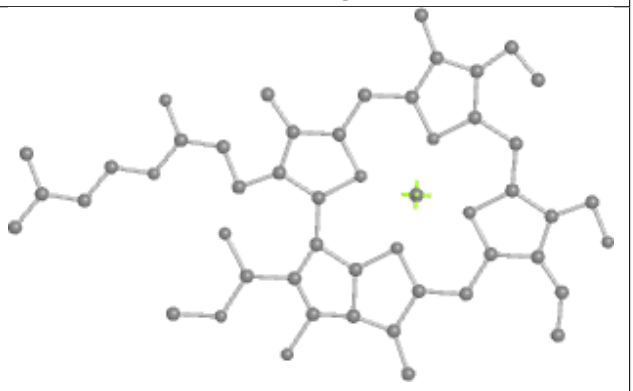
Bond lengths



Bond angles



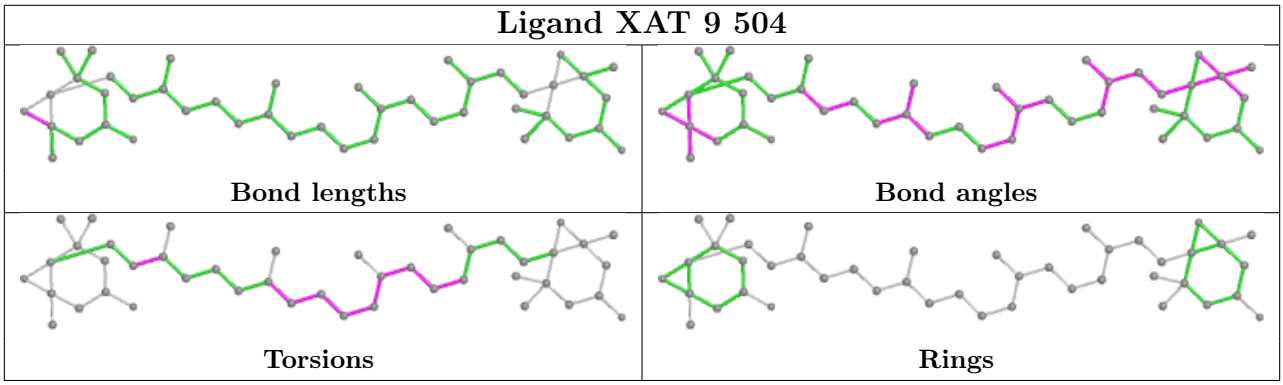
Torsions



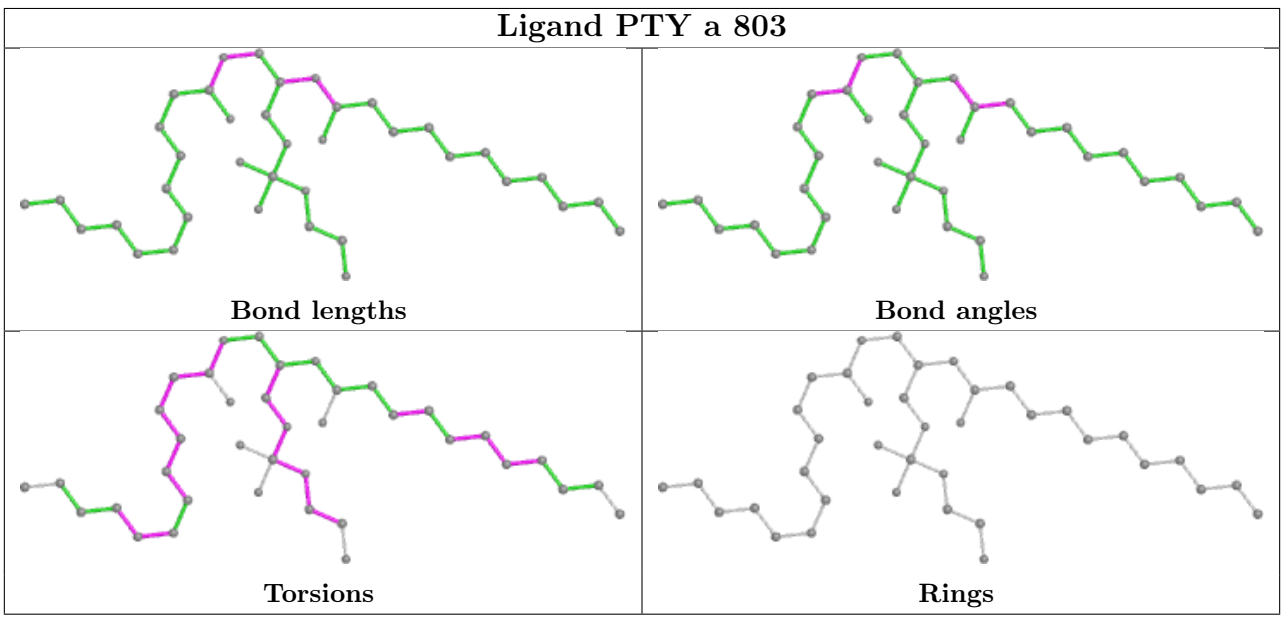
Rings

## Ligand LUT 5 505

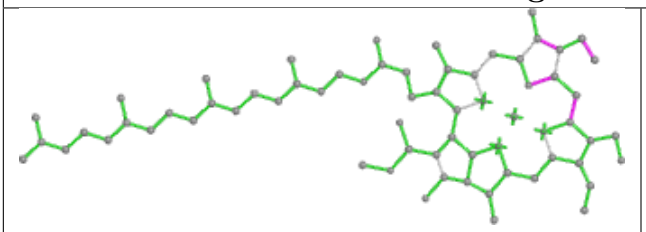
## Ligand XAT 9 504



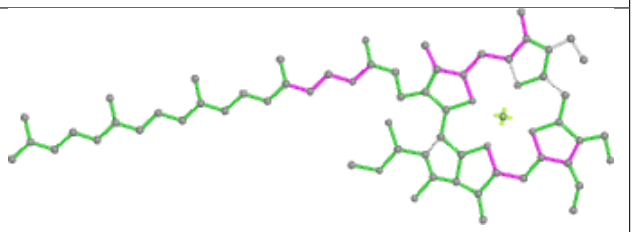

## Ligand PTY a 803



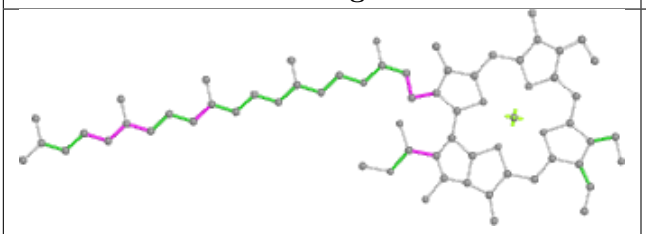
## Ligand CHL 1 604



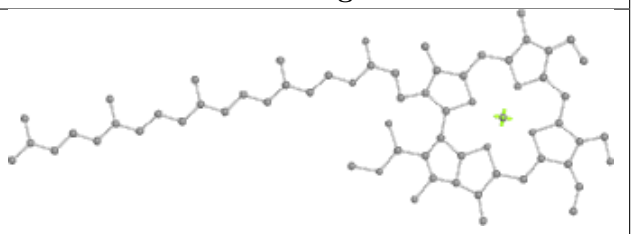
Bond lengths



Bond angles

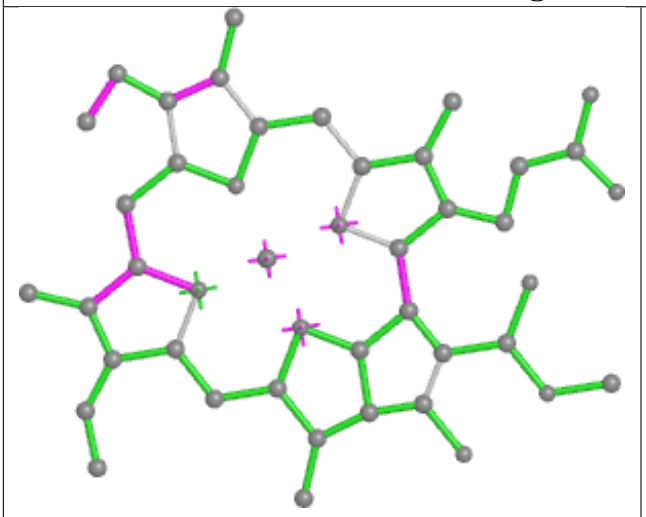


Torsions

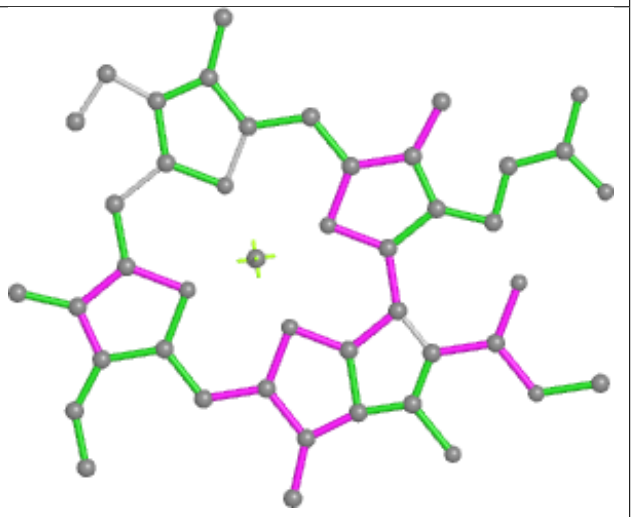


Rings

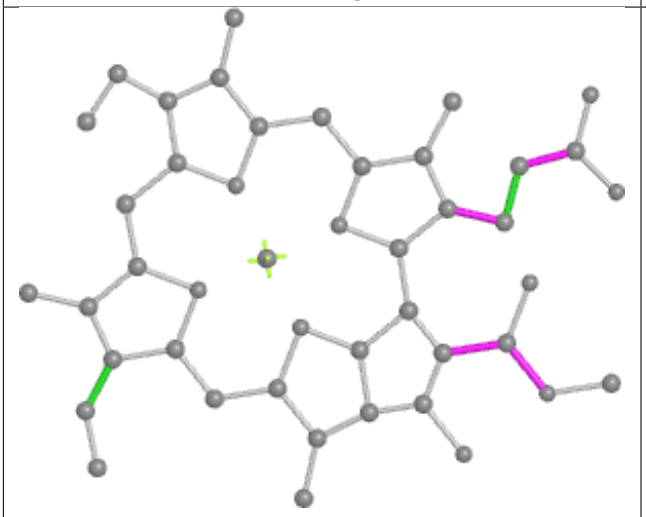
## Ligand CLA 2 608



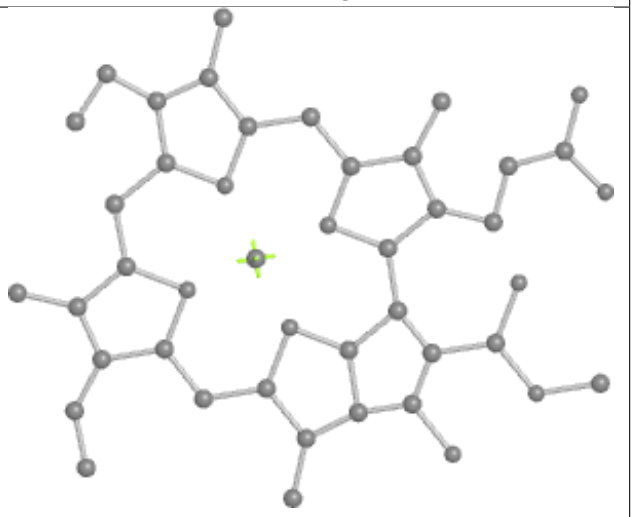
Bond lengths



Bond angles

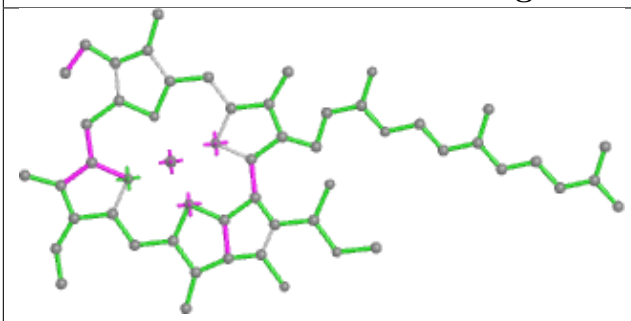


Torsions

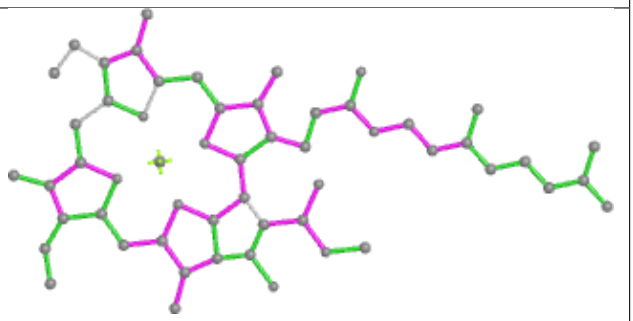


Rings

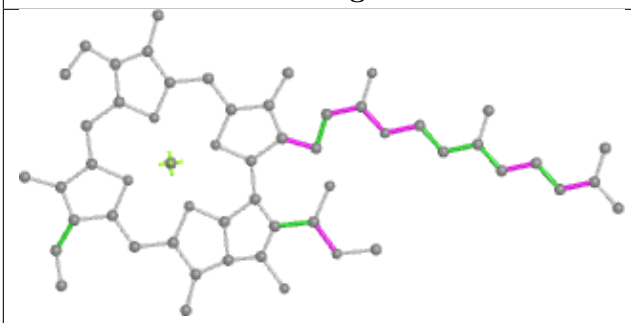
## Ligand CLA B 1211



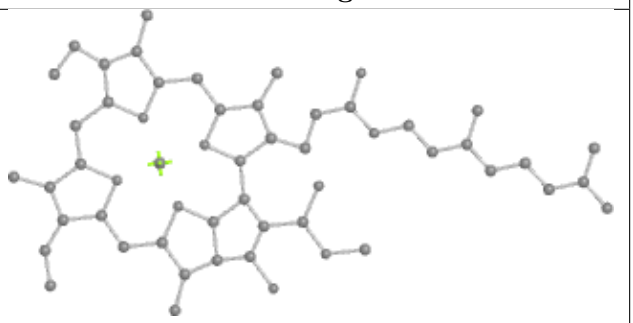
Bond lengths



Bond angles

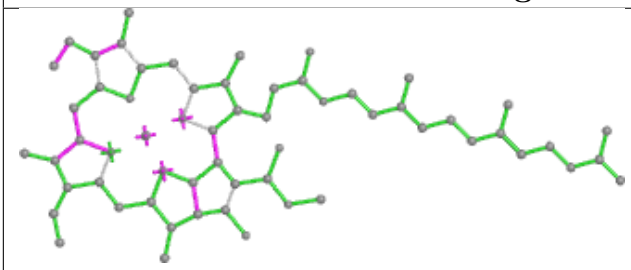


Torsions

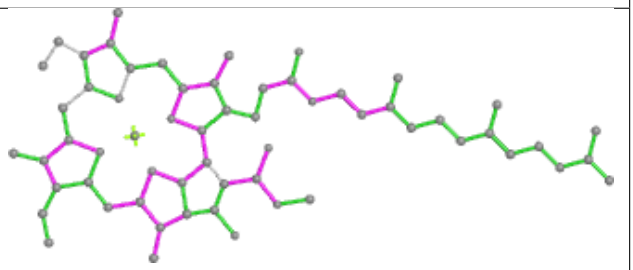


Rings

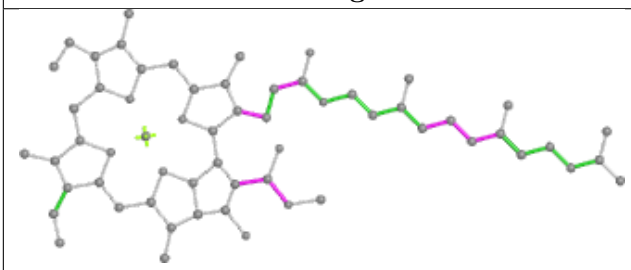
## Ligand CLA K 1402



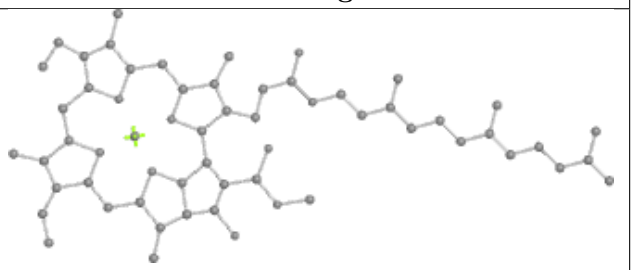
Bond lengths



Bond angles

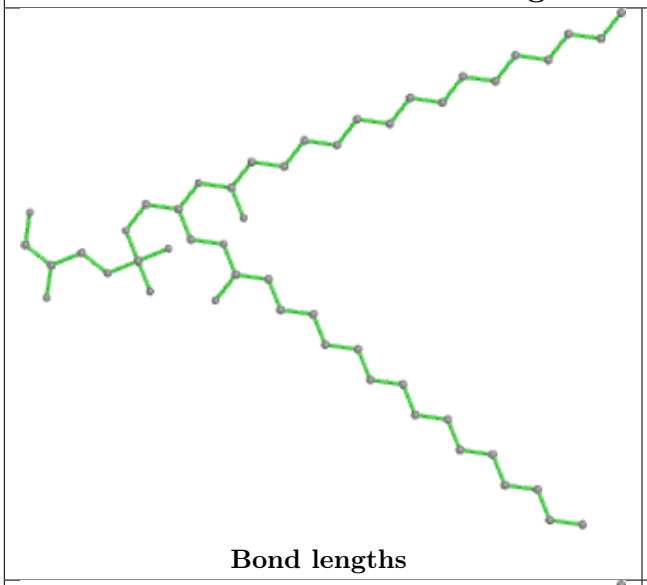


Torsions

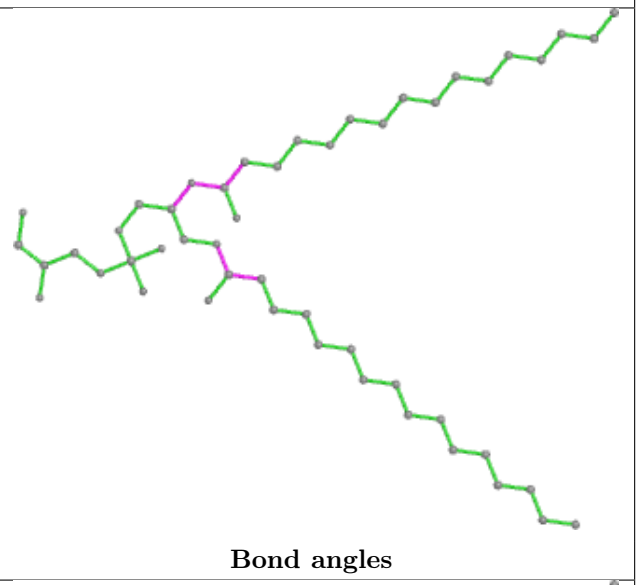


Rings

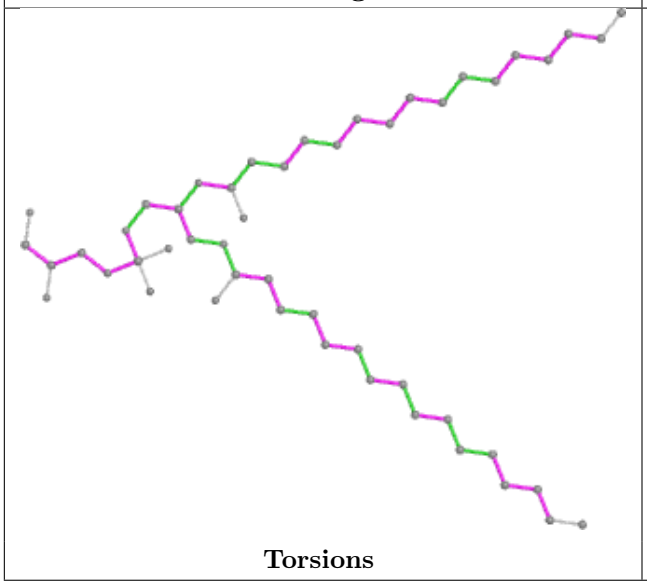
## Ligand LHG 1 802



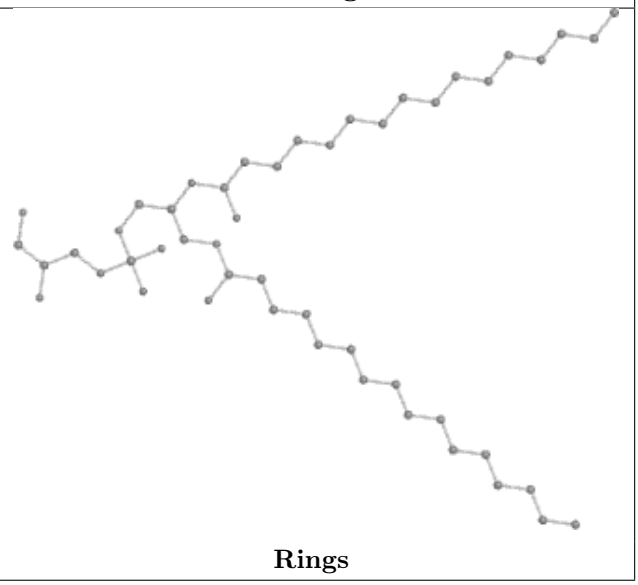
Bond lengths



Bond angles

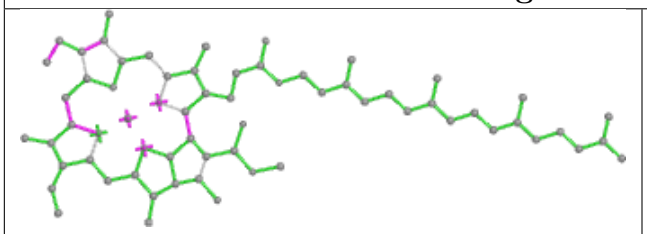


Torsions

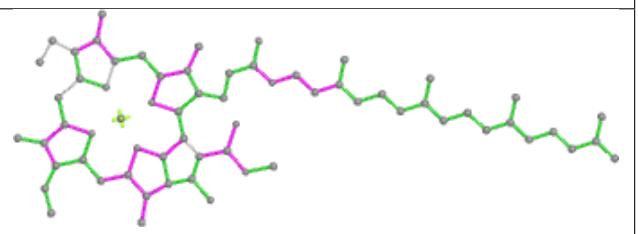


Rings

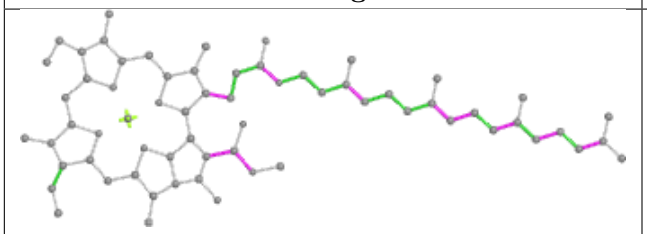
## Ligand CLA A 1117



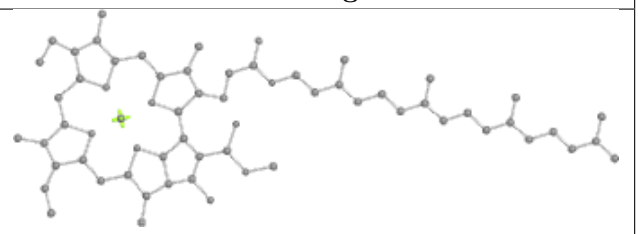
Bond lengths



Bond angles

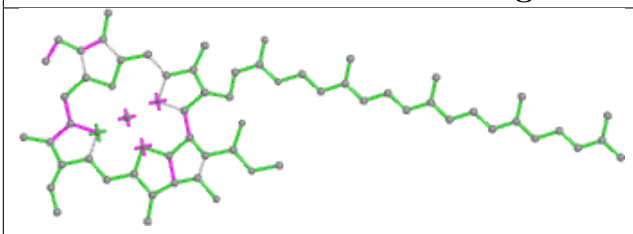


Torsions

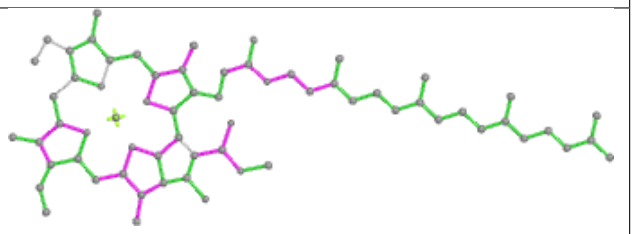


Rings

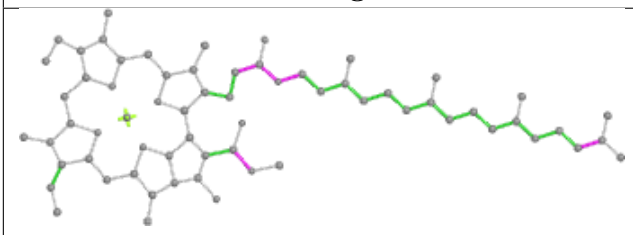
## Ligand CLA B 1238



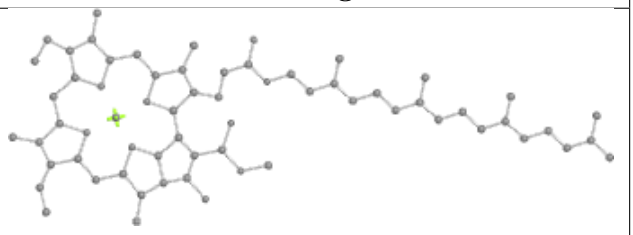
Bond lengths



Bond angles

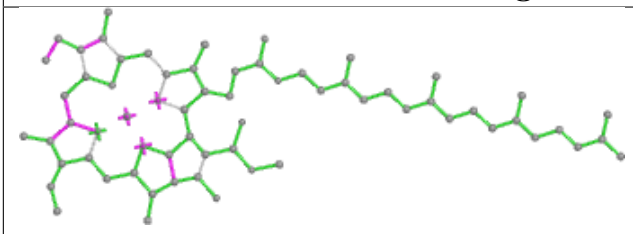


Torsions

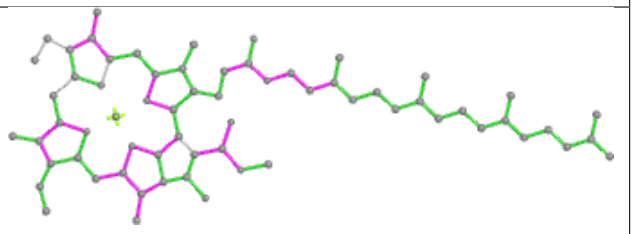


Rings

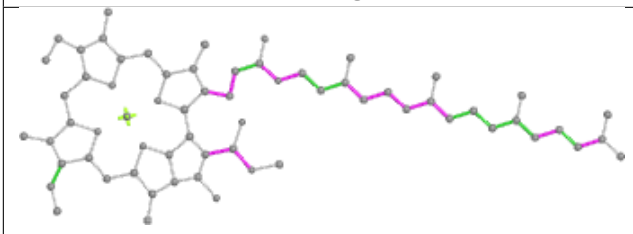
## Ligand CLA A 1119



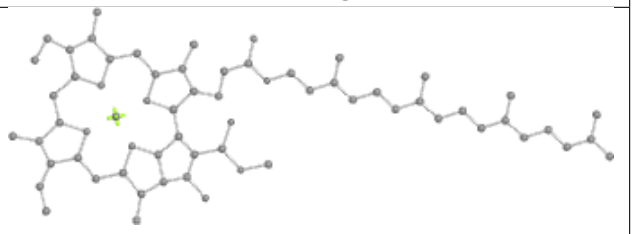
Bond lengths



Bond angles

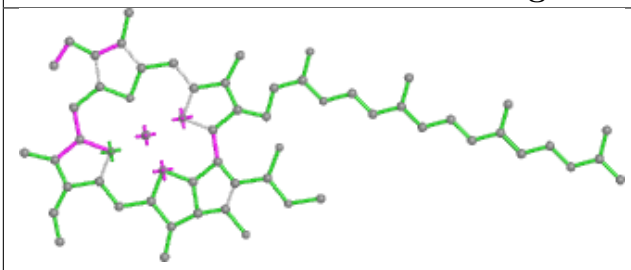


Torsions

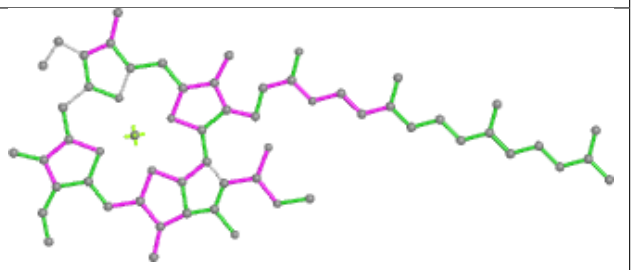


Rings

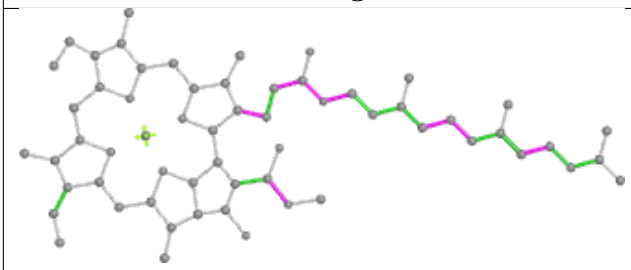
## Ligand CLA 2 601



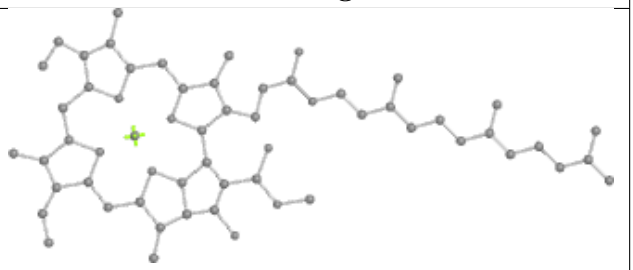
Bond lengths



Bond angles

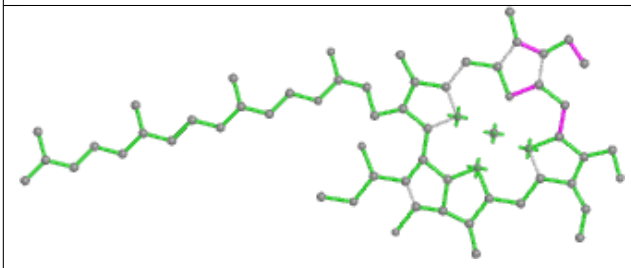


Torsions

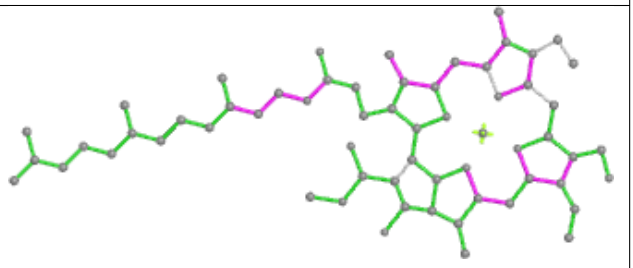


Rings

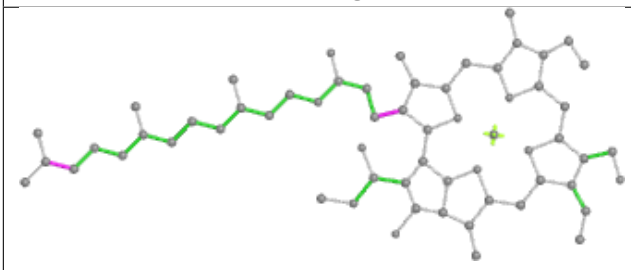
## Ligand CHL 8 601



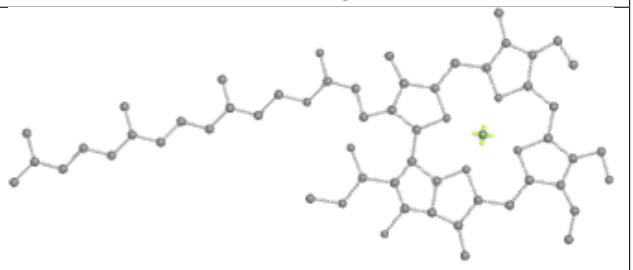
Bond lengths



Bond angles

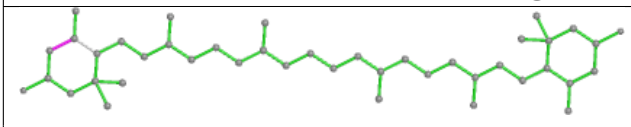


Torsions

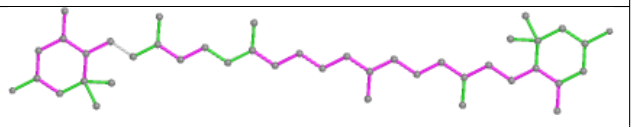


Rings

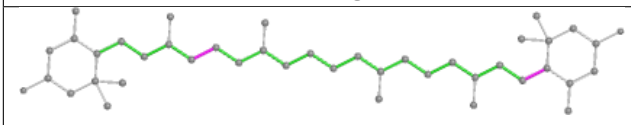
## Ligand LUT 3 501



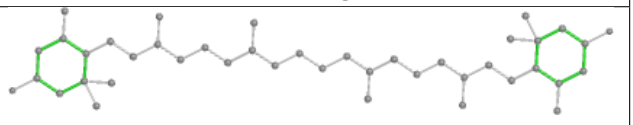
Bond lengths



Bond angles

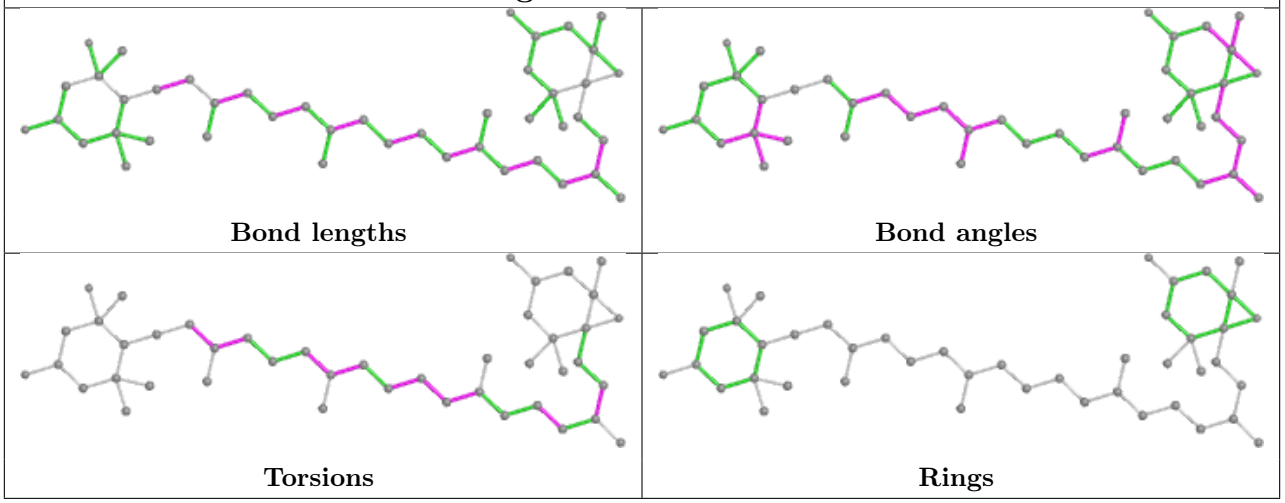


Torsions

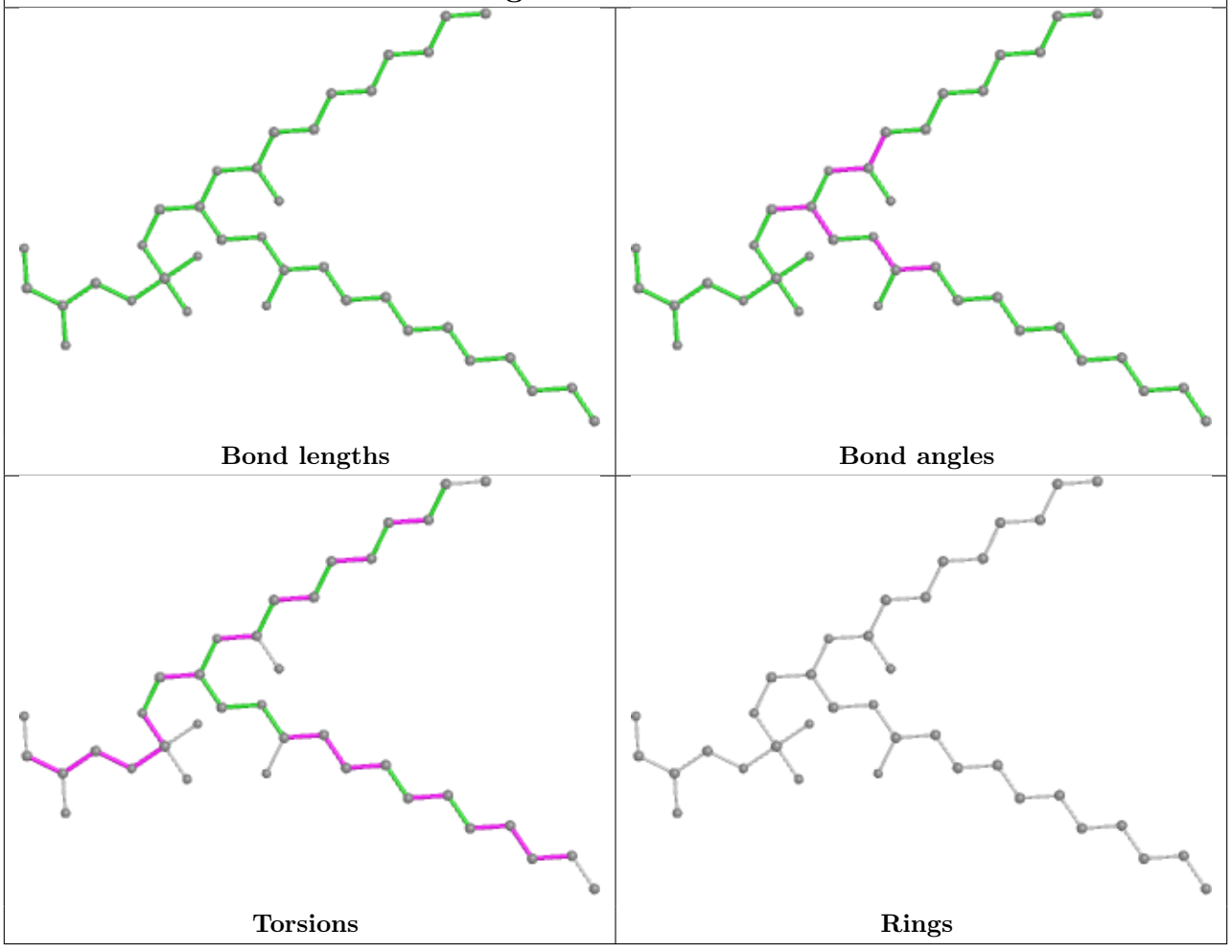


Rings

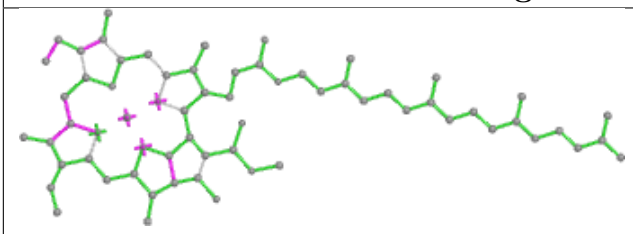
## Ligand NEX F 4001



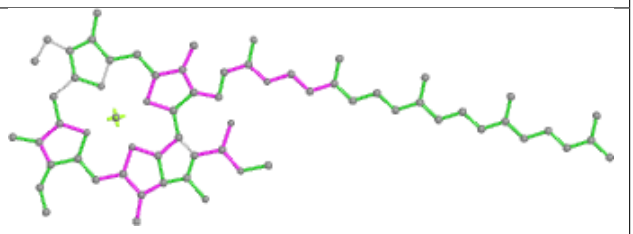

## Ligand LHG 6 802



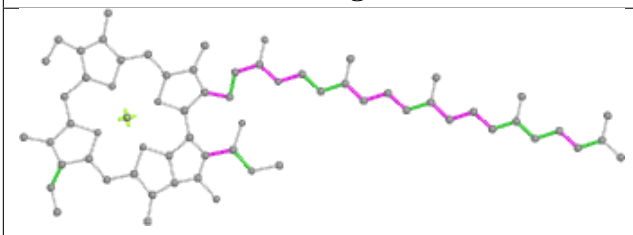
## Ligand CLA A 1108



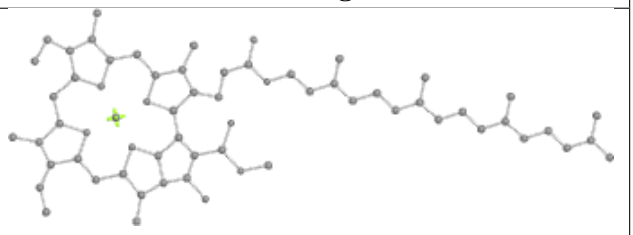
Bond lengths



Bond angles

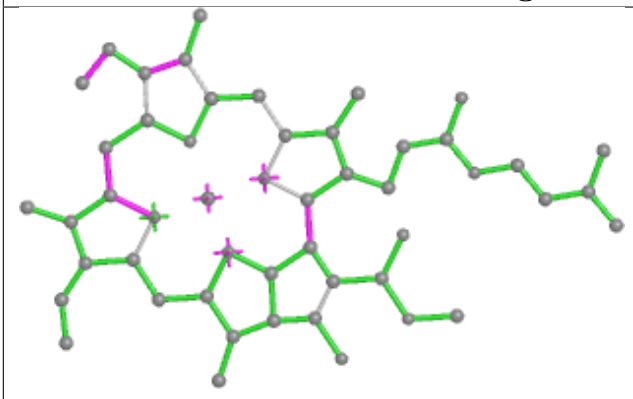


Torsions

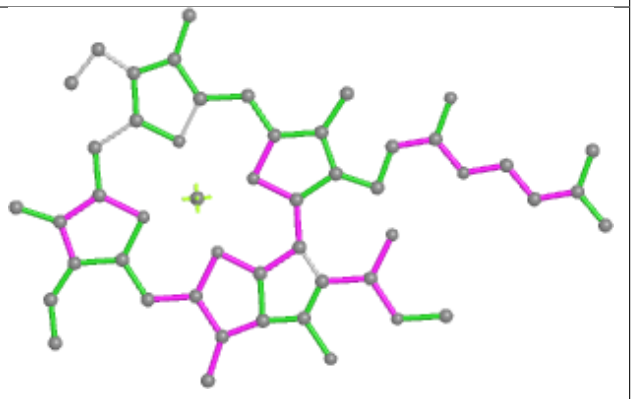


Rings

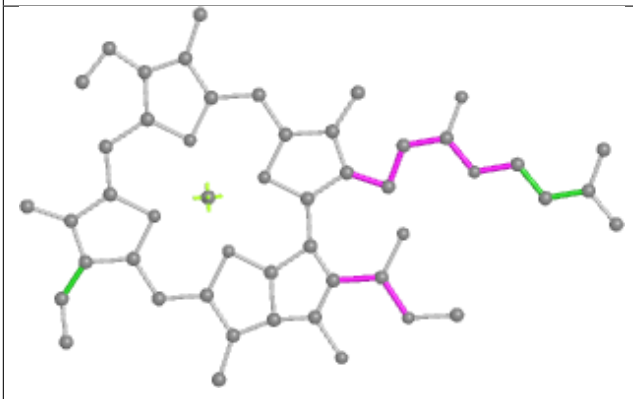
## Ligand CLA F 1301



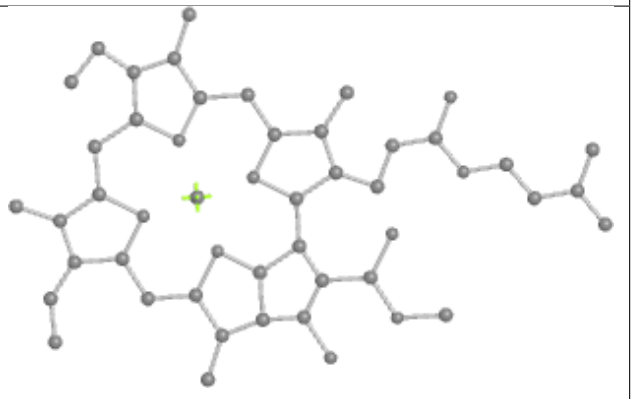
Bond lengths



Bond angles



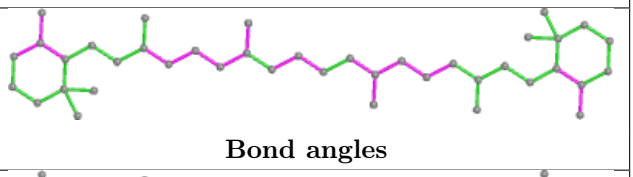
Torsions



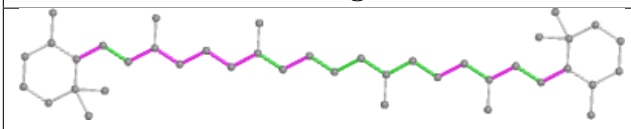
Rings

## Ligand BCR 8 503

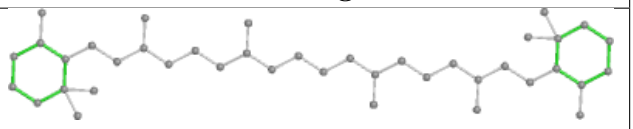
Bond lengths



Bond angles

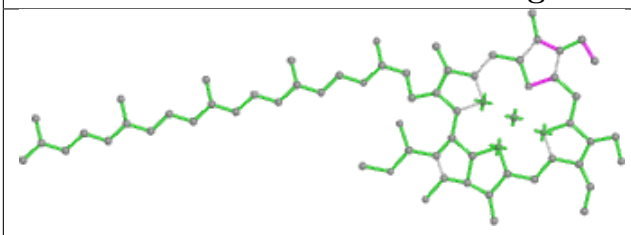


Torsions

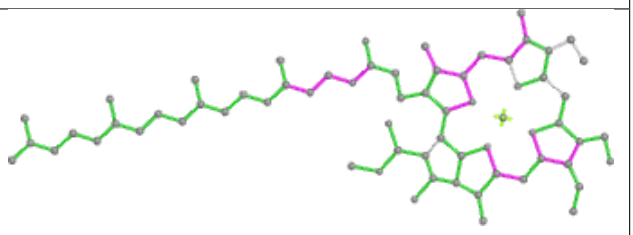


Rings

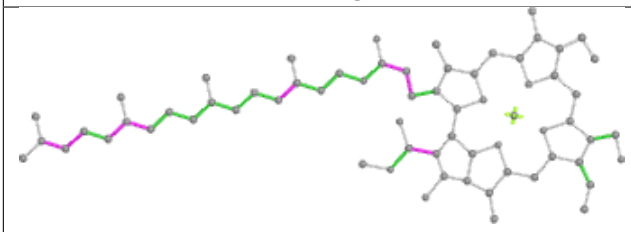
## Ligand CHL 4 609



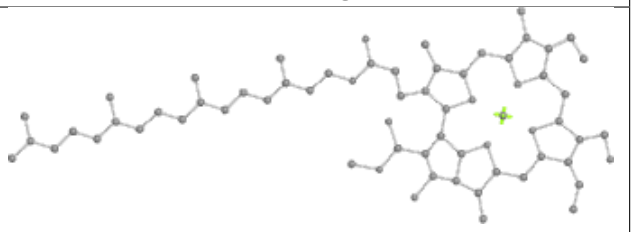
Bond lengths



Bond angles

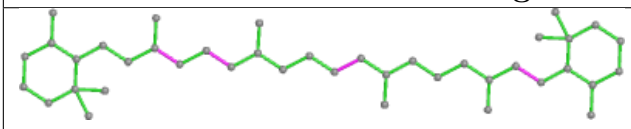


Torsions

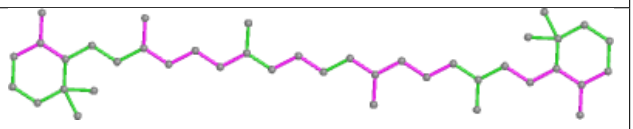


Rings

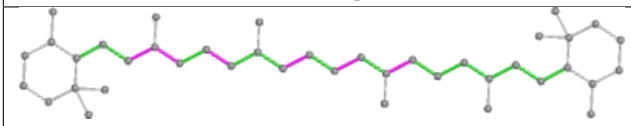
## Ligand BCR A 4002



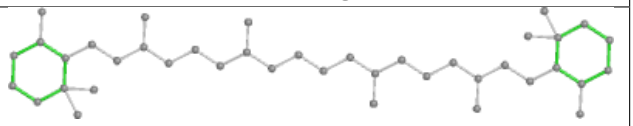
Bond lengths



Bond angles

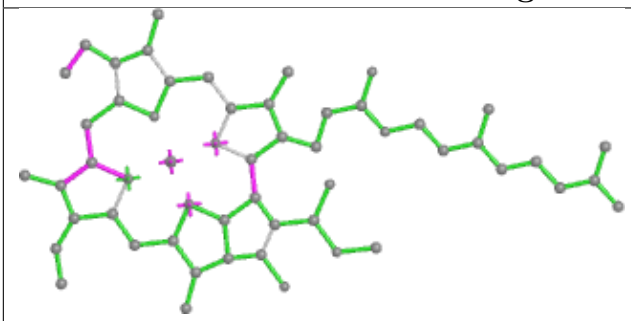


Torsions

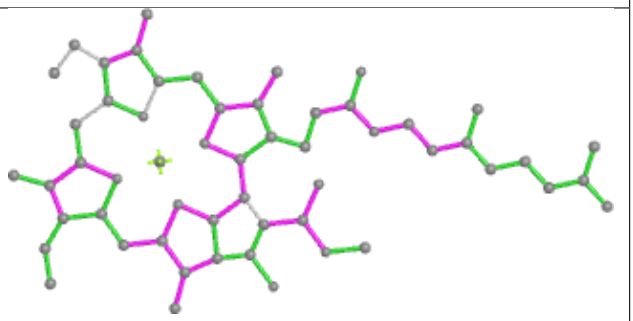


Rings

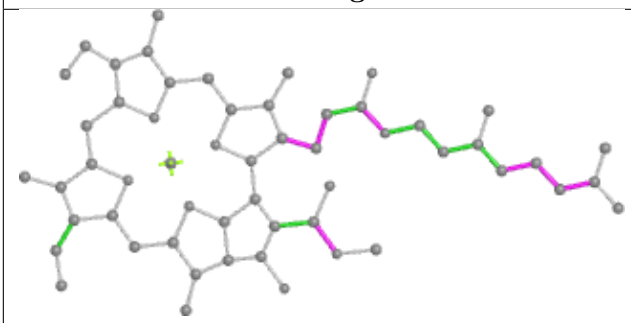
## Ligand CLA F 1302



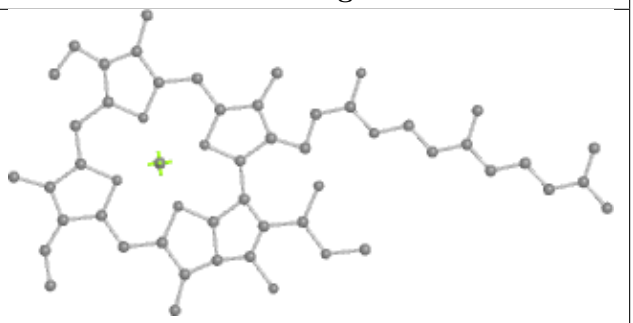
Bond lengths



Bond angles

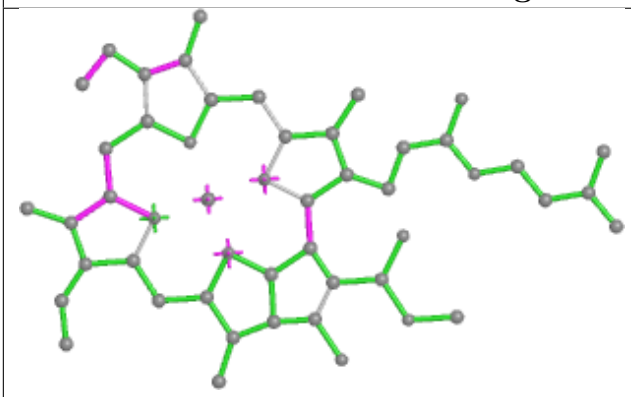


Torsions

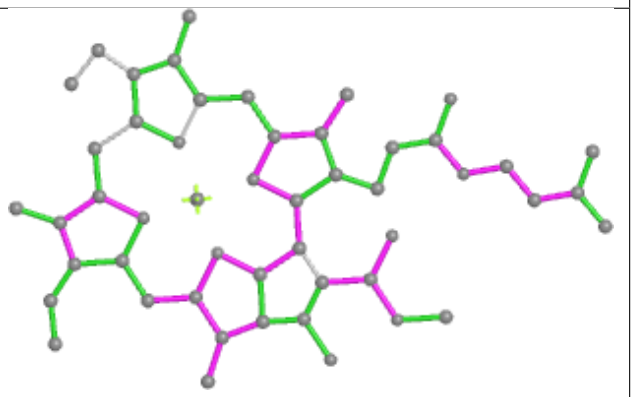


Rings

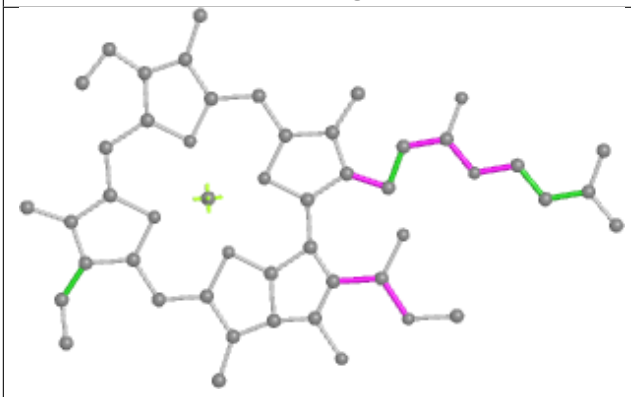
## Ligand CLA G 1601



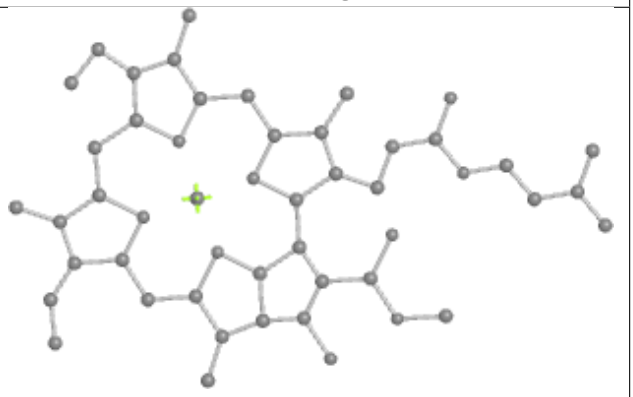
Bond lengths



Bond angles

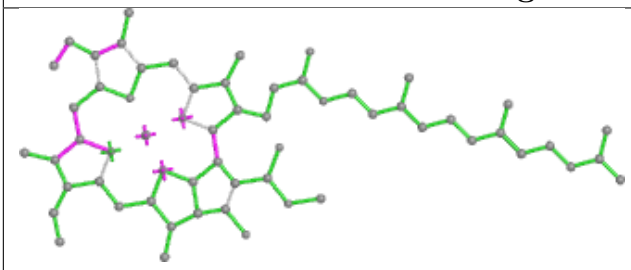


Torsions

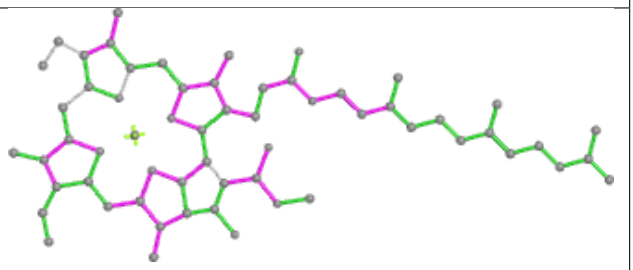


Rings

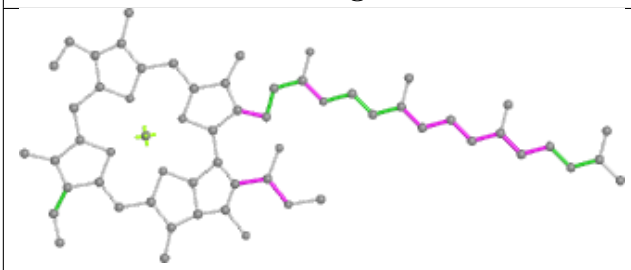
## Ligand CLA L 1502



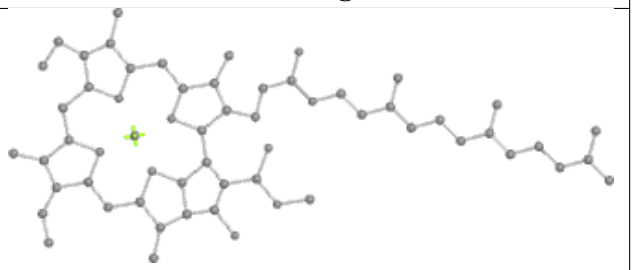
Bond lengths



Bond angles

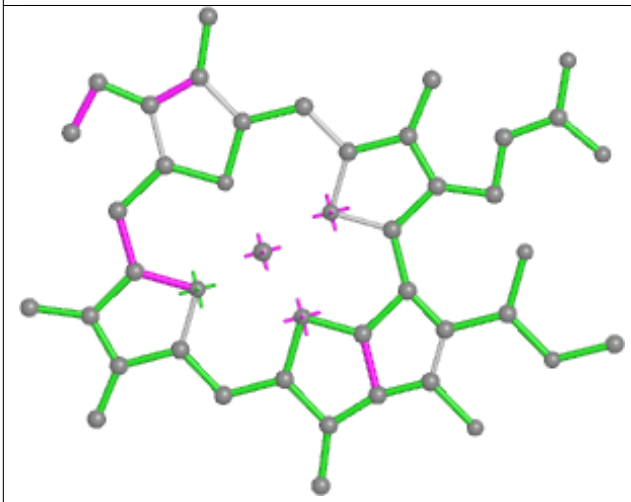


Torsions

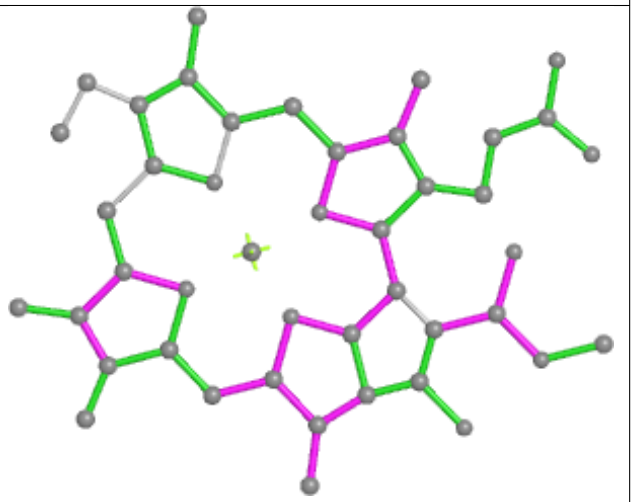


Rings

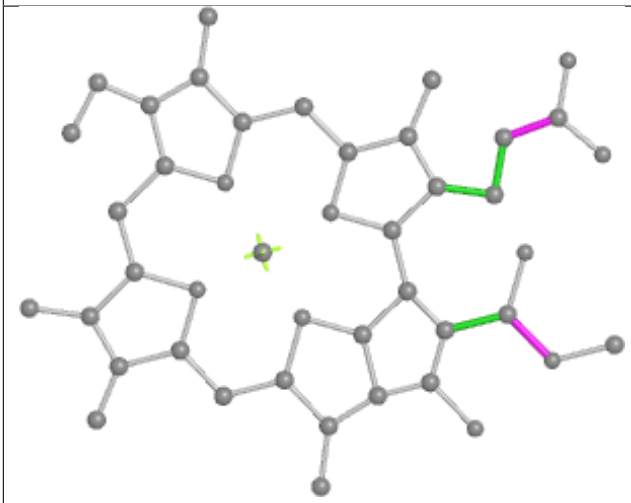
## Ligand CLA 7 602



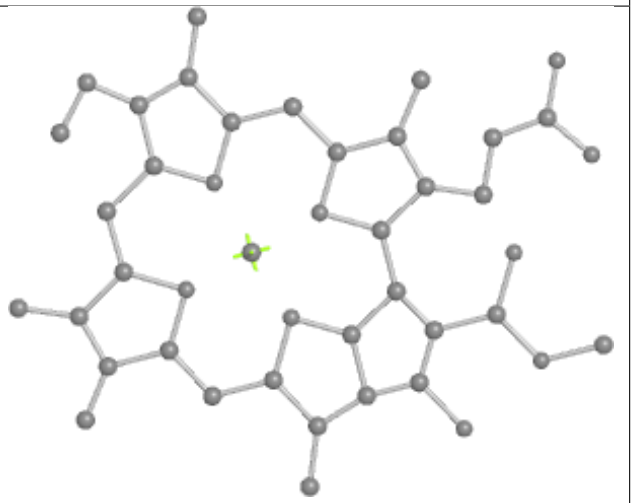
Bond lengths



Bond angles

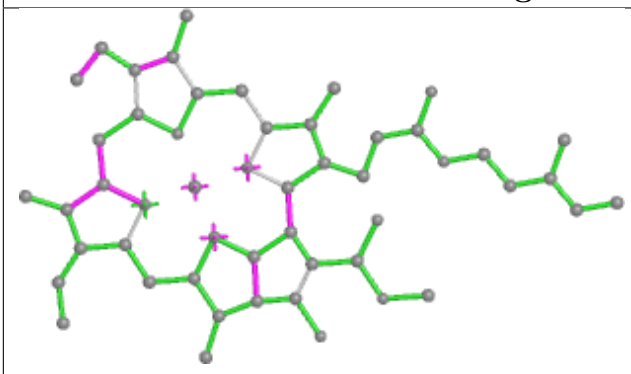


Torsions

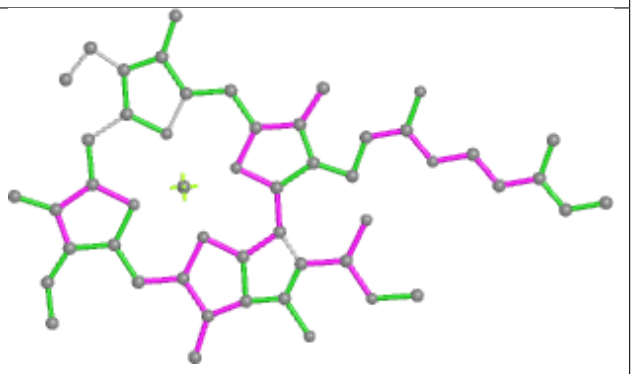


Rings

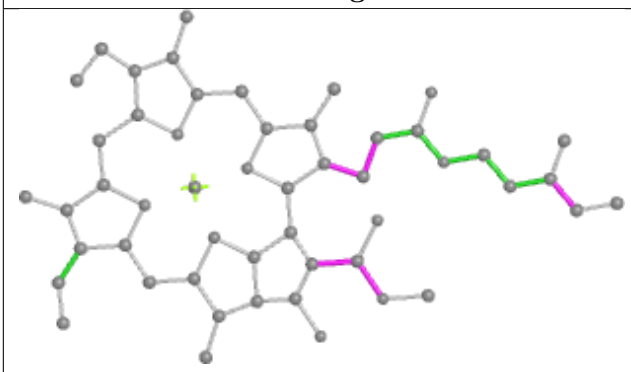
## Ligand CLA A 1135



Bond lengths



Bond angles



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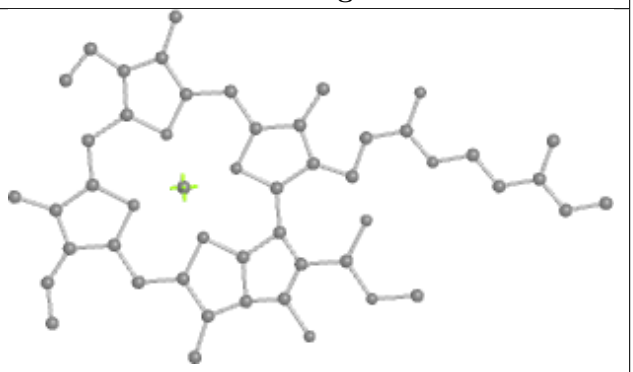
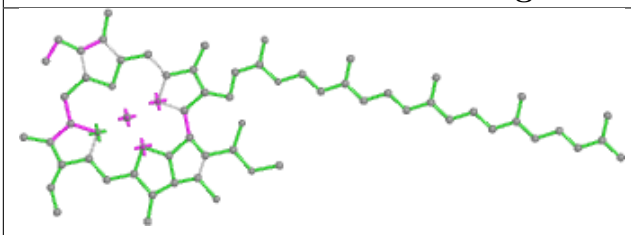
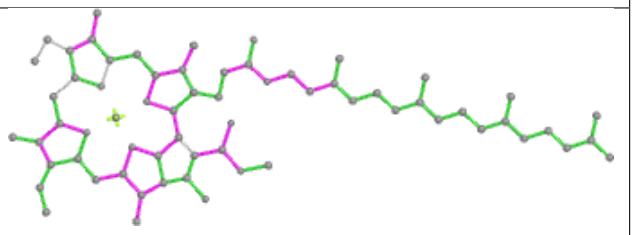


Rings

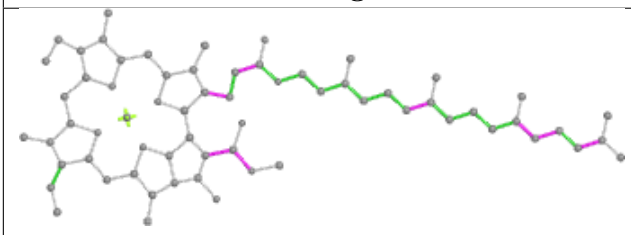
## Ligand CLA B 1240



Bond lengths



Bond angles



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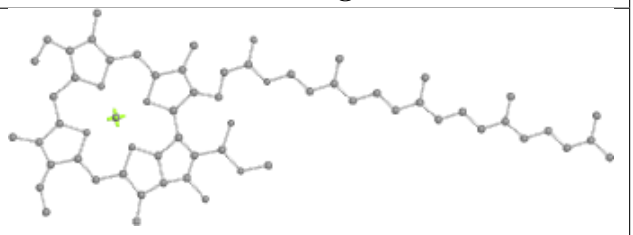
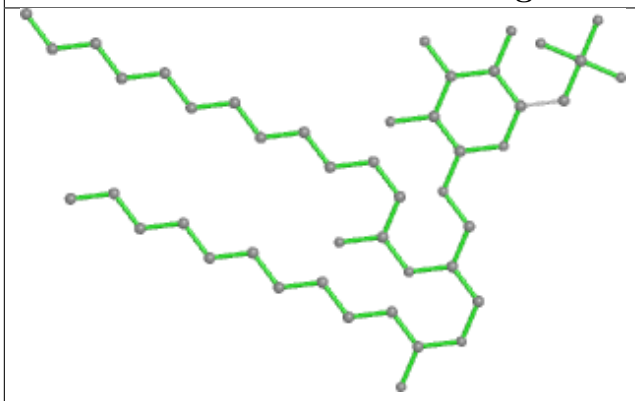
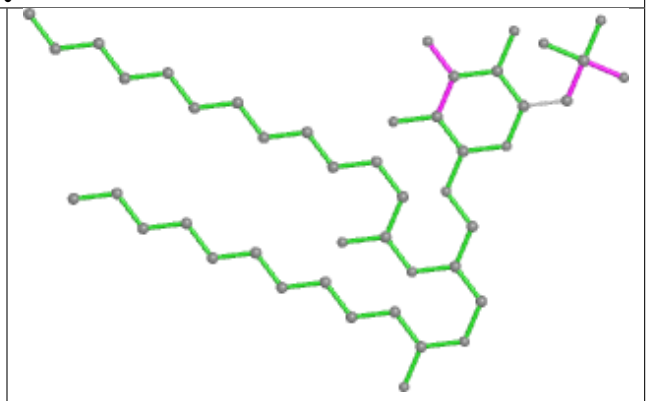


Rings

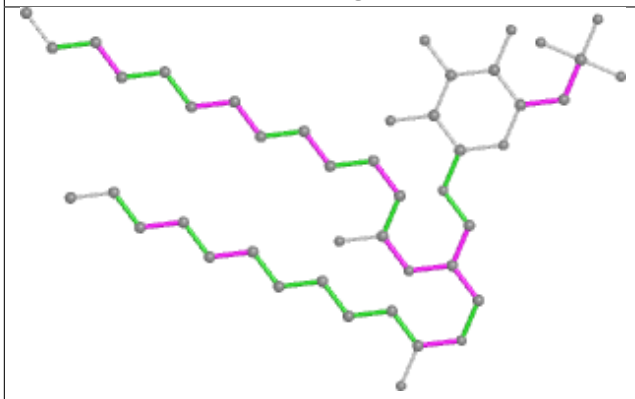
## Ligand SQD G 5001



Bond lengths



Bond angles



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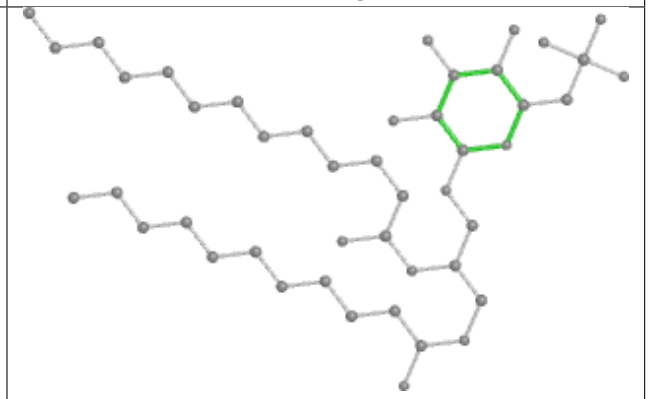
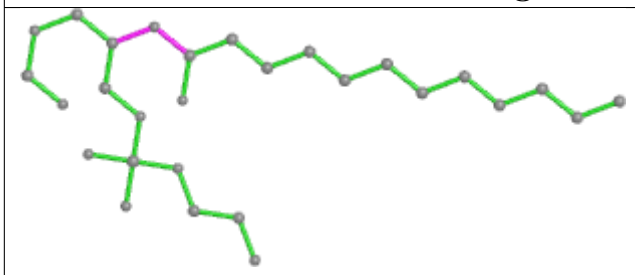
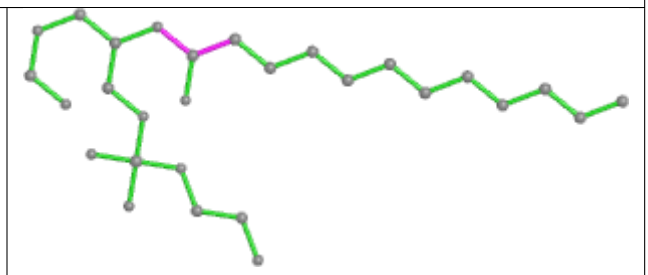


Rings

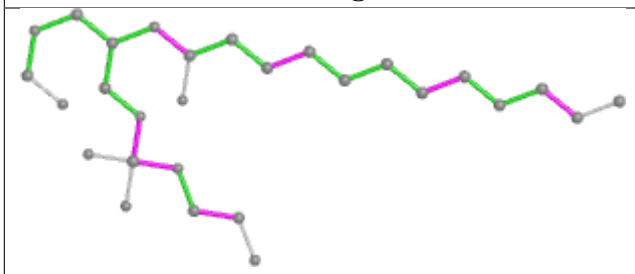
## Ligand PTY G 5002



Bond lengths



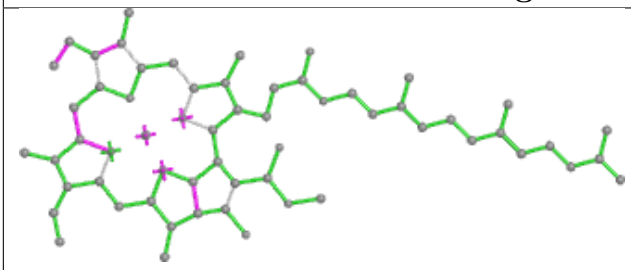
Bond angles



Torsions

Rings

## Ligand CLA B 1207



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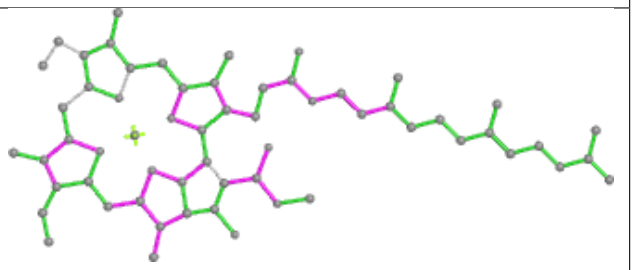
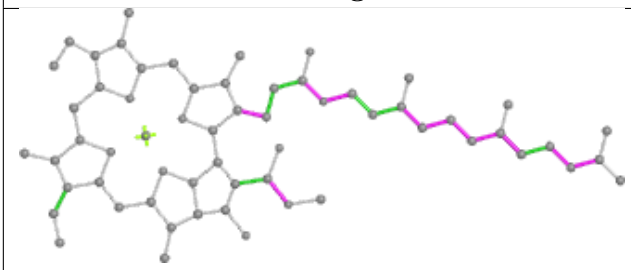
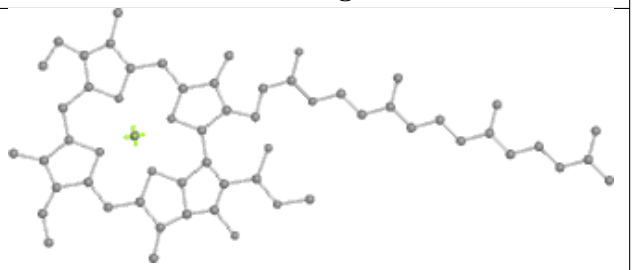


Bond angles

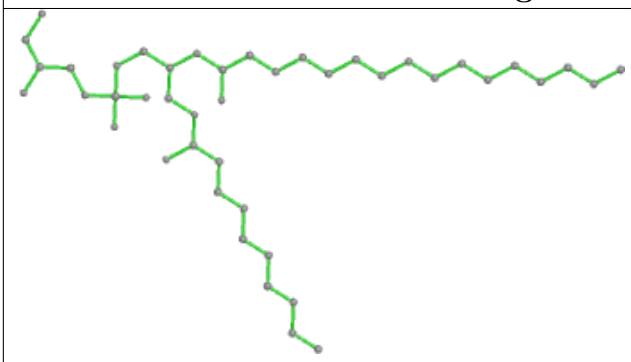


Torsions

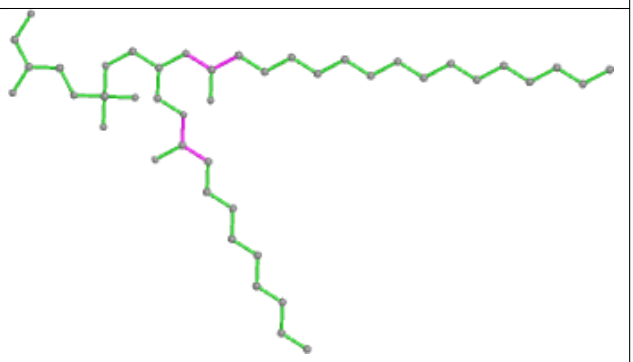


Rings

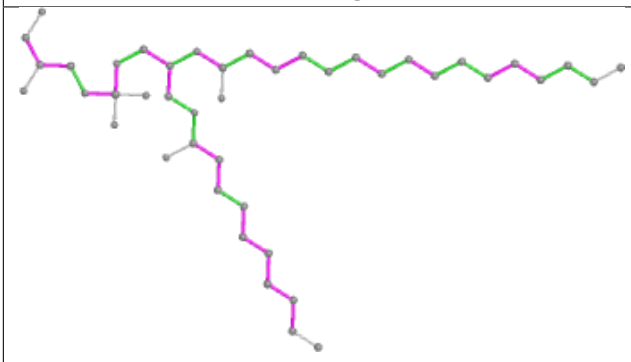
## Ligand LHG F 5001



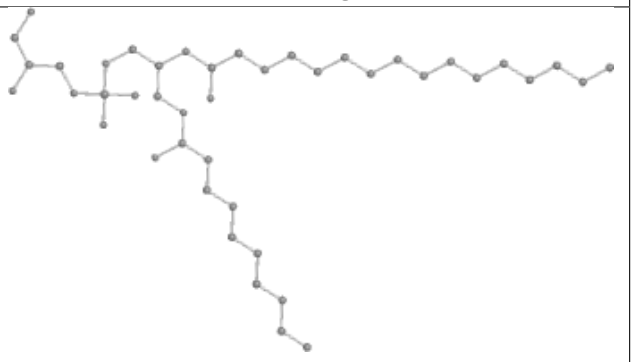
Bond lengths



Bond angles

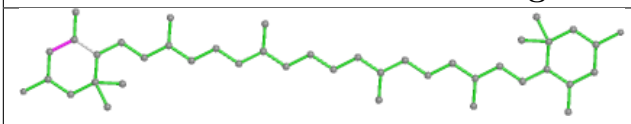


Torsions



Rings

## Ligand LUT 2 507



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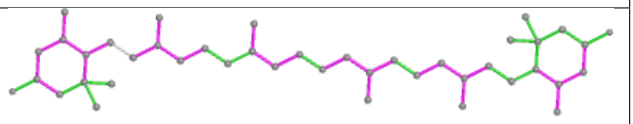
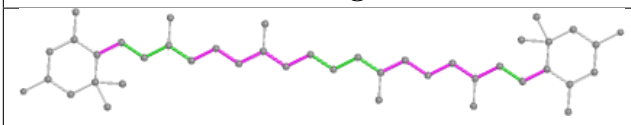


Bond angles



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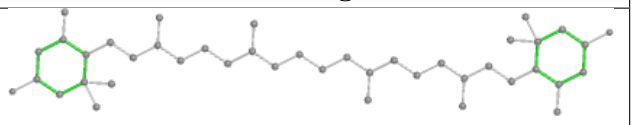
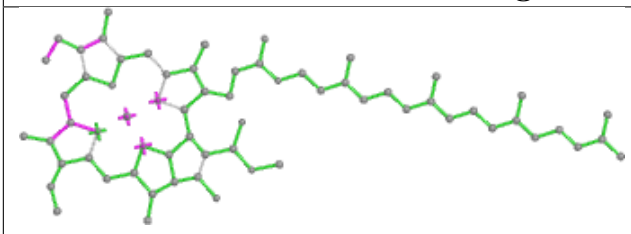


Rings

## Ligand CLA A 1013



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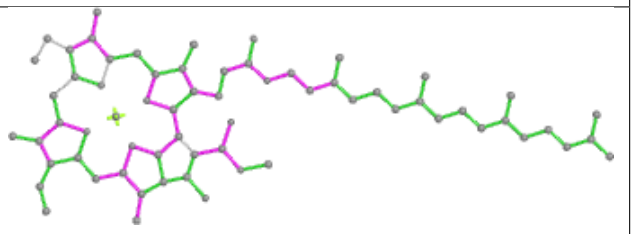
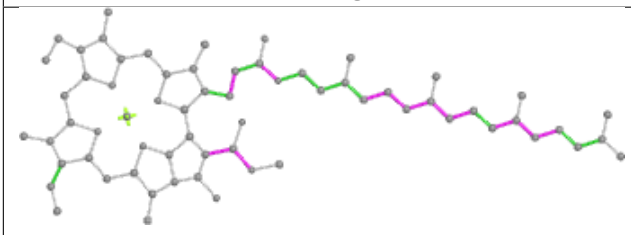


Bond angles



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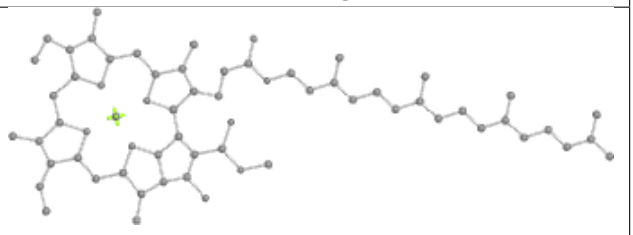
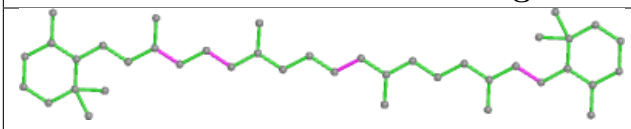


Rings

## Ligand BCR A 4005



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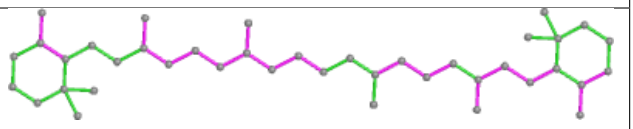
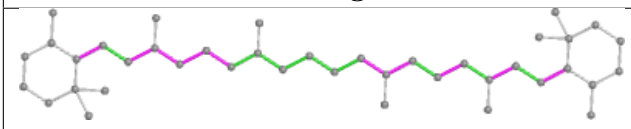
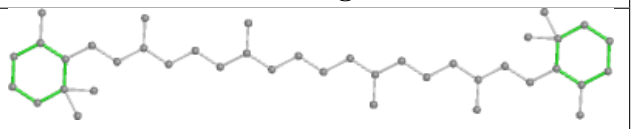


Bond angles

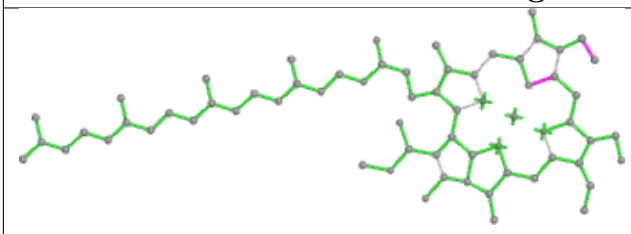


Torsions

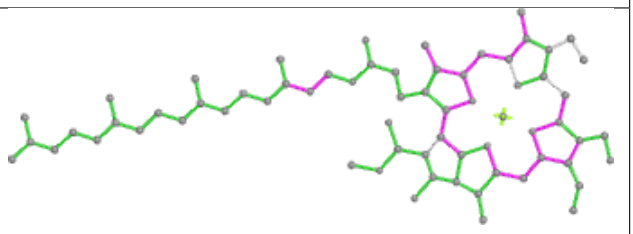


Rings

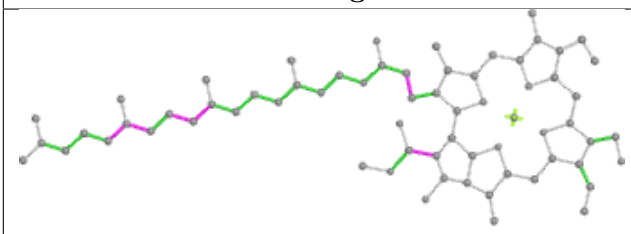
## Ligand CHL 6 609



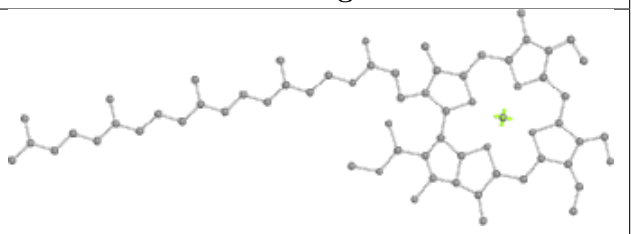
Bond lengths



Bond angles

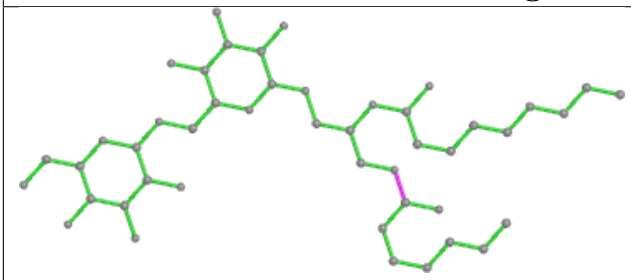


Torsions



Rings

## Ligand DGD 8 803



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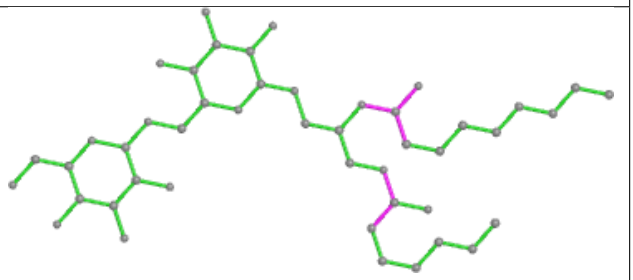
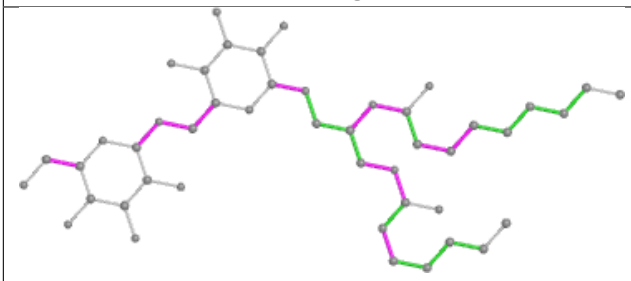
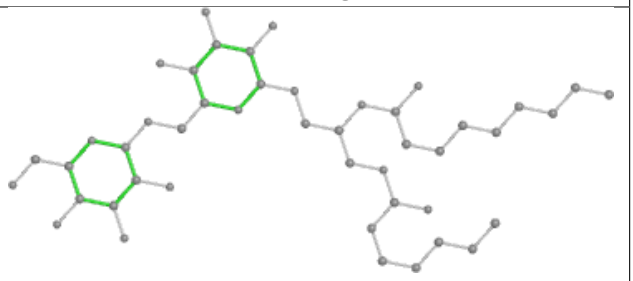


Bond angles

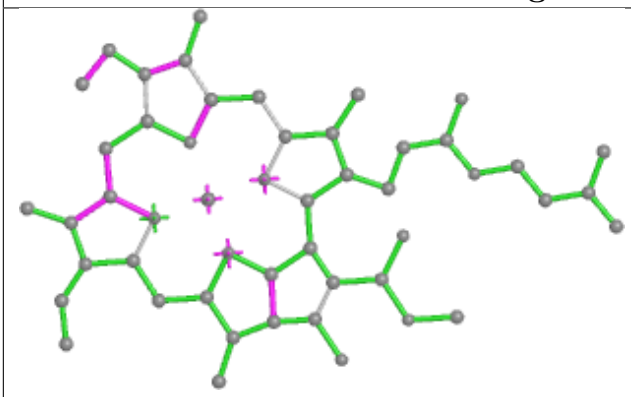


Torsions

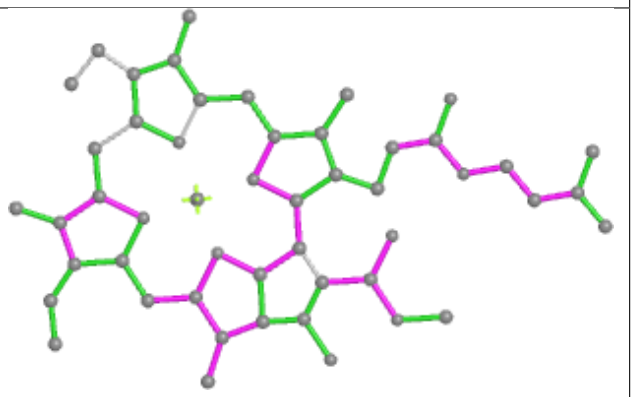


Rings

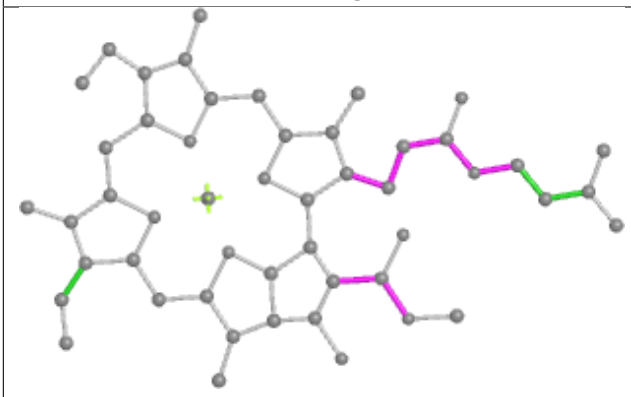
**Ligand CLA 2 612**



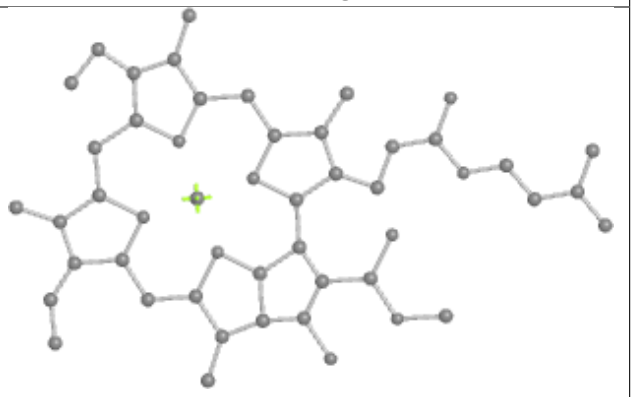
**Bond lengths**



**Bond angles**

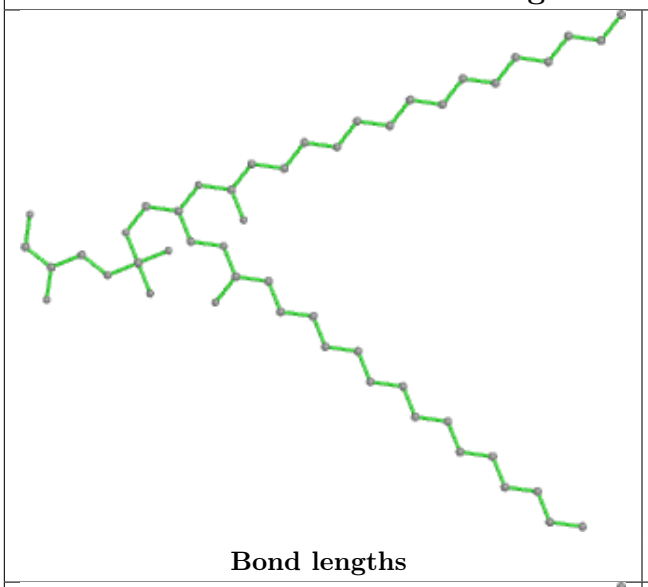


**Torsions**



**Rings**

**Ligand LHG 2 801**



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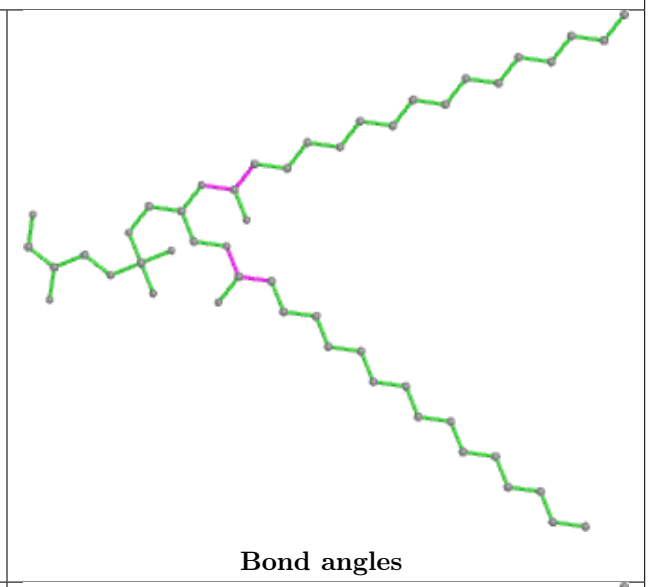

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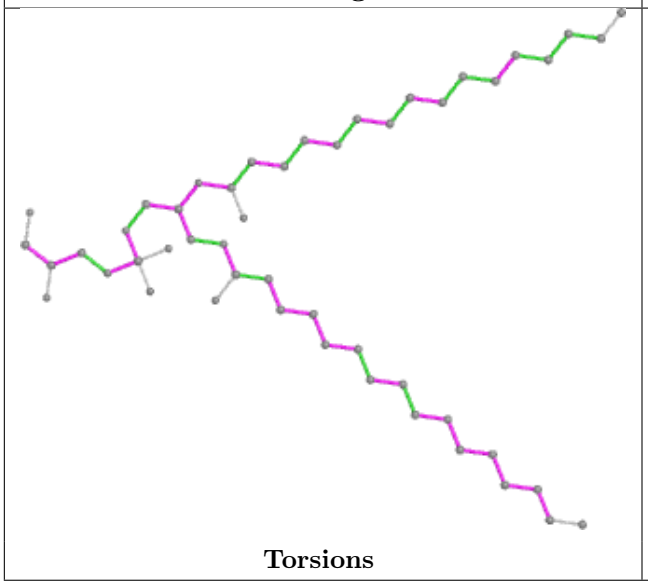

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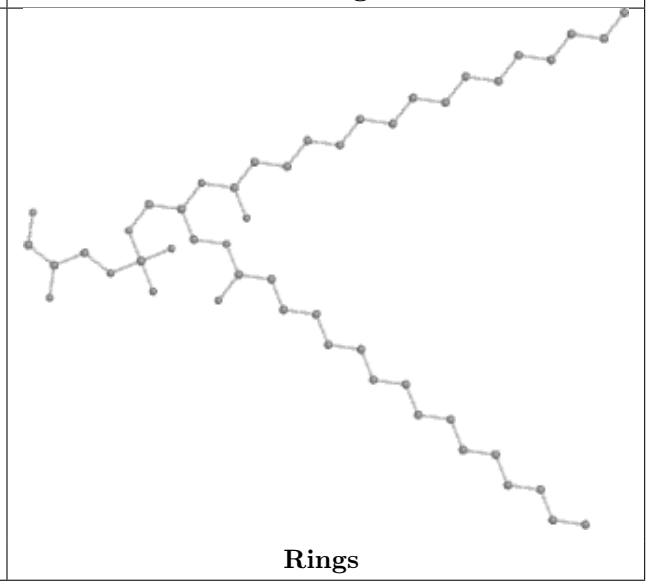
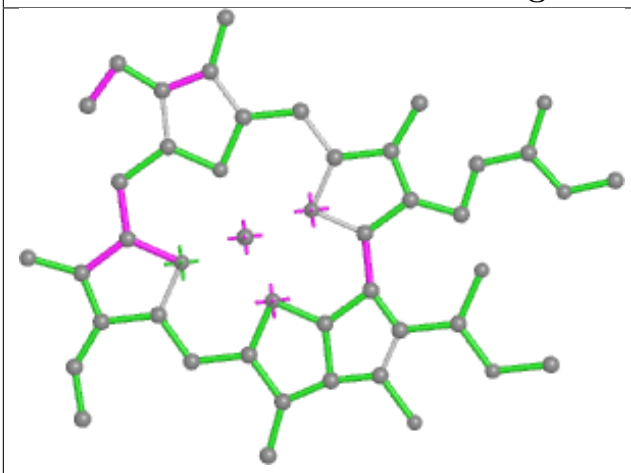
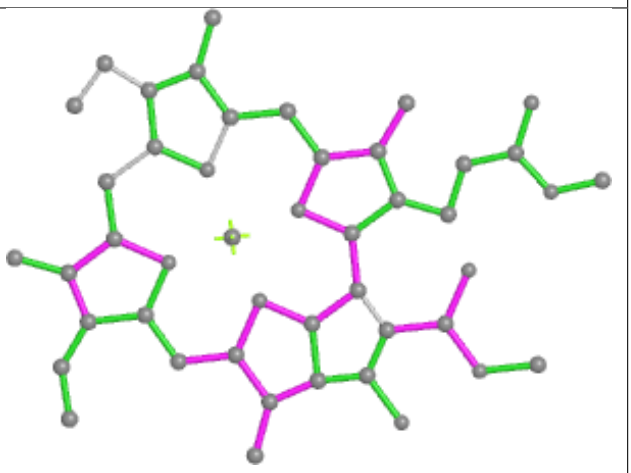


**Rings**

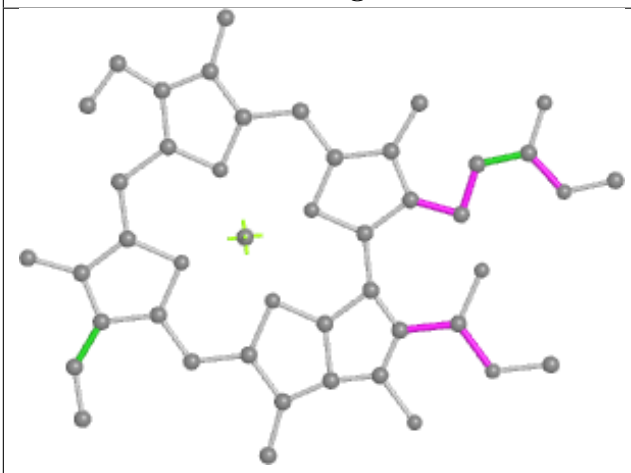
## Ligand CLA 8 615



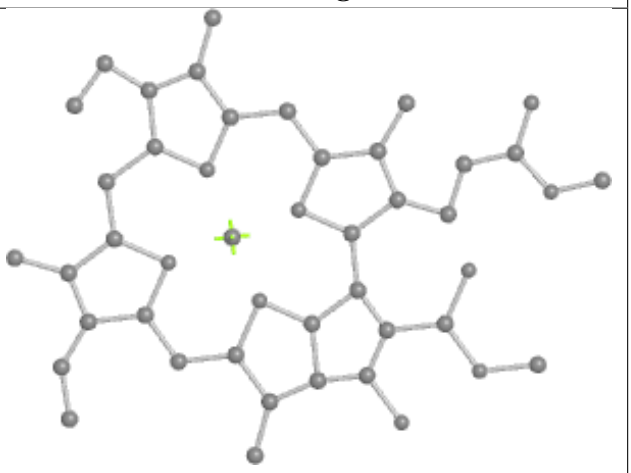
Bond lengths



Bond angles

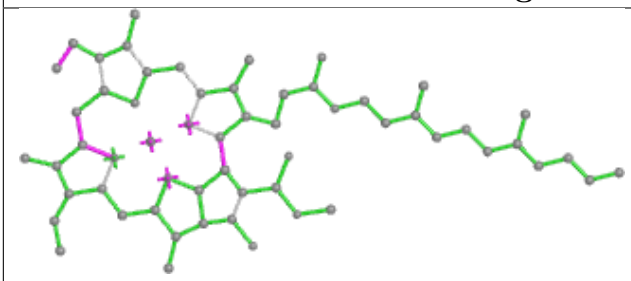


Torsions



Rings

## Ligand CLA B 1230



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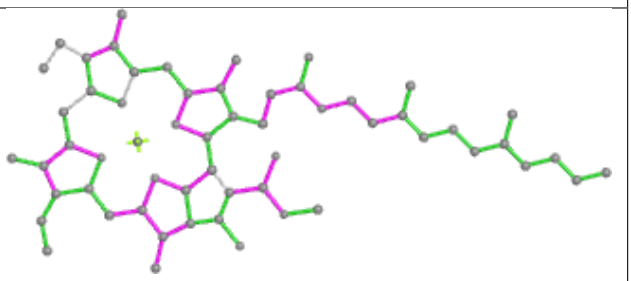
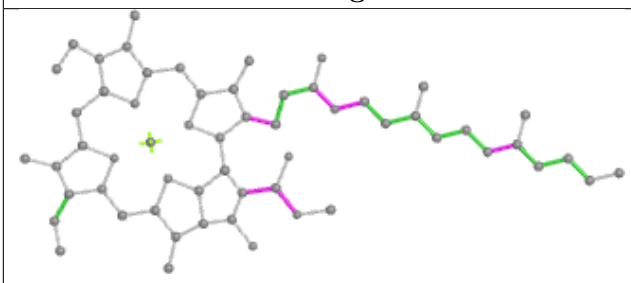


Bond angles



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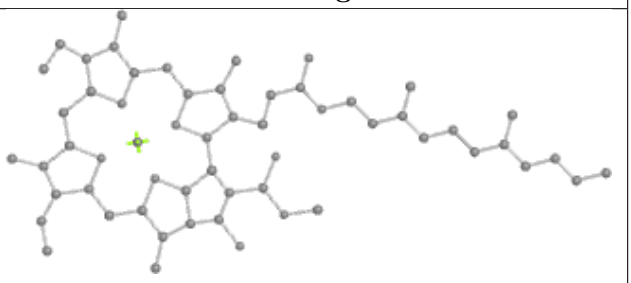
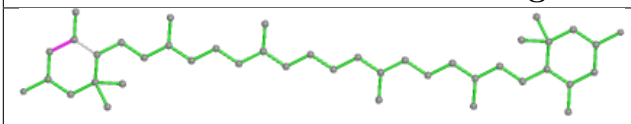


Rings

## Ligand LUT 8 501



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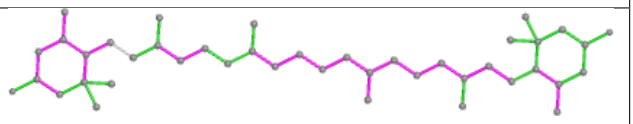
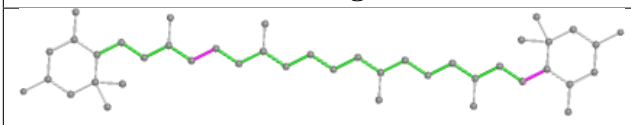


Bond angles



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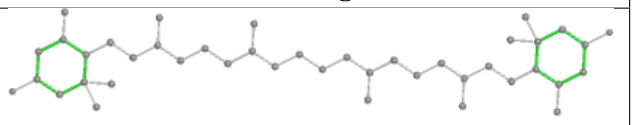
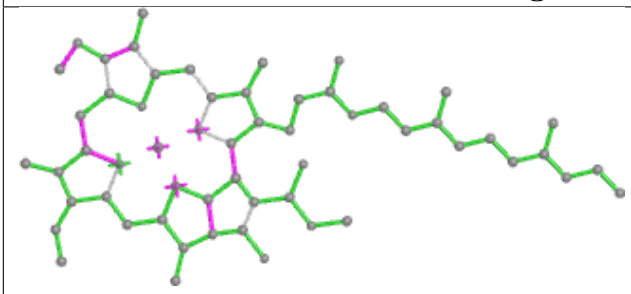


Rings

## Ligand CLA 3 610



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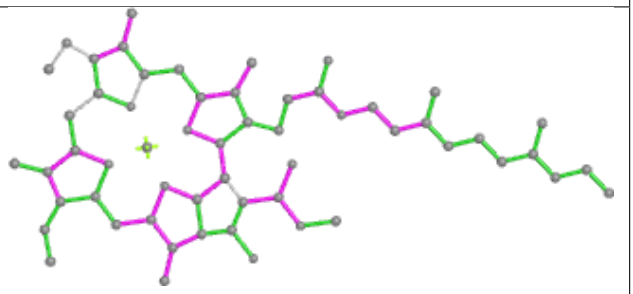
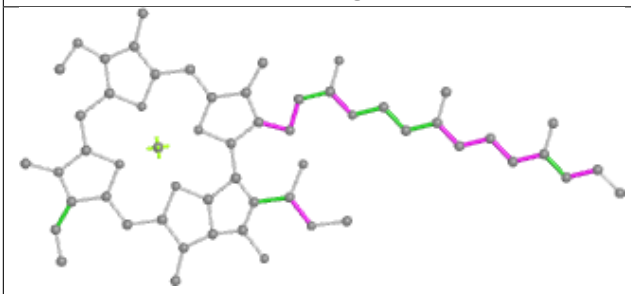


Bond angles



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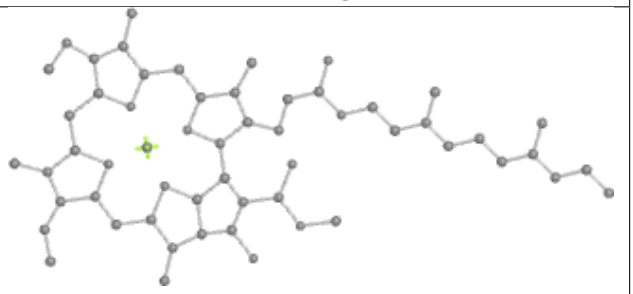
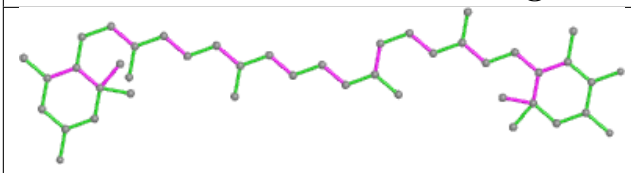
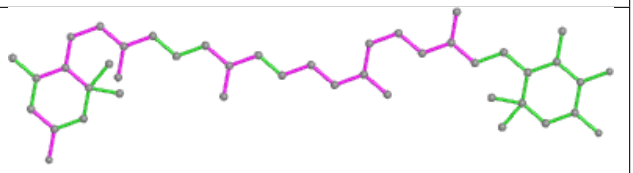


Rings

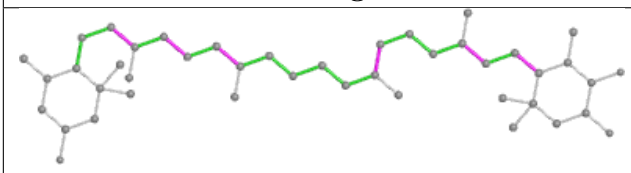
## Ligand AXT 1 502



Bond lengths



Bond angles



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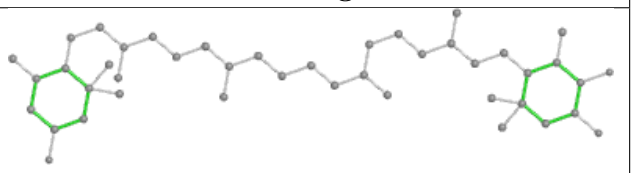

Rings

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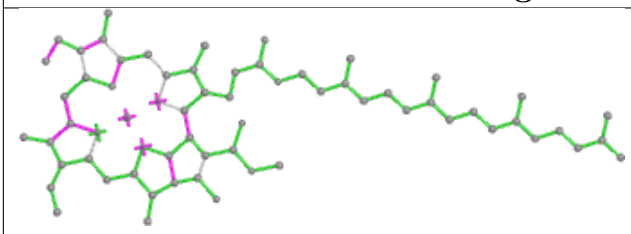

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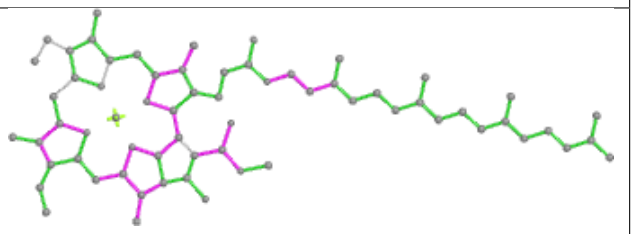
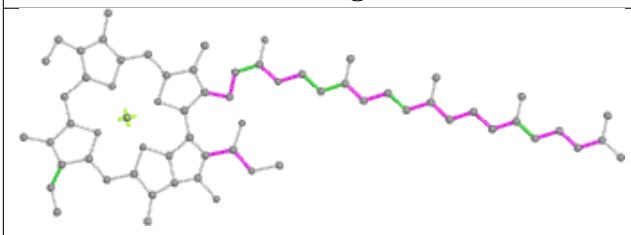
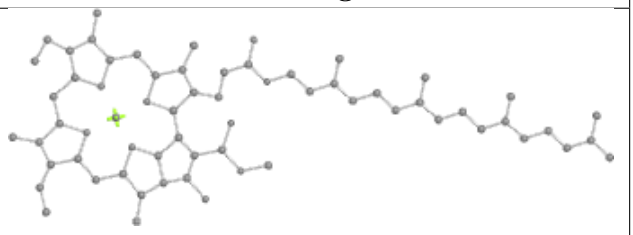


Bond angles

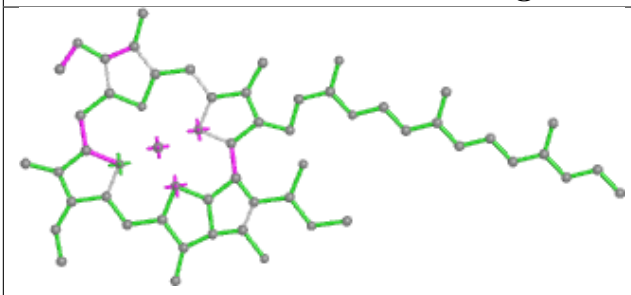


Torsions



Rings

## Ligand CLA B 1212



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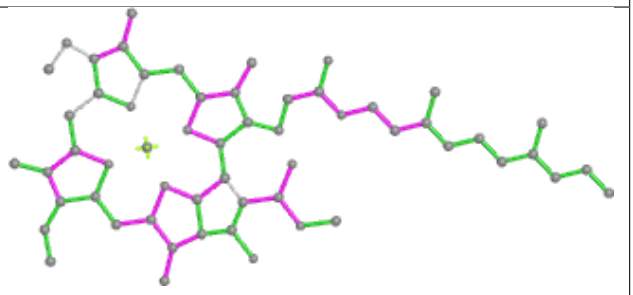
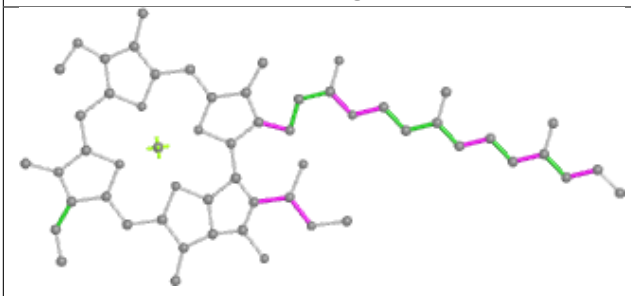


Bond angles



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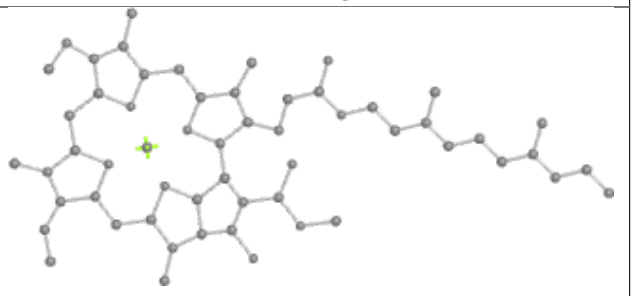
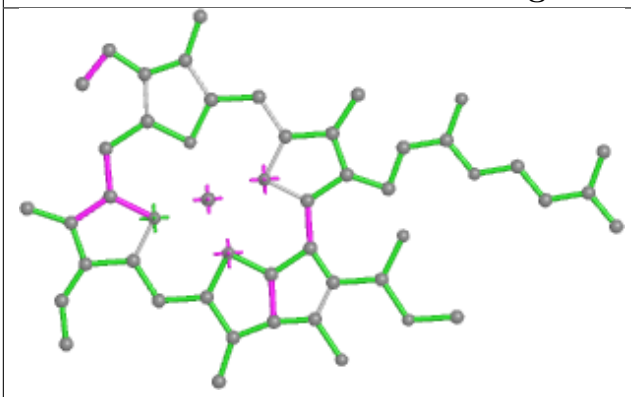


Rings

## Ligand CLA 4 606



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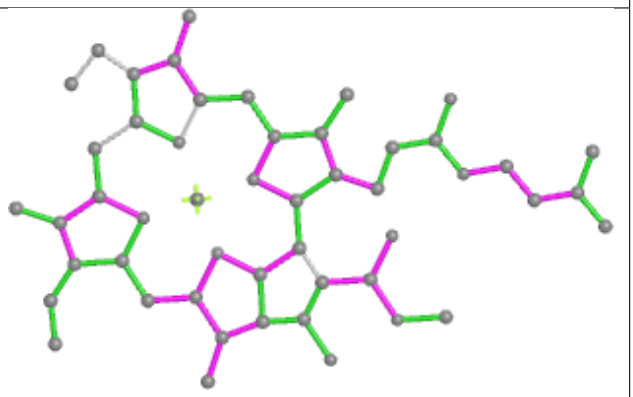
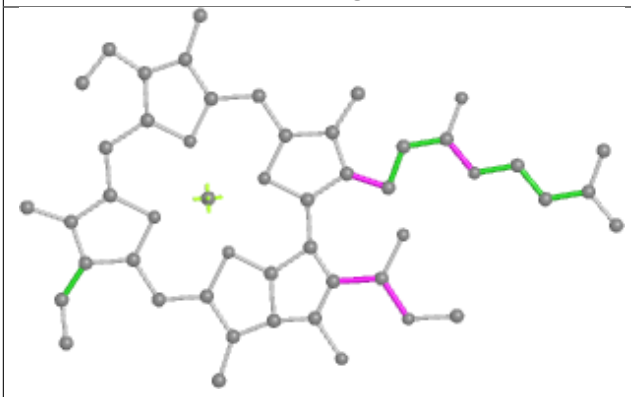


Bond angles



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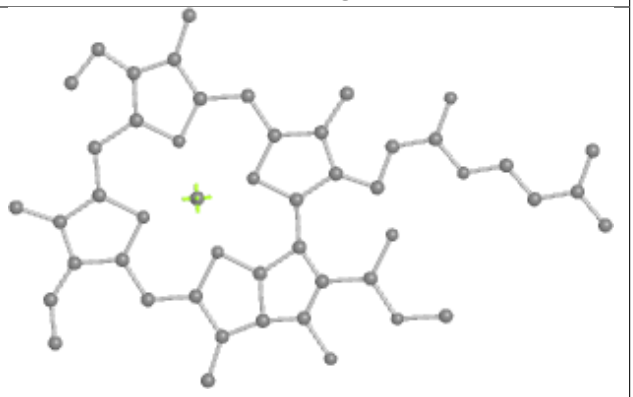
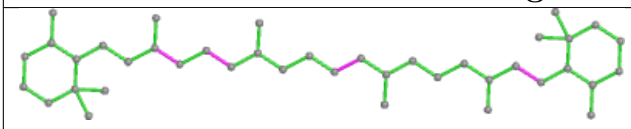


Rings

## Ligand BCR 3 505



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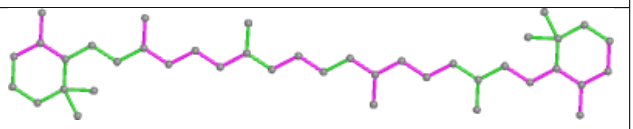
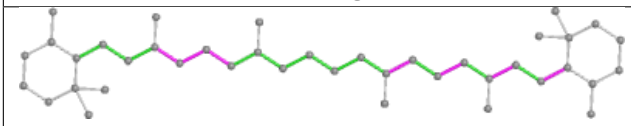


Bond angles



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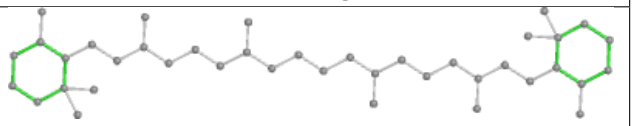
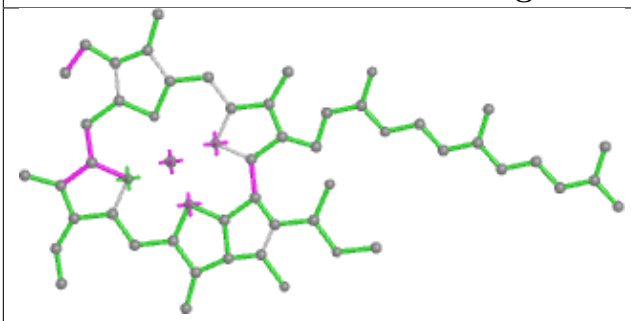


Rings

## Ligand CLA B 1213



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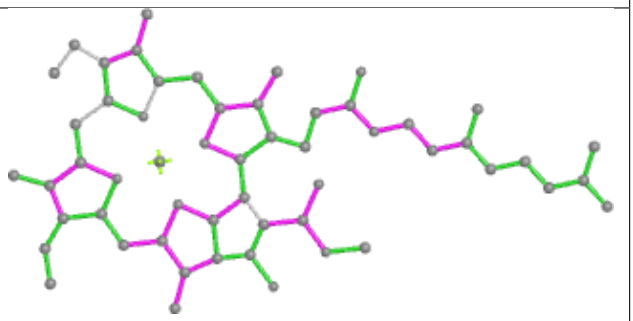
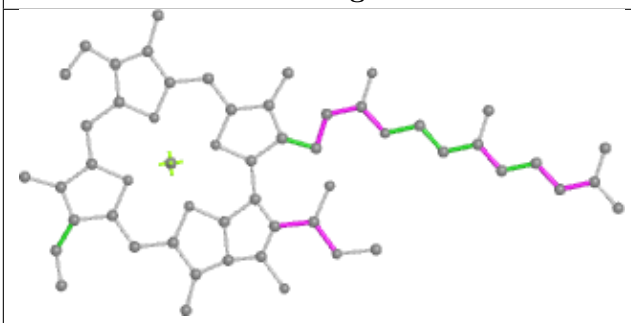


Bond angles



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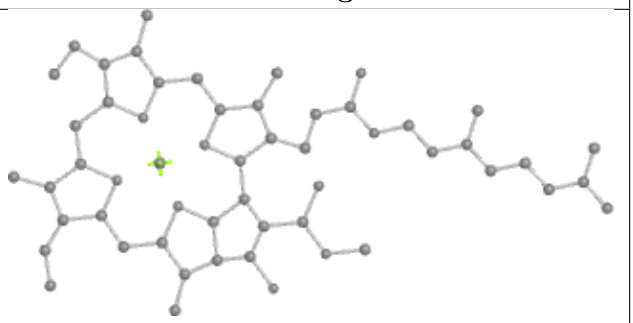
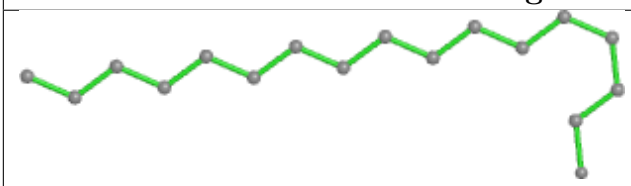


Rings

## Ligand PLM 8 806



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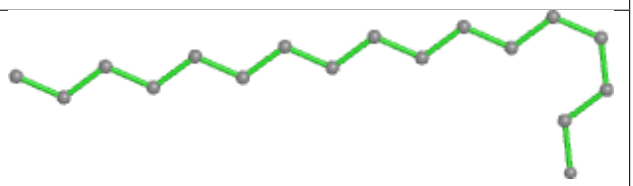
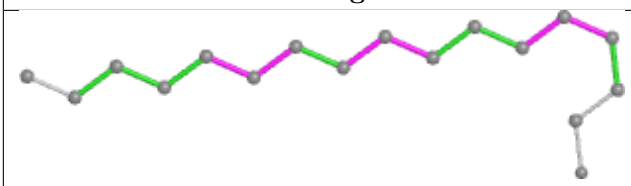


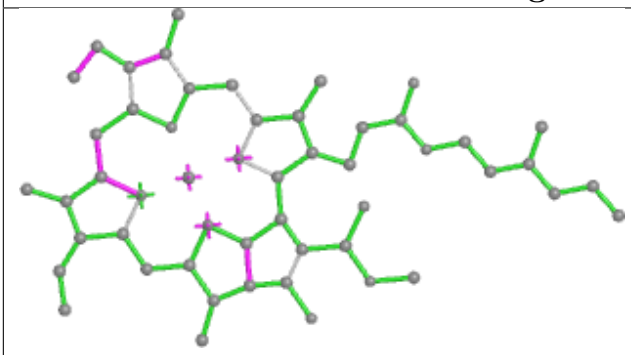
Bond angles



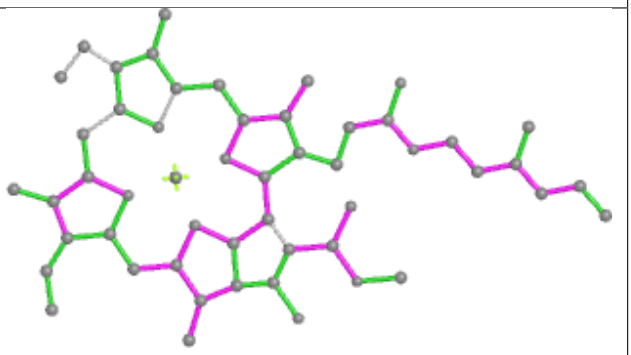
Torsions

Rings

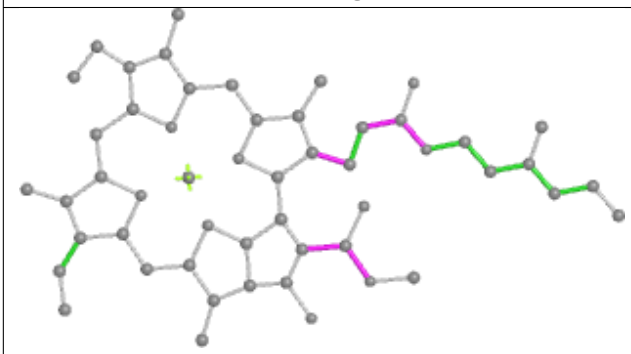
## Ligand CLA 8 608



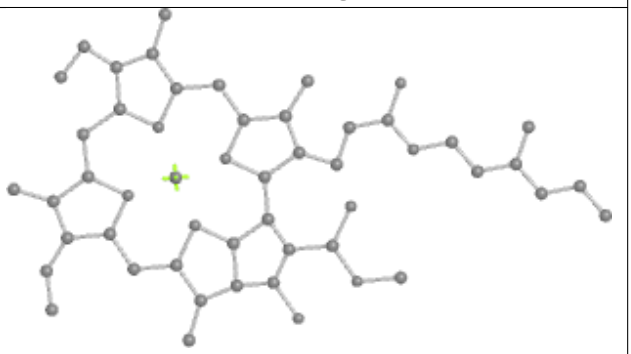
Bond lengths



Bond angles

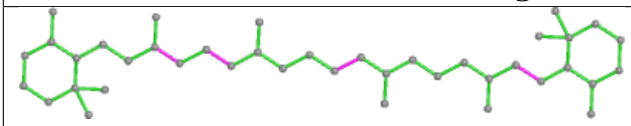


Torsions

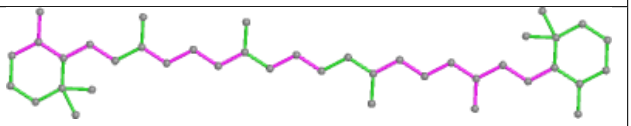


Rings

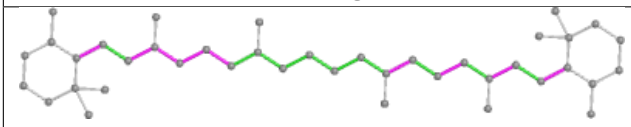
## Ligand BCR B 4005



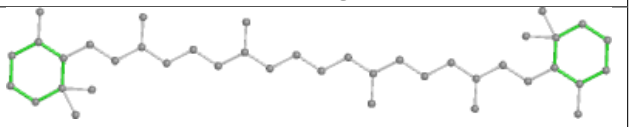
Bond lengths



Bond angles

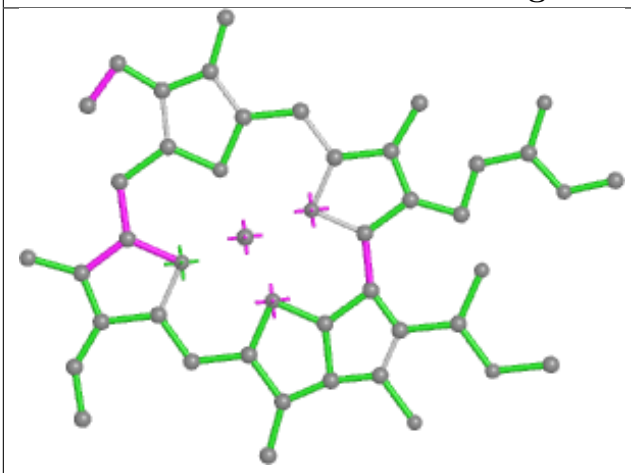


Torsions

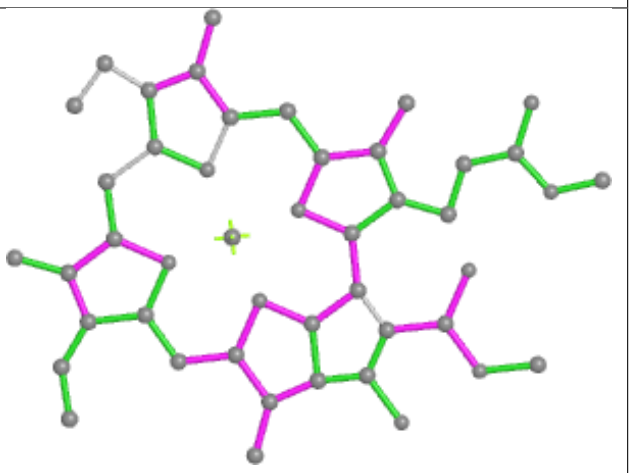


Rings

## Ligand CLA 1 615



Bond lengths



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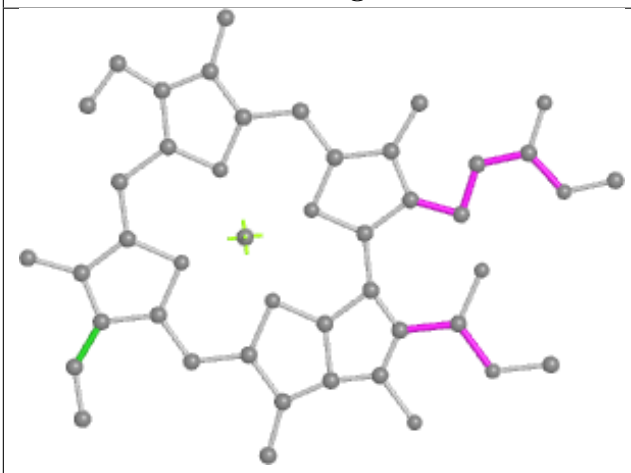
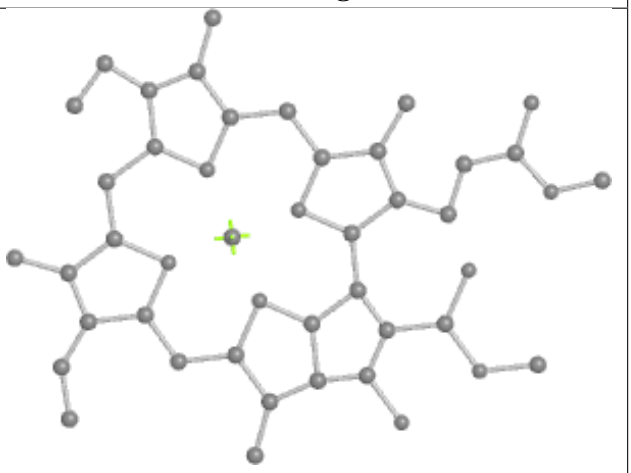
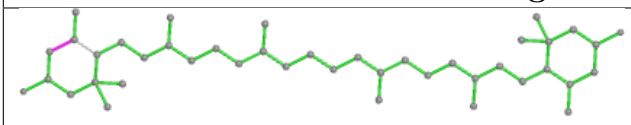


Torsions



Rings

## Ligand LUT 1 501



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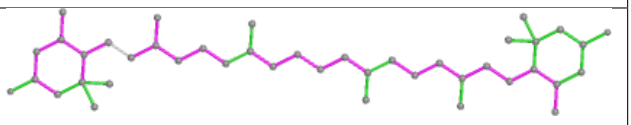
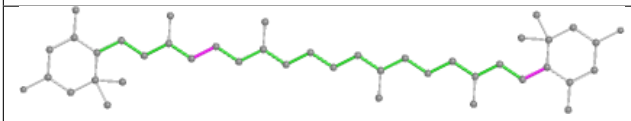


Bond angles



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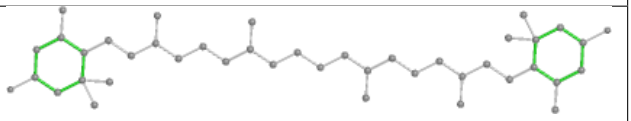
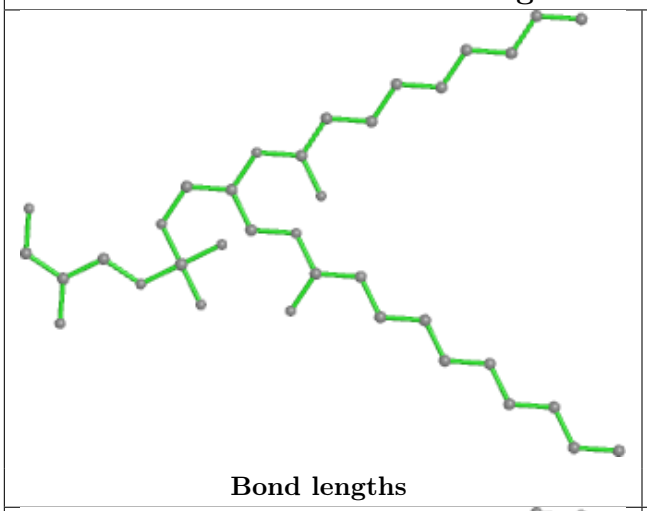


Rings

## Ligand LHG F 5002



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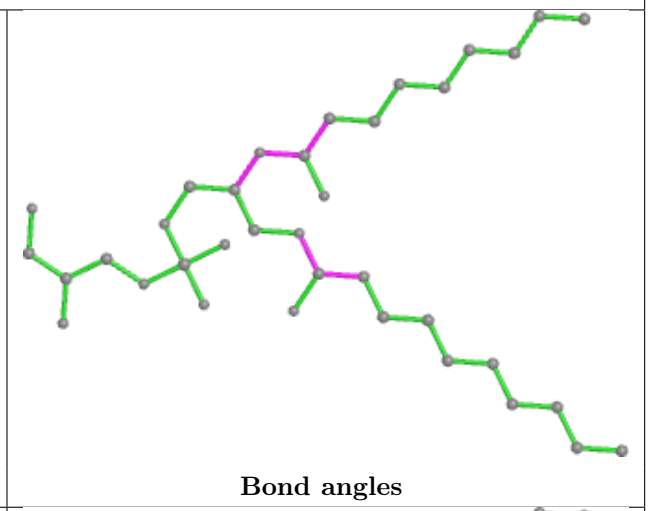
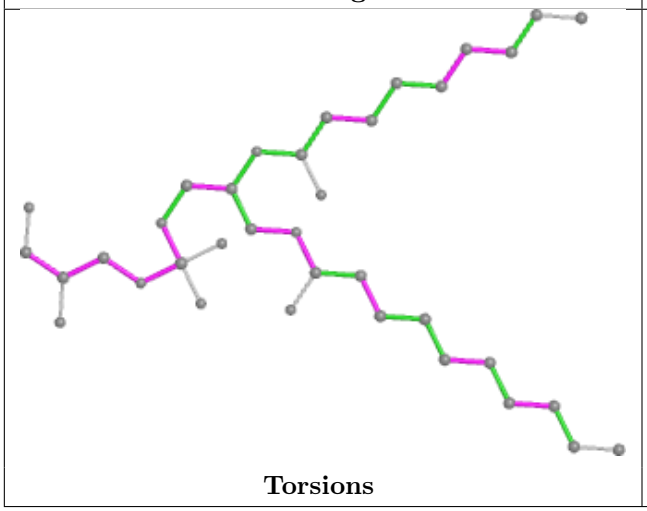


Bond angles



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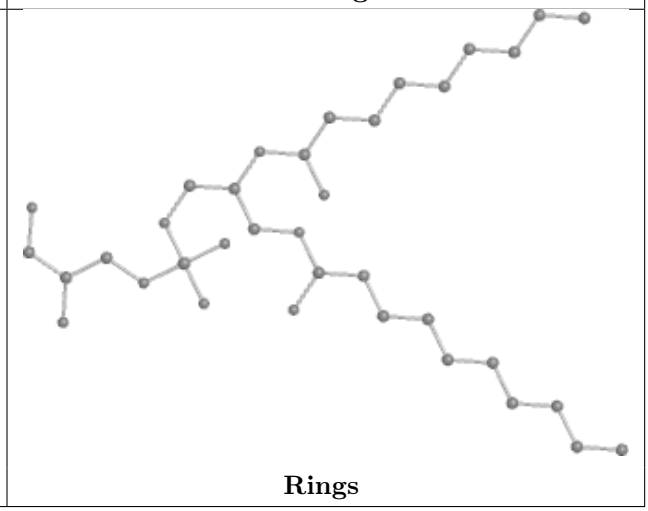
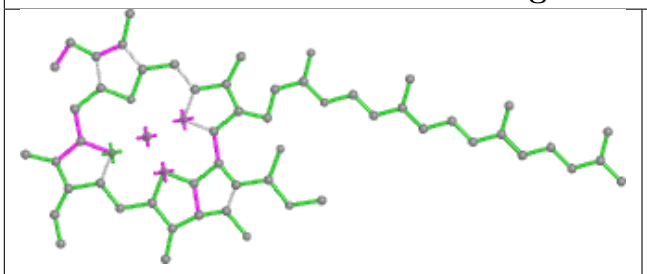


Rings

## Ligand CLA 1 608



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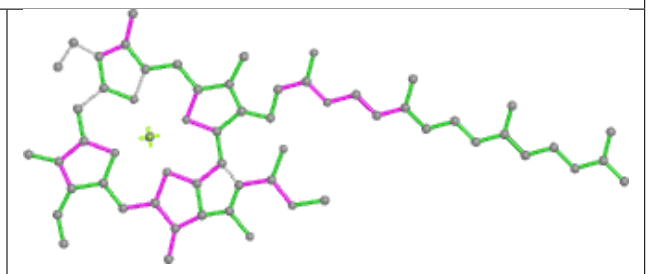
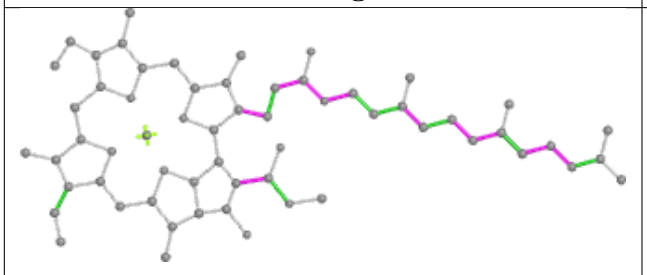


Bond angles



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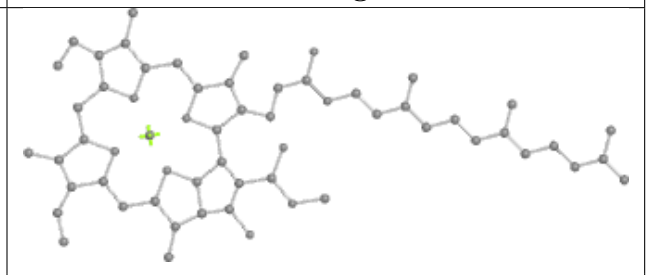
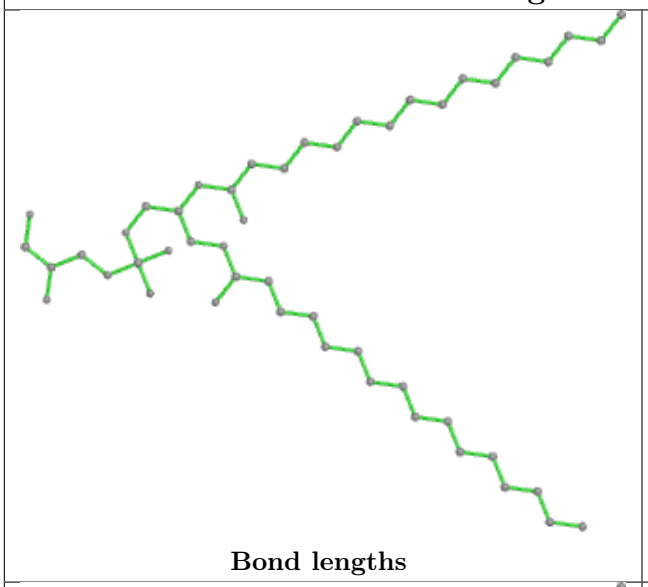
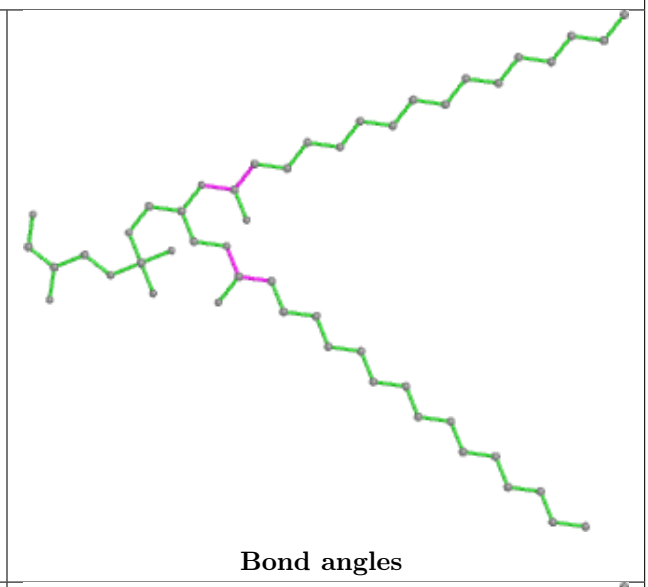


Rings

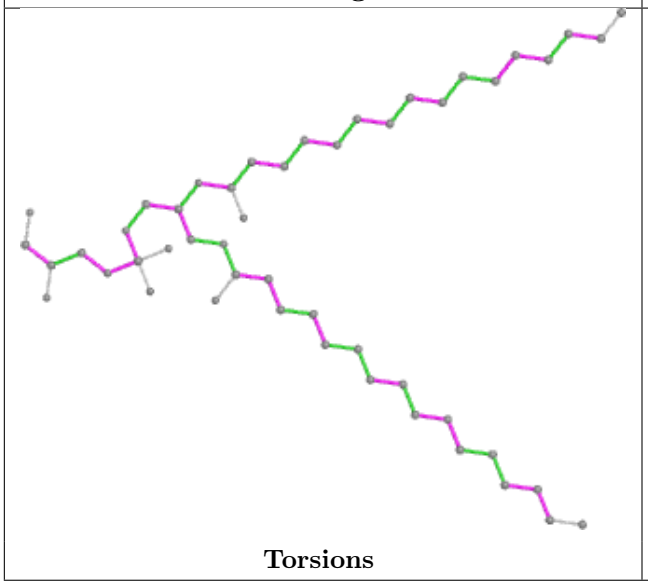
**Ligand LHG 4 801**



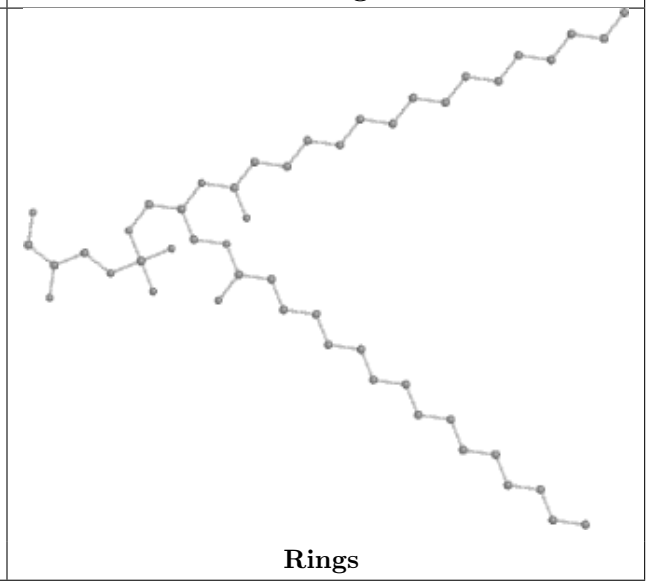
**Bond lengths**



**Bond angles**

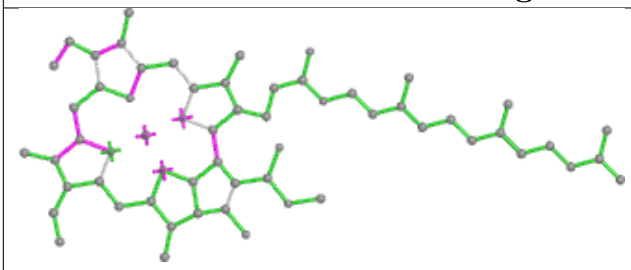


**Torsions**

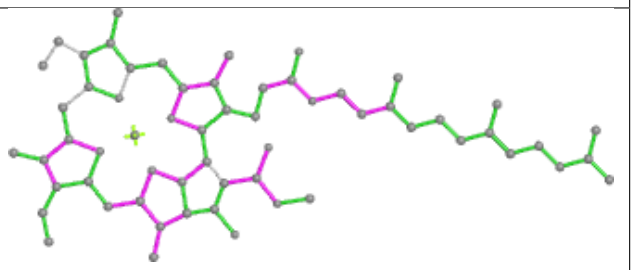


**Rings**

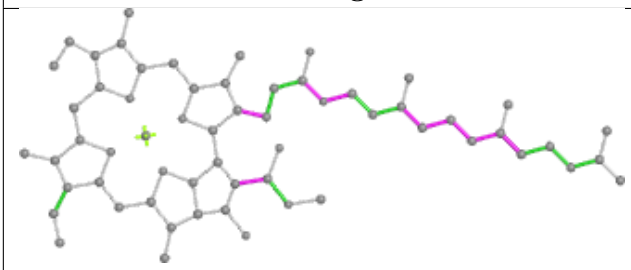
## Ligand CLA B 1220



Bond lengths



Bond angles



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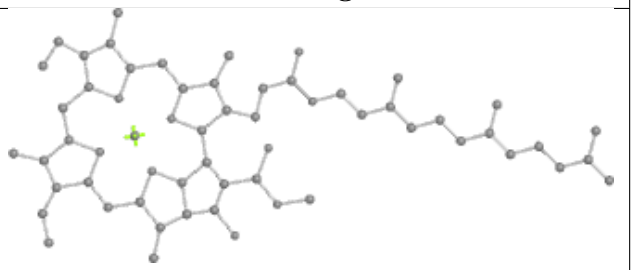
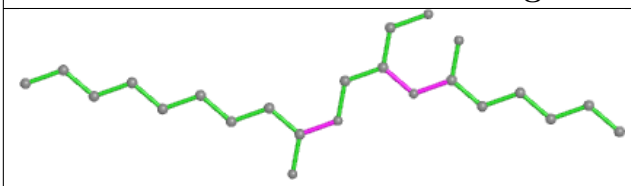


Rings

## Ligand DGA 5 803



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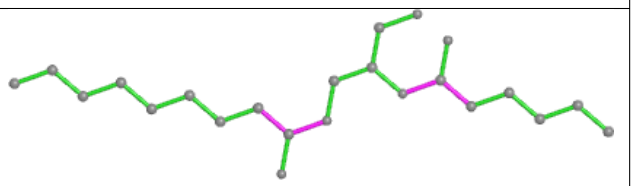
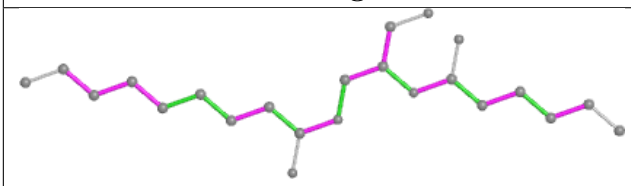
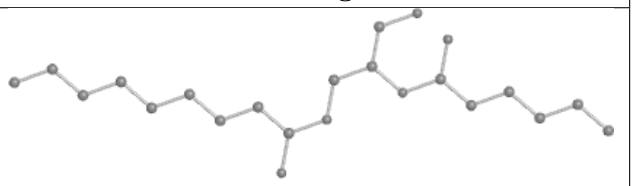


Bond angles

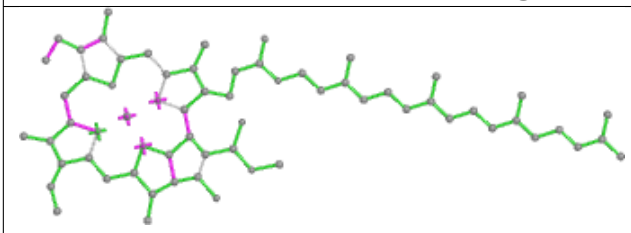


Torsions



Rings

## Ligand CLA A 1128



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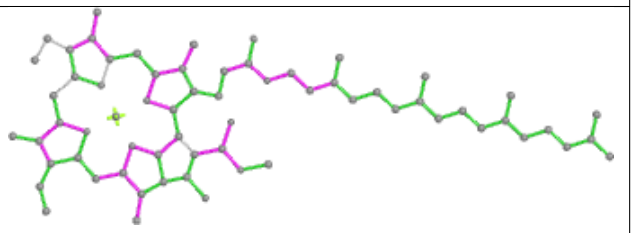
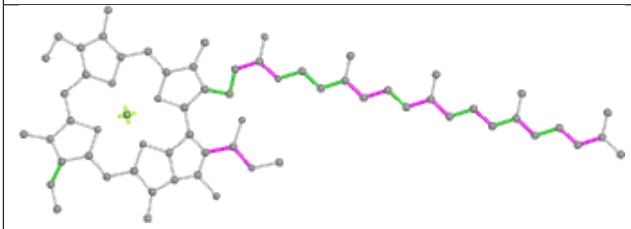
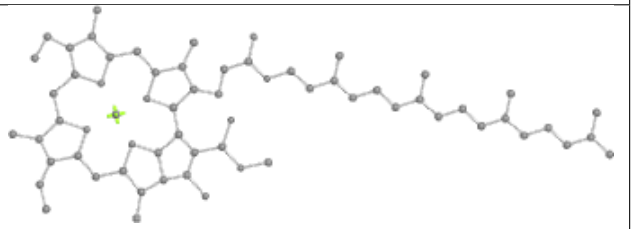


Bond angles

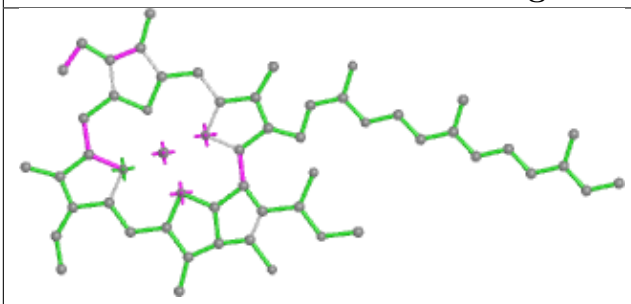


Torsions



Rings

## Ligand CLA 4 611



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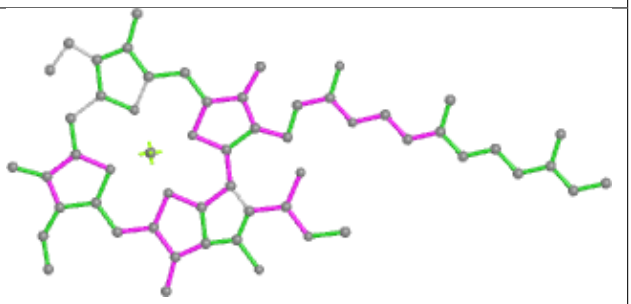
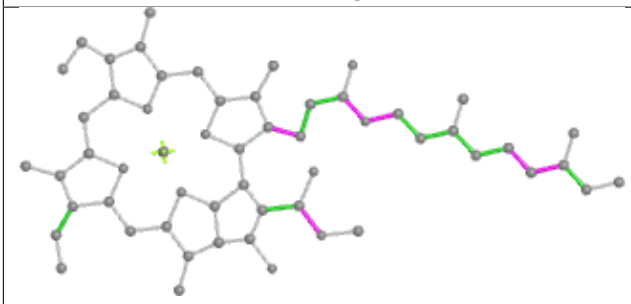


Bond angles



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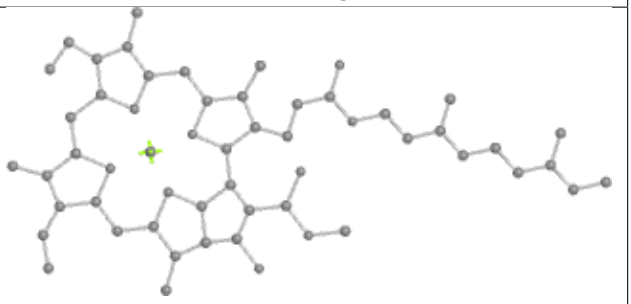
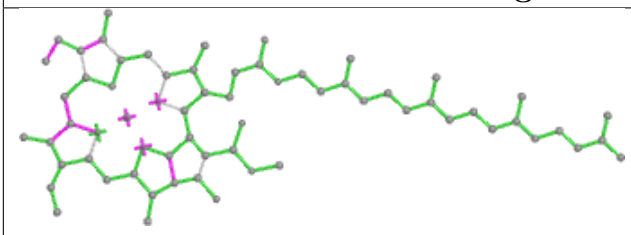


Rings

## Ligand CLA A 1012



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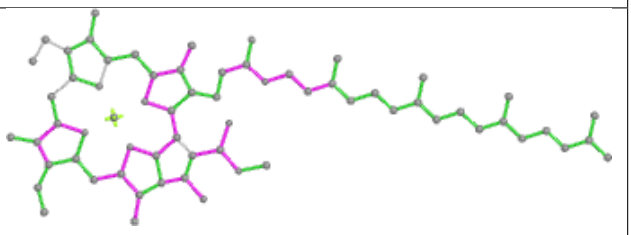
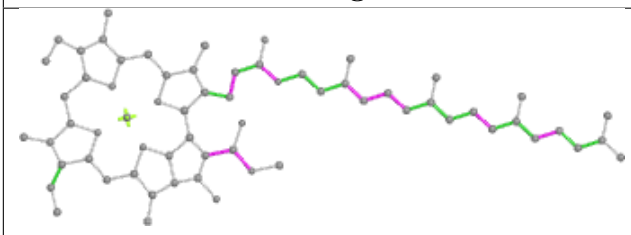


Bond angles



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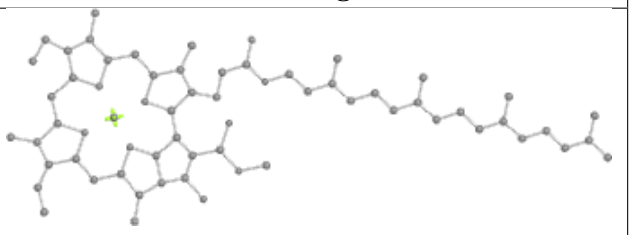
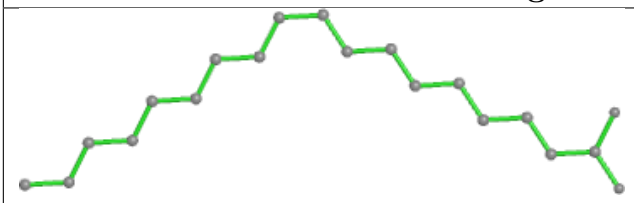
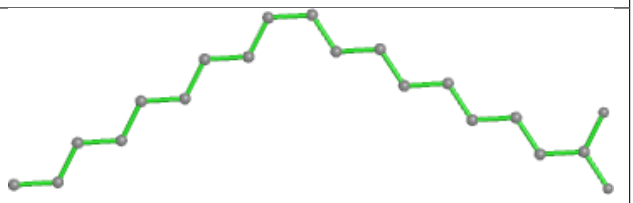


Rings

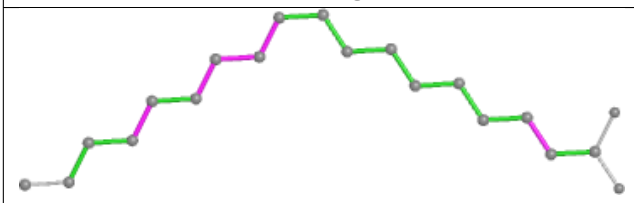
## Ligand OLA 8 808



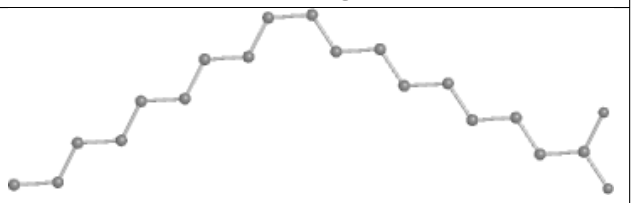
Bond lengths



Bond angles

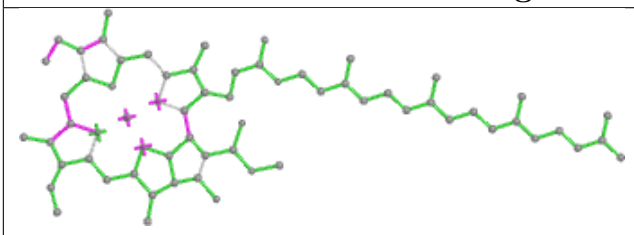


Torsions

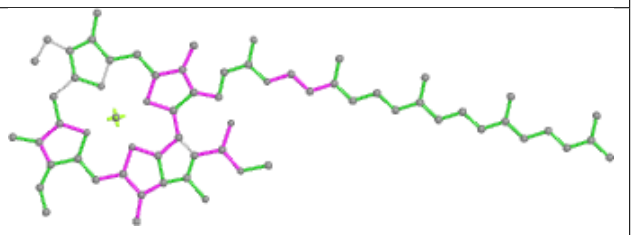


Rings

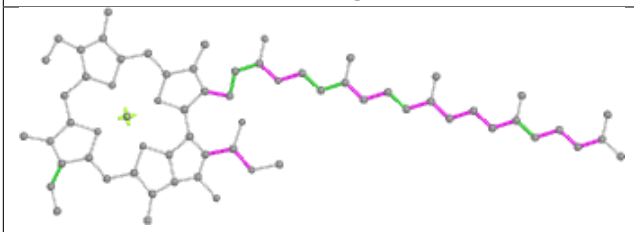
## Ligand CLA A 1101



Bond lengths



Bond angles



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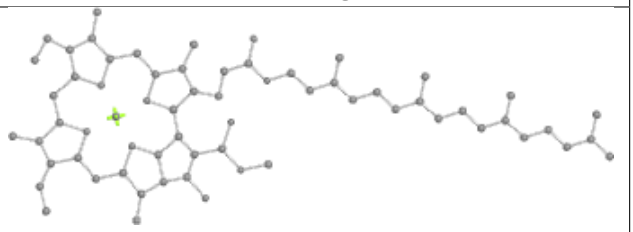
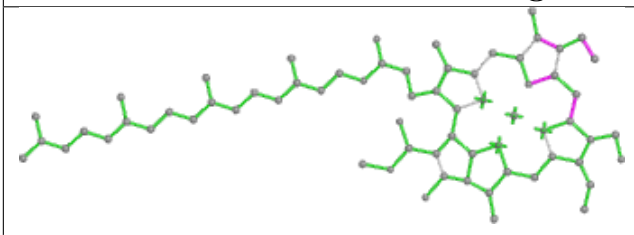
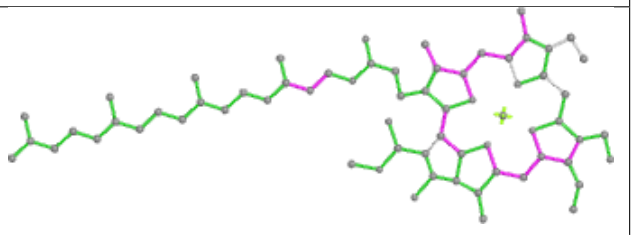


Rings

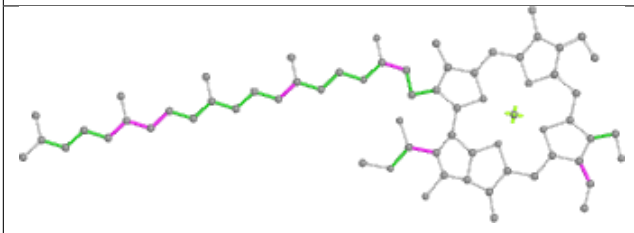
## Ligand CHL 2 609



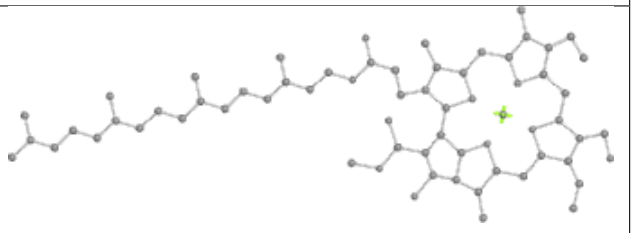
Bond lengths



Bond angles

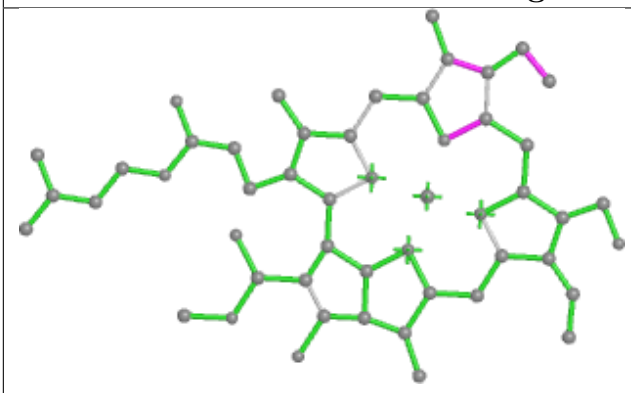


Torsions

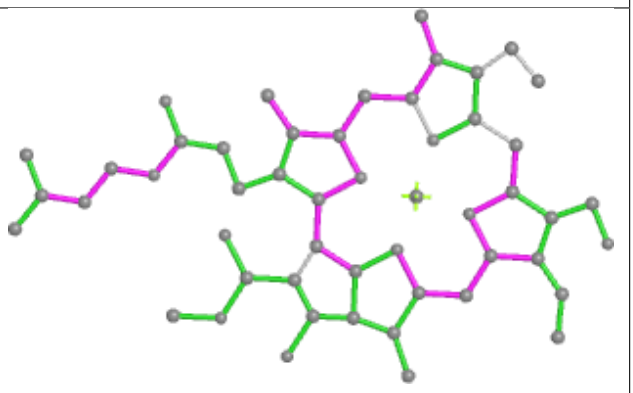


Rings

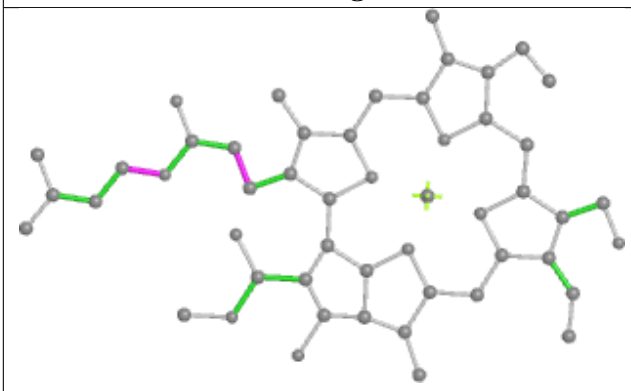
## Ligand CHL 9 610



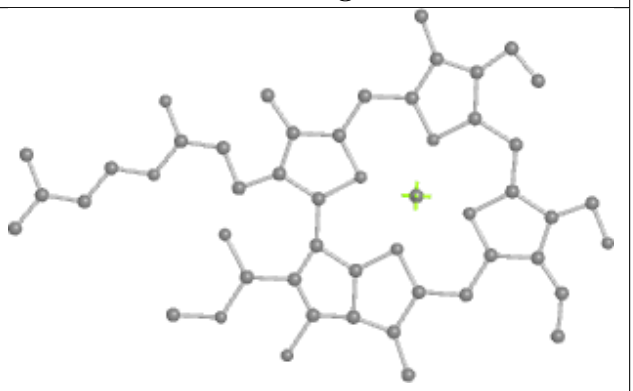
Bond lengths



Bond angles

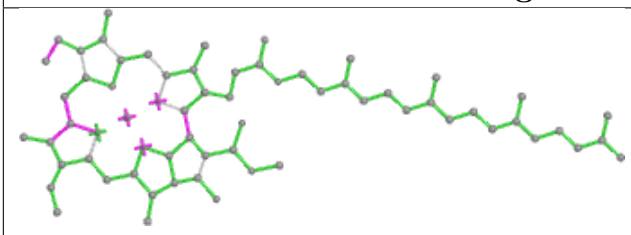


Torsions



Rings

## Ligand CLA B 1201



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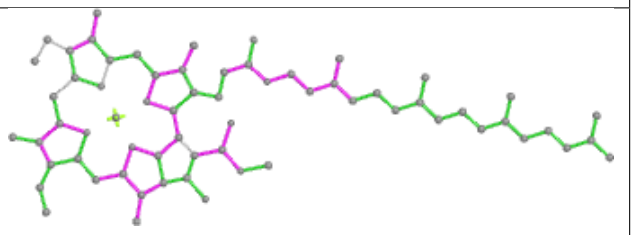
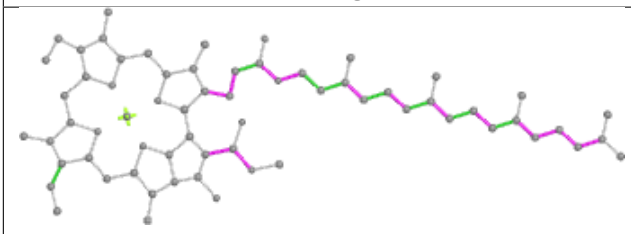
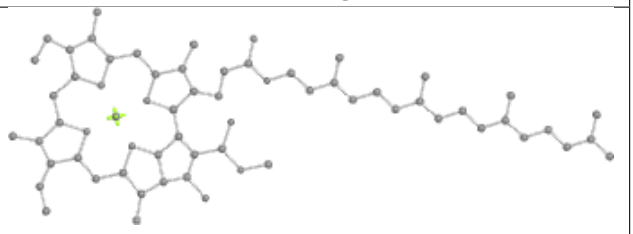


Bond angles

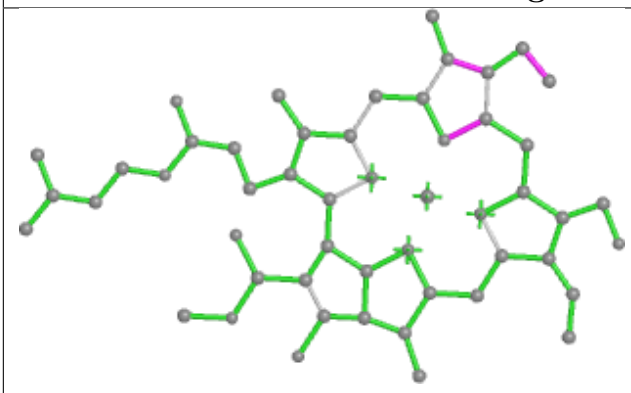


Torsions

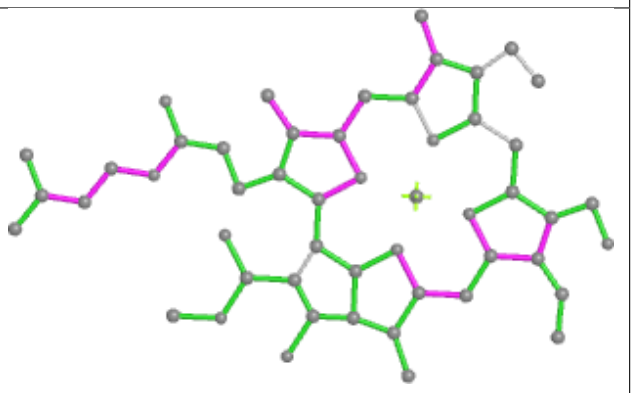


Rings

**Ligand CHL 8 613**



**Bond lengths**



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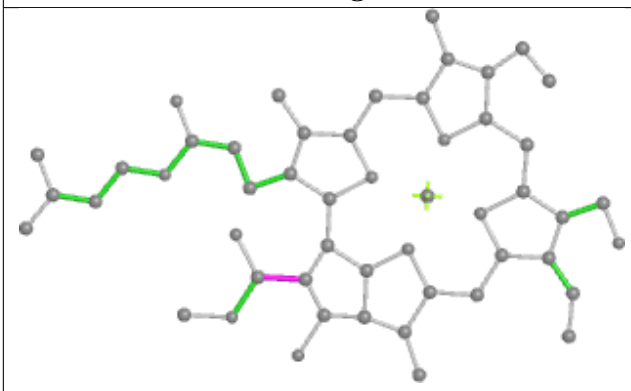

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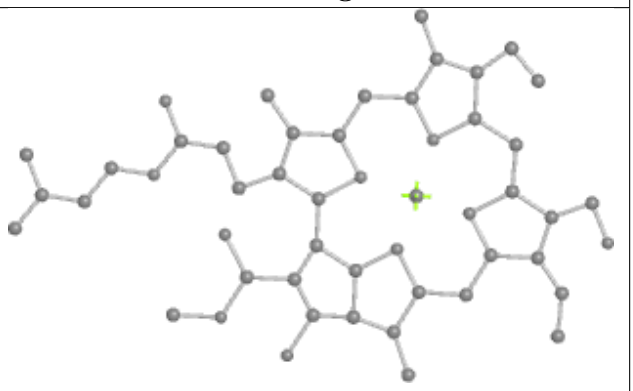
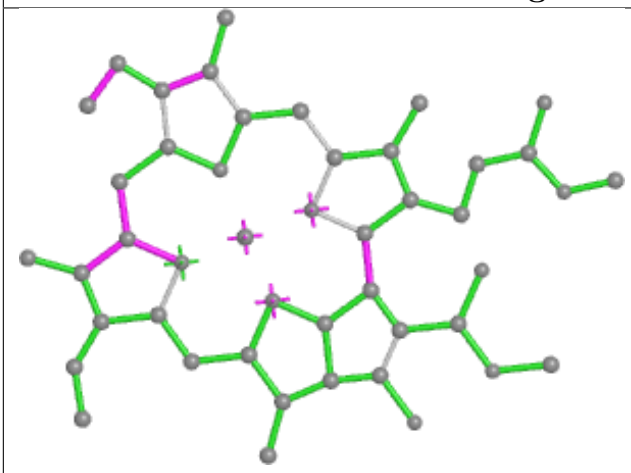
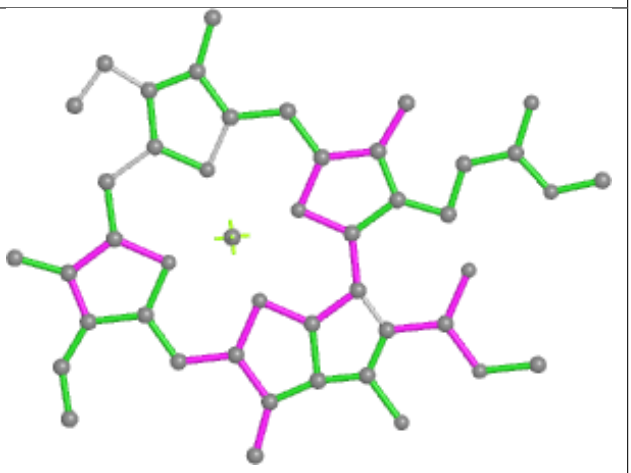


**Rings**

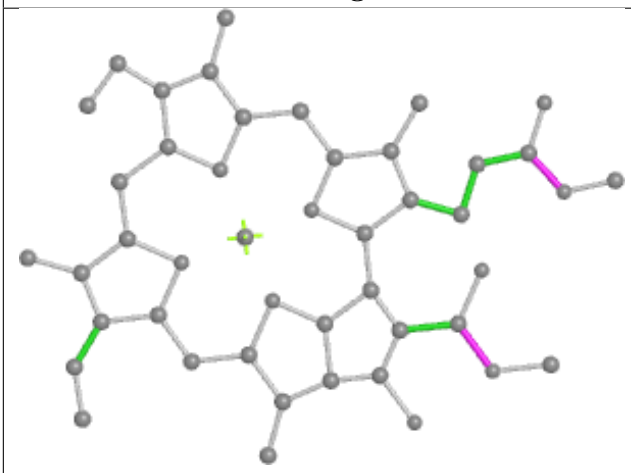
**Ligand CLA a 615**



**Bond lengths**



**Bond angles**



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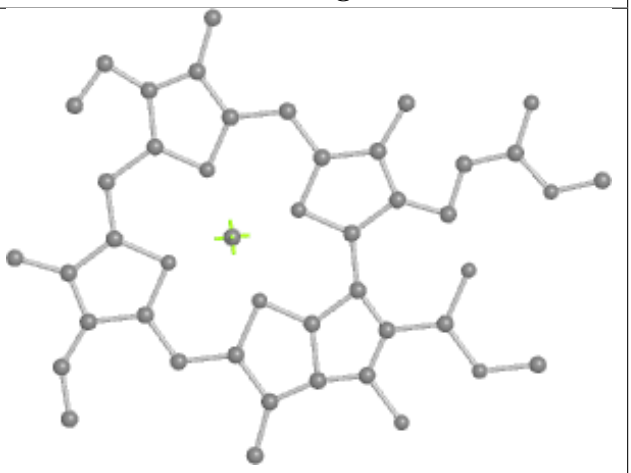
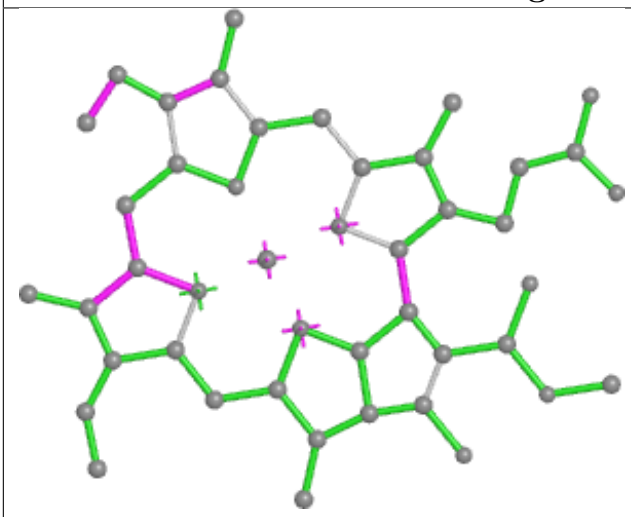


**Rings**

**Ligand CLA 5 608**



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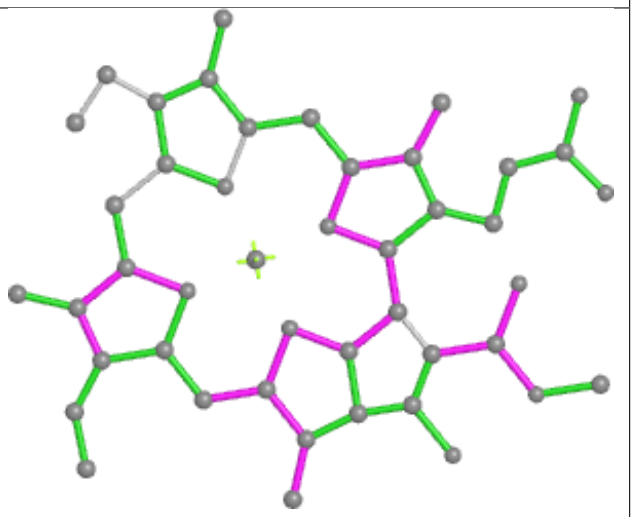

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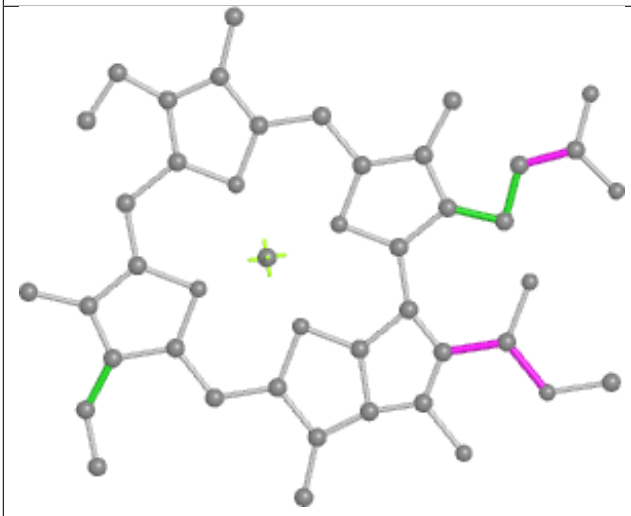
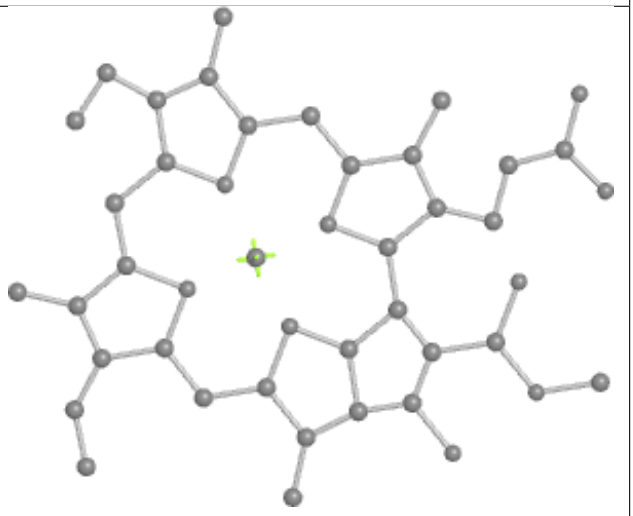
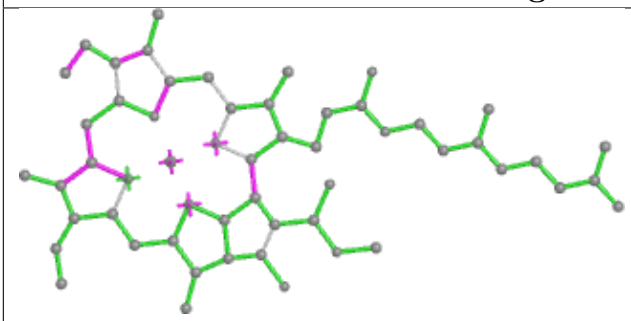


**Torsions**



**Rings**

## Ligand CLA a 608



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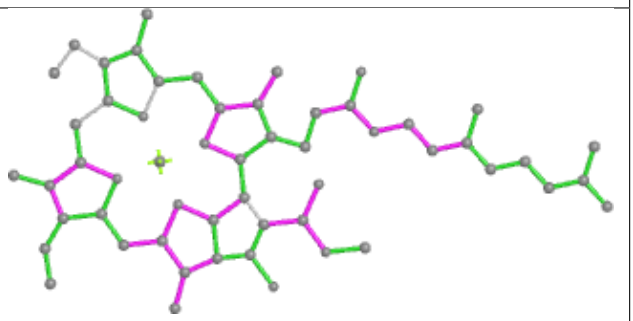
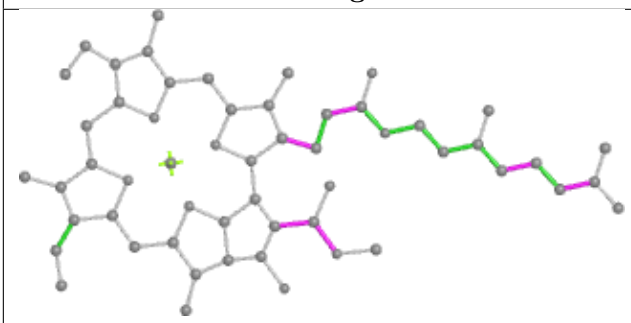


Bond angles



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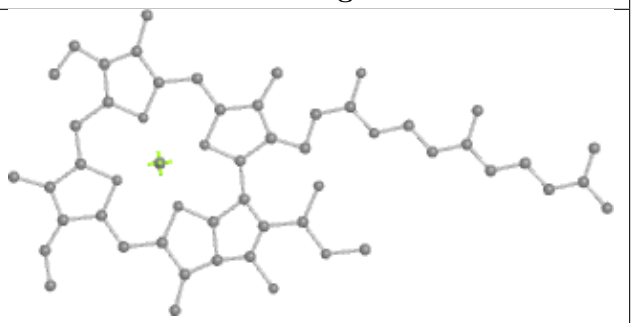
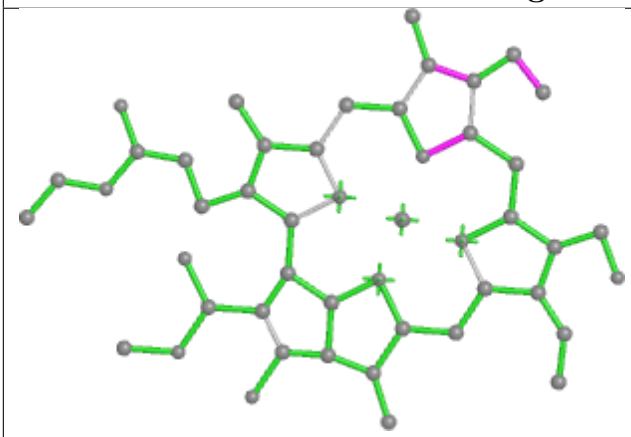


Rings

## Ligand CHL 9 608



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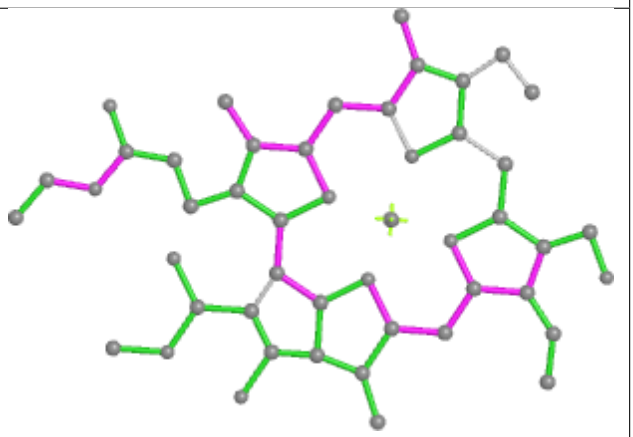
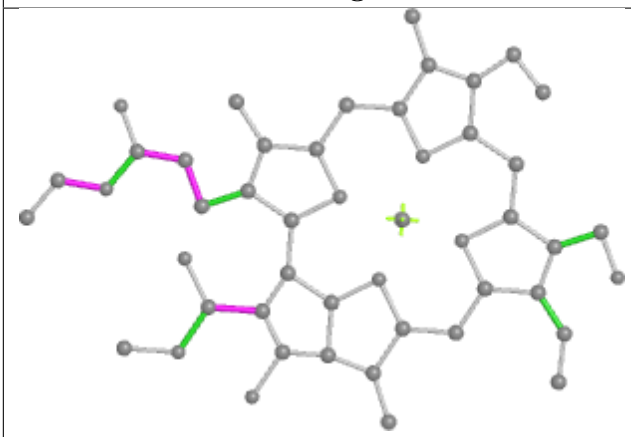


Bond angles



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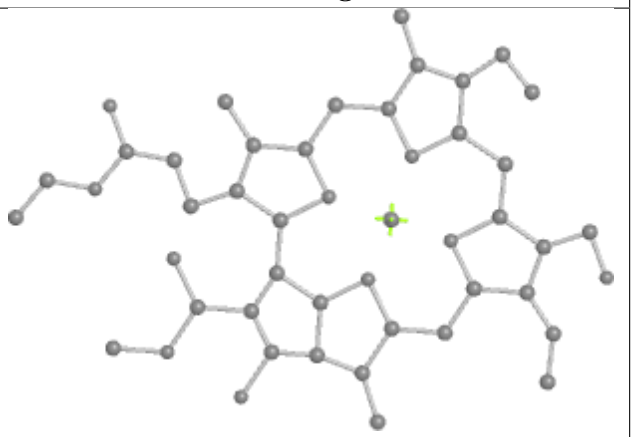
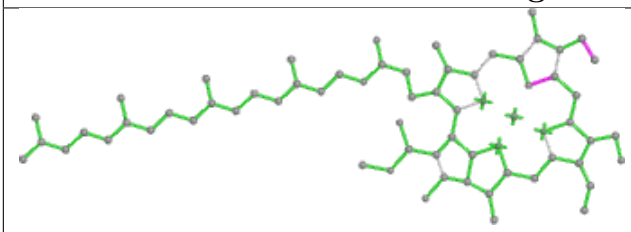


Rings

## Ligand CHL 6 619



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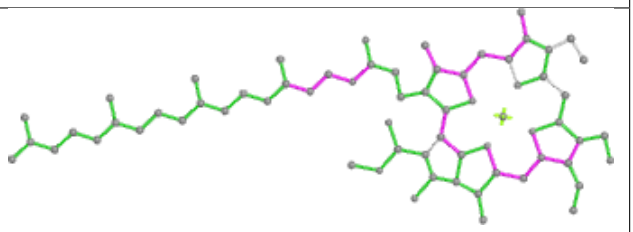
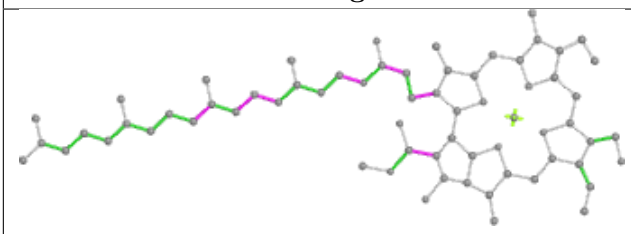


Bond angles



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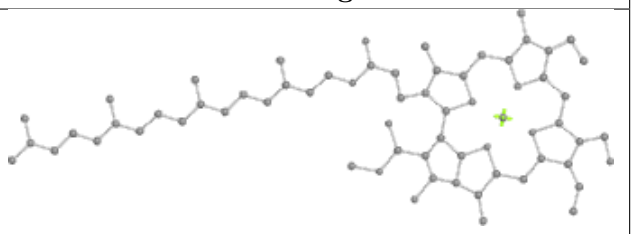
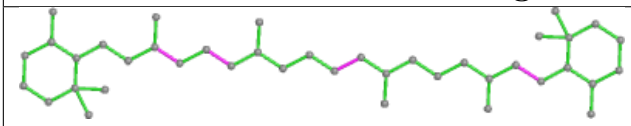


Rings

## Ligand BCR A 4001



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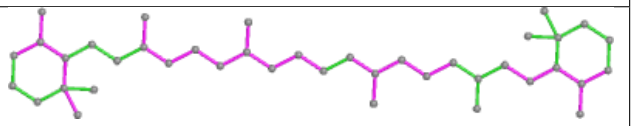
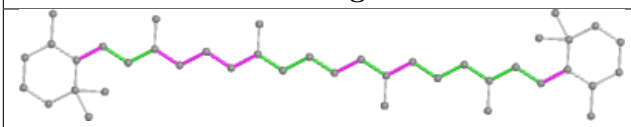
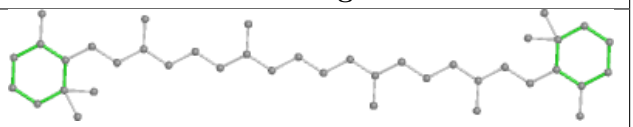


Bond angles

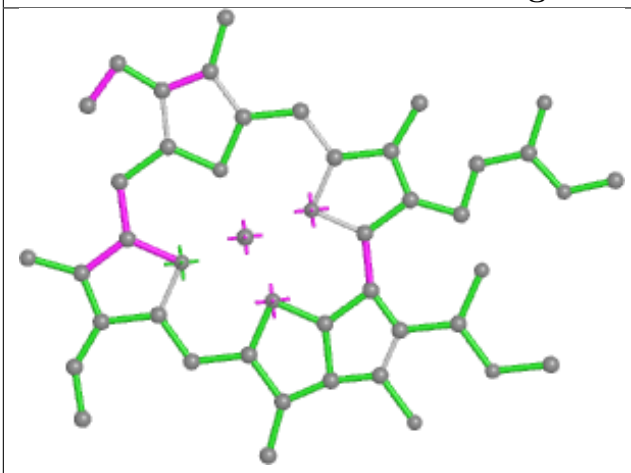


Torsions



Rings

## Ligand CLA 5 614



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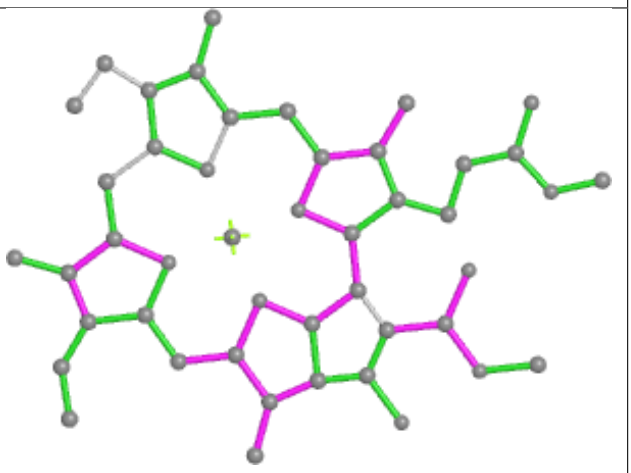
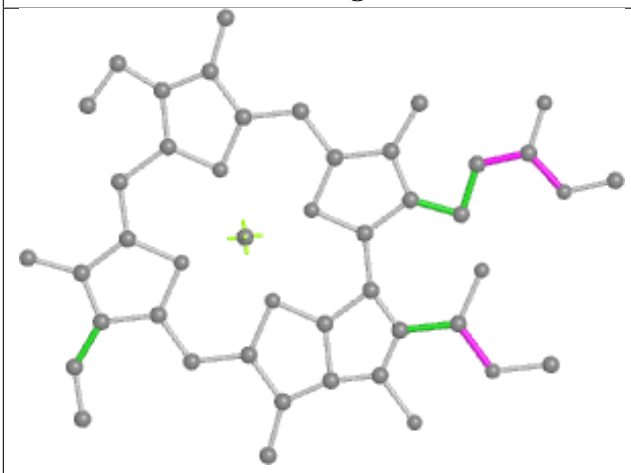
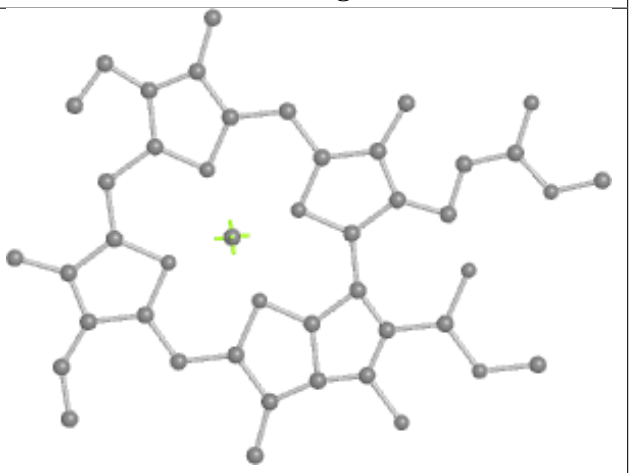


Bond angles

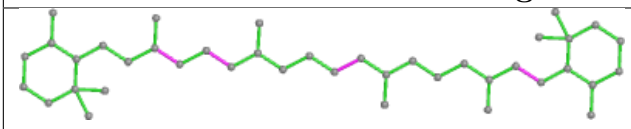


Torsions



Rings

## Ligand BCR L 4003



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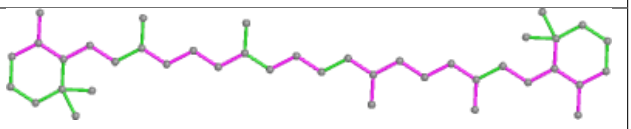
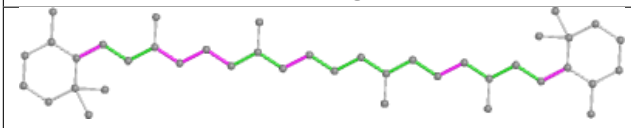


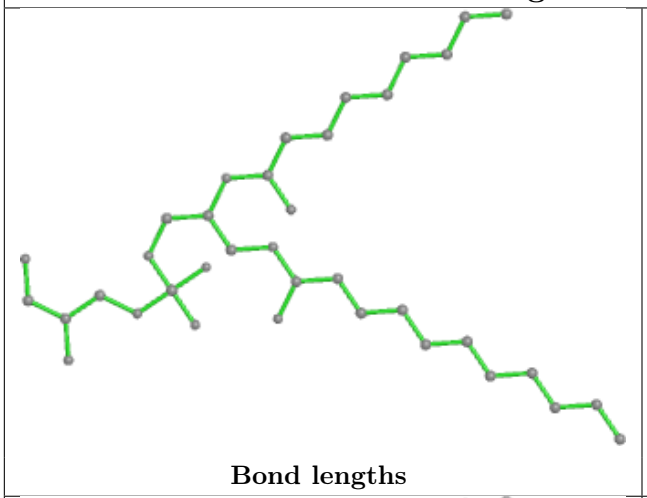
Bond angles



Torsions

Rings

## Ligand LHG 8 801



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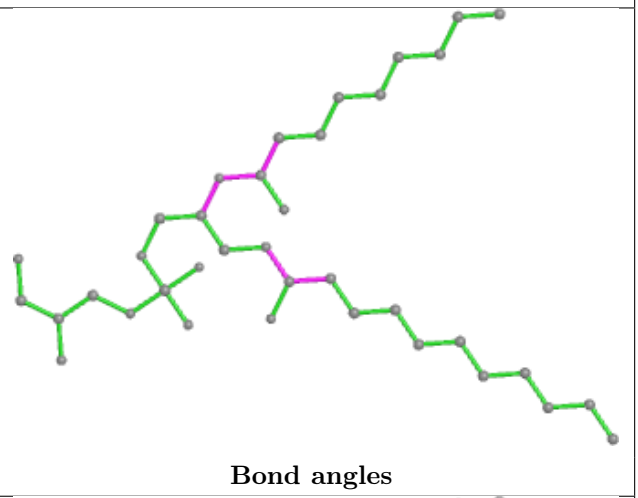
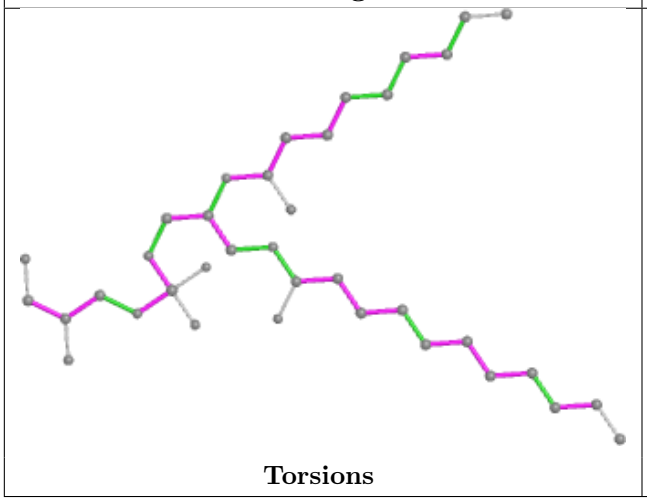
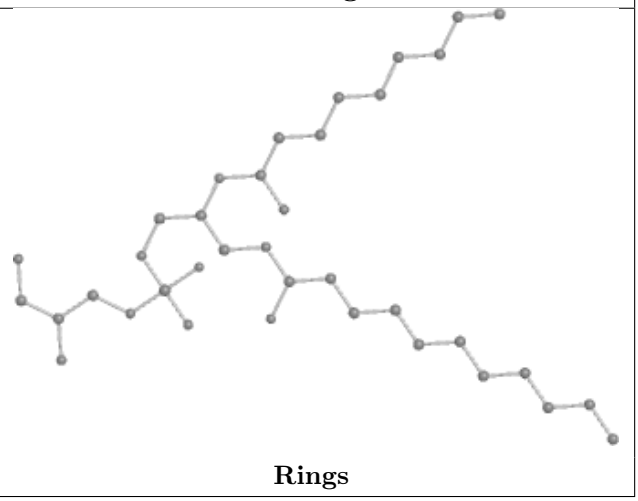


Bond angles

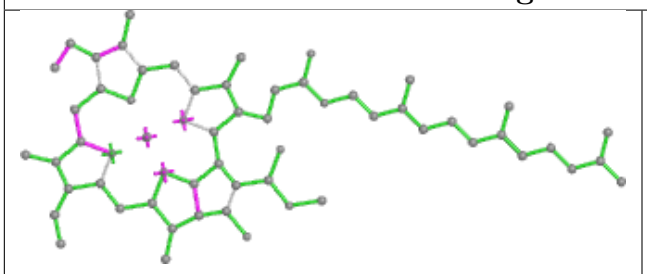


Torsions

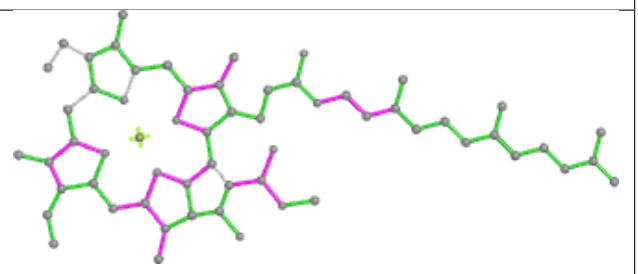


Rings

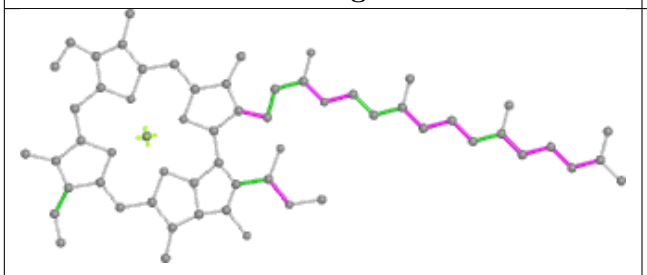
## Ligand CLA B 1215



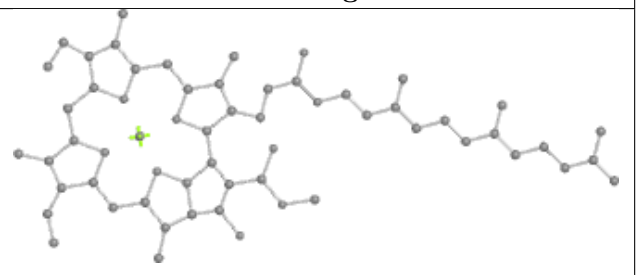
Bond lengths



Bond angles

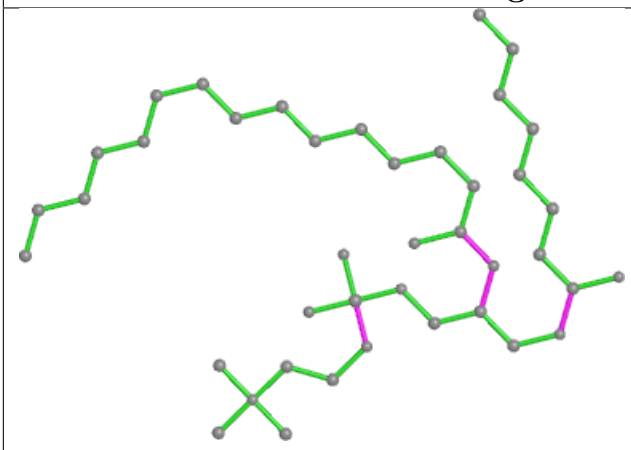


Torsions

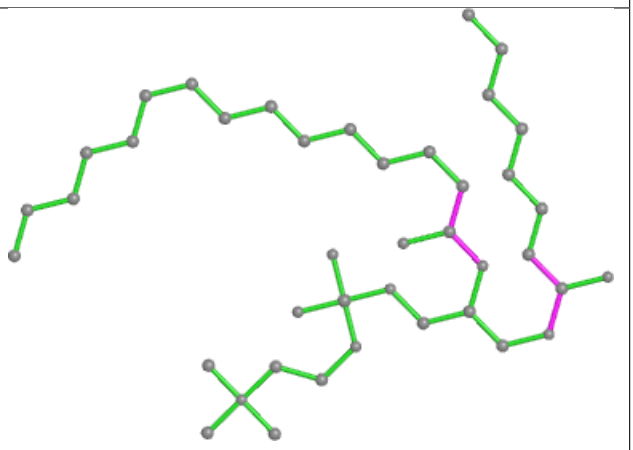


Rings

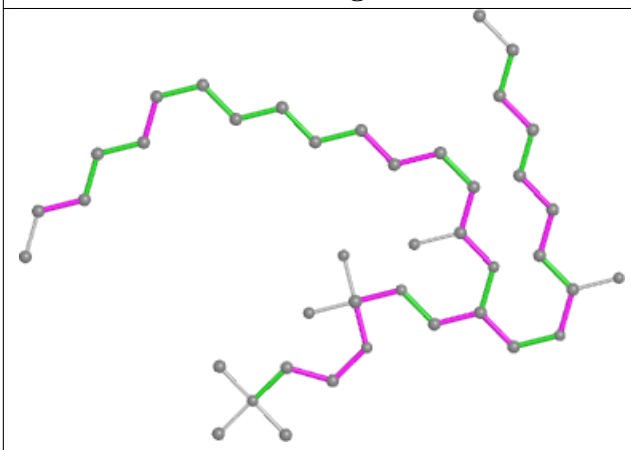
## Ligand PCW K 5001



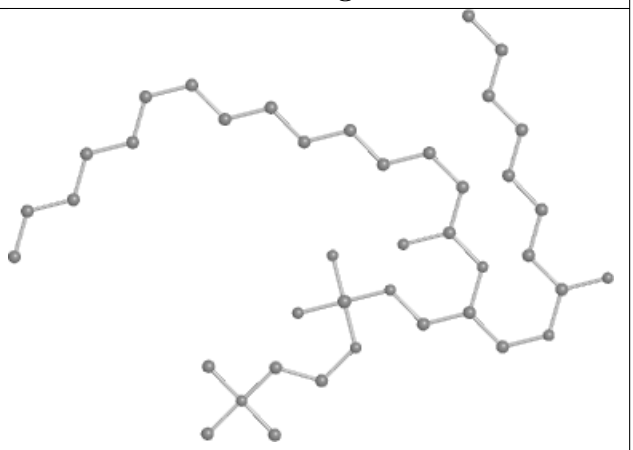
Bond lengths



Bond angles

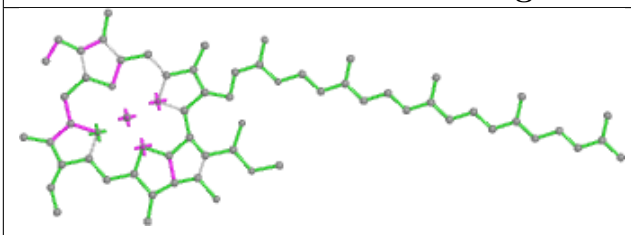


Torsions

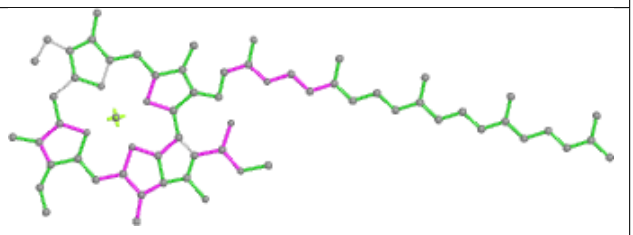


Rings

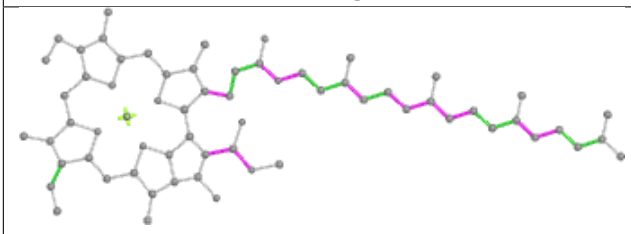
## Ligand CLA B 1231



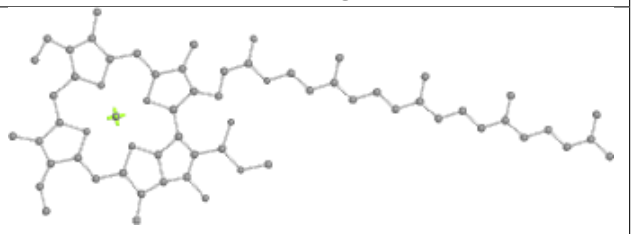
Bond lengths



Bond angles

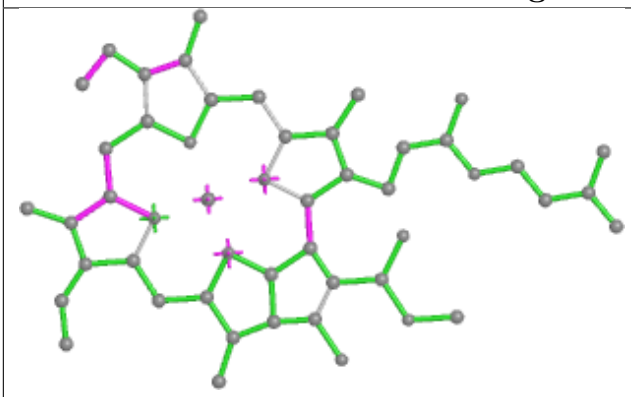


Torsions



Rings

## Ligand CLA 6 612



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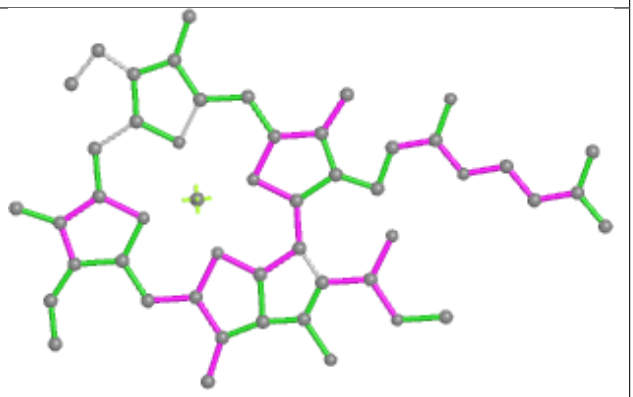
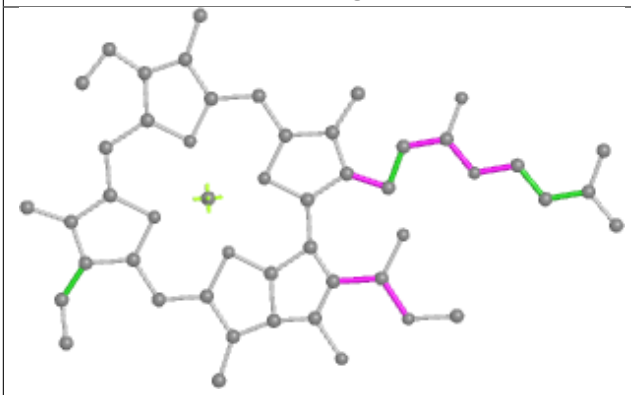
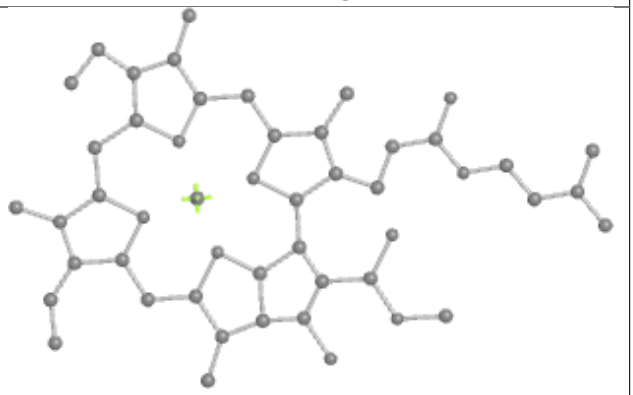


Bond angles

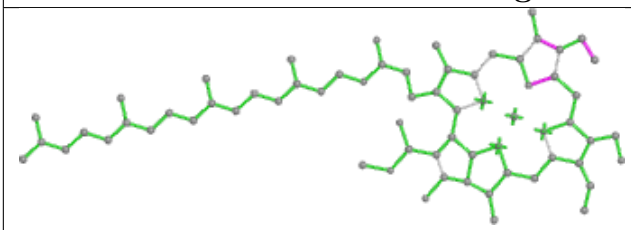


Torsions



Rings

## Ligand CHL A 1114



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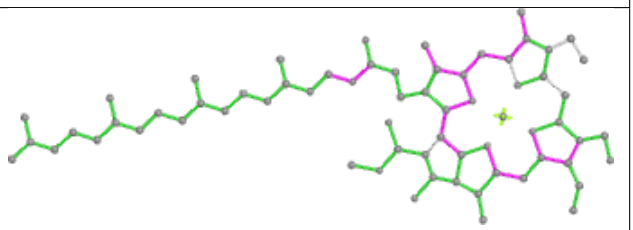
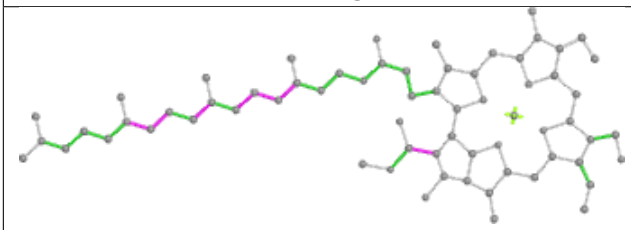


Bond angles



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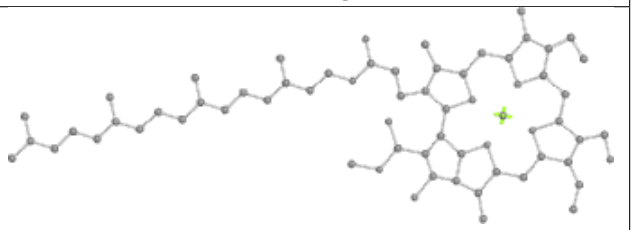
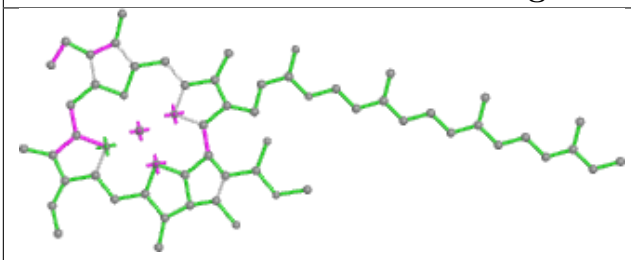
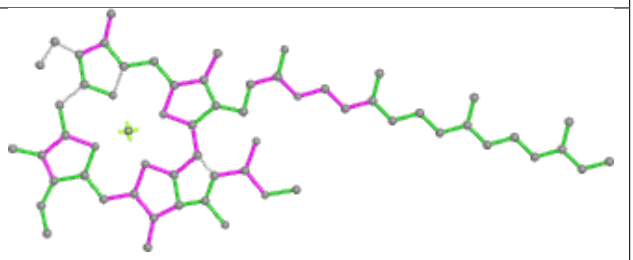


Rings

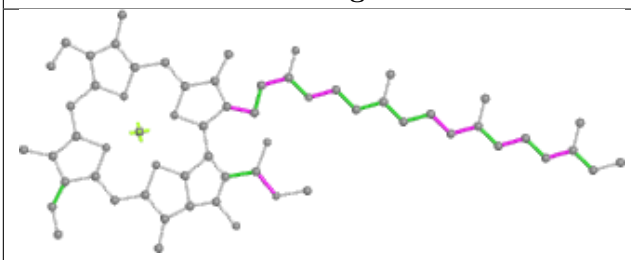
## Ligand CLA 3 613



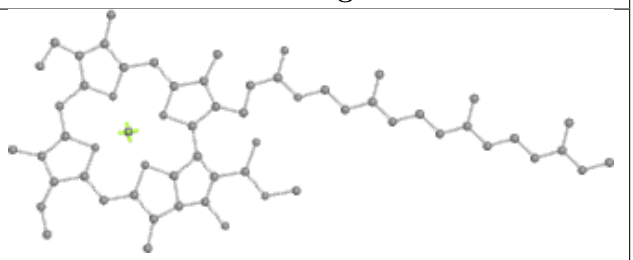
Bond lengths



Bond angles

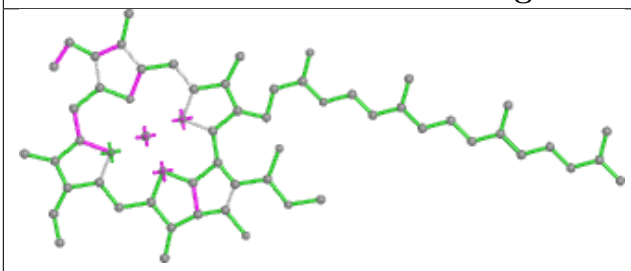


Torsions

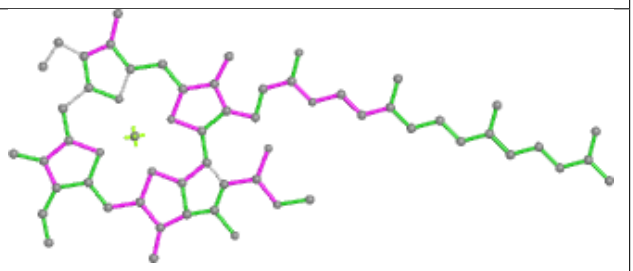


Rings

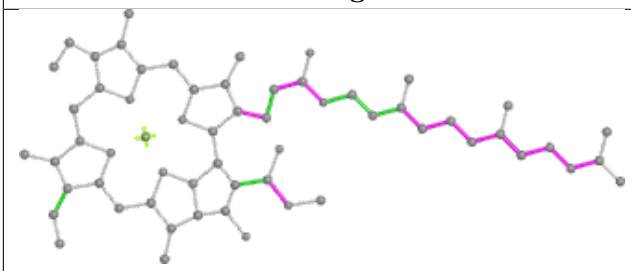
## Ligand CLA A 1121



Bond lengths



Bond angles



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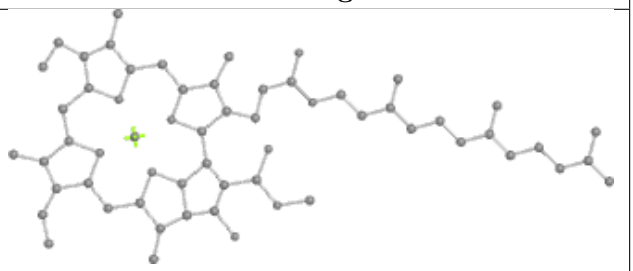
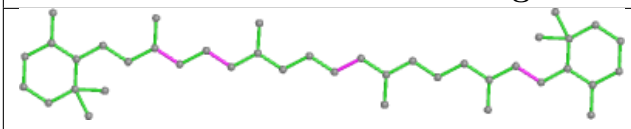


Rings

## Ligand BCR K 4002



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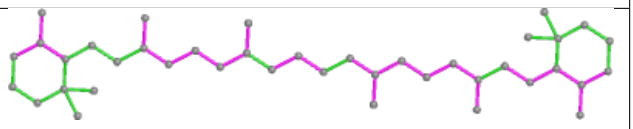
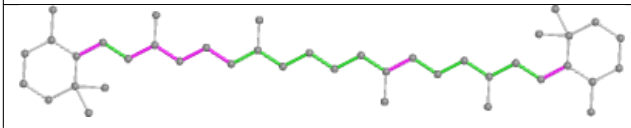


Bond angles



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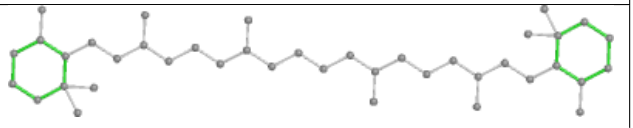
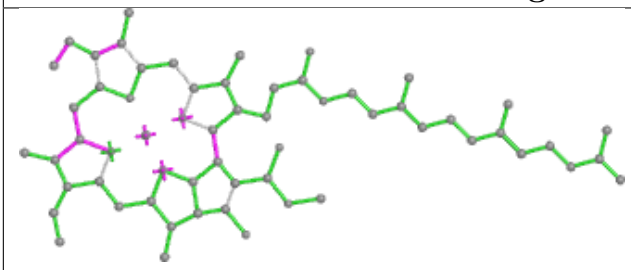


Rings

## Ligand CLA 5 607



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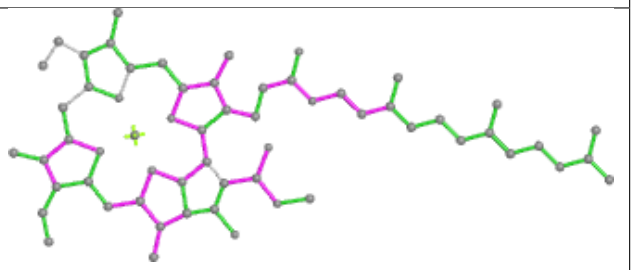
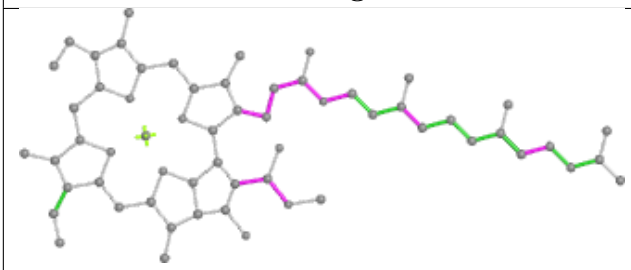


Bond angles



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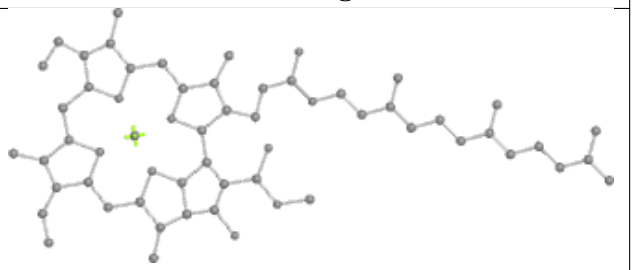
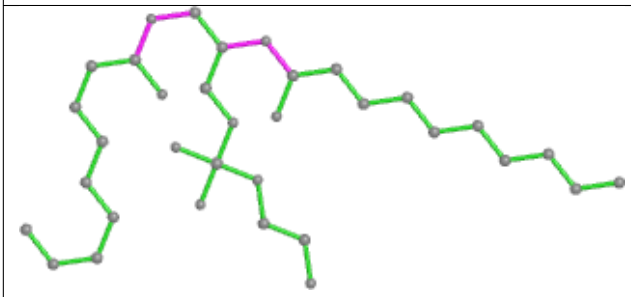


Rings

## Ligand PTY A 5006



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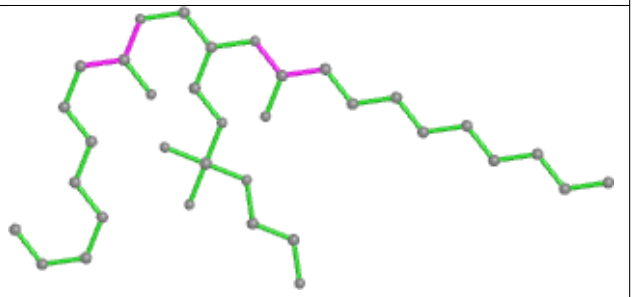
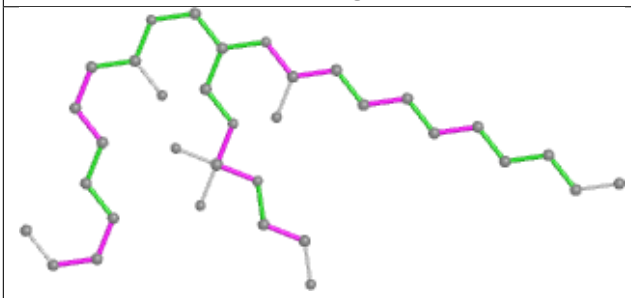


Bond angles



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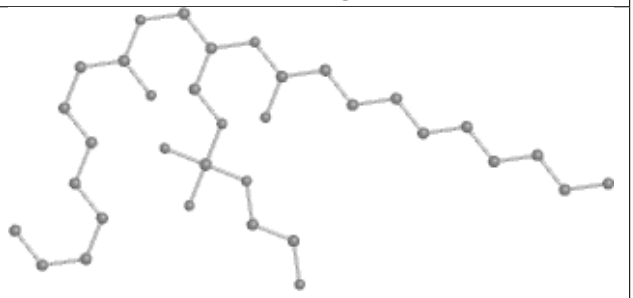
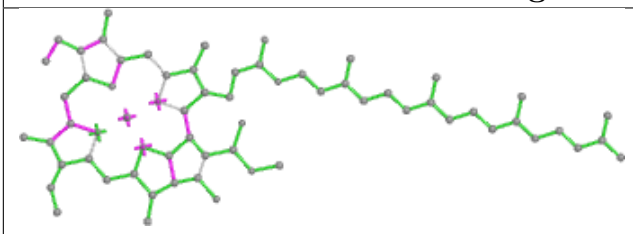
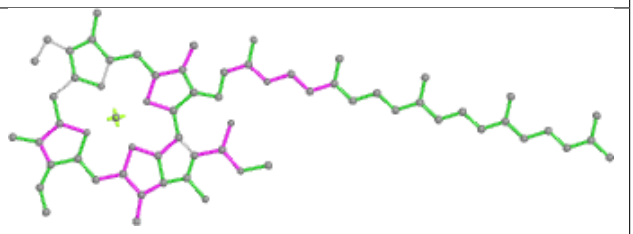


Rings

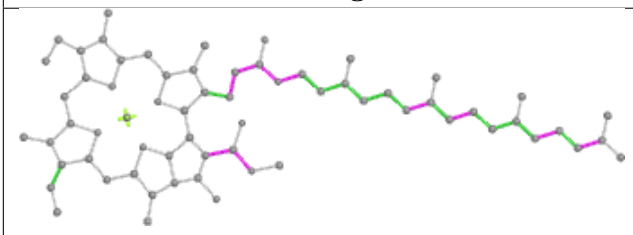
## Ligand CLA 6 603



Bond lengths



Bond angles



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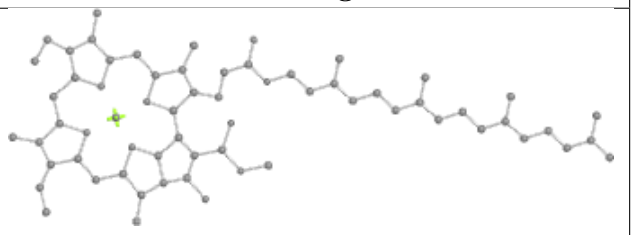
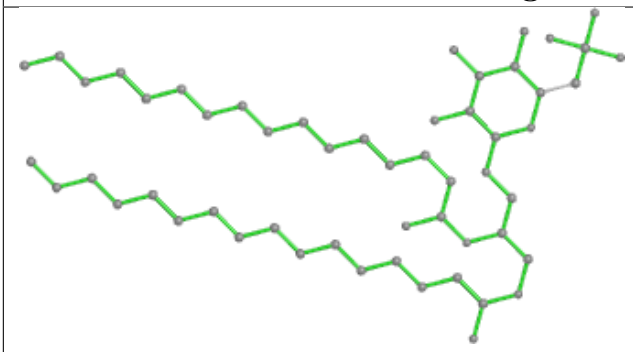


Rings

## Ligand SQD I 5001



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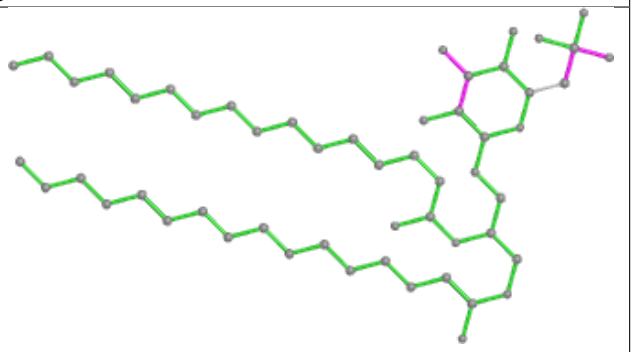
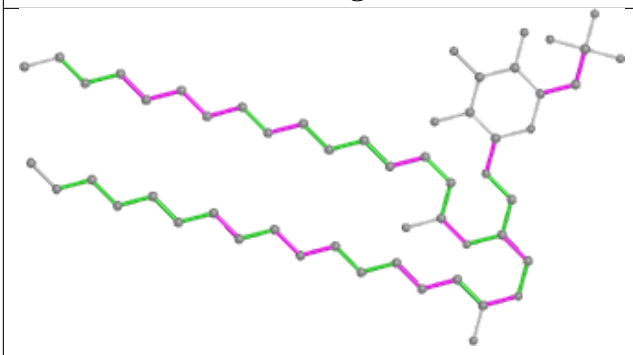


Bond angles



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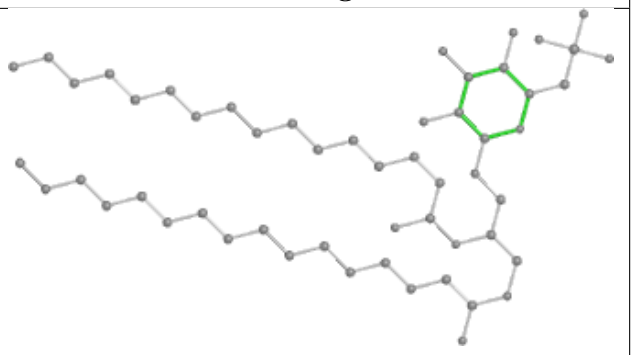
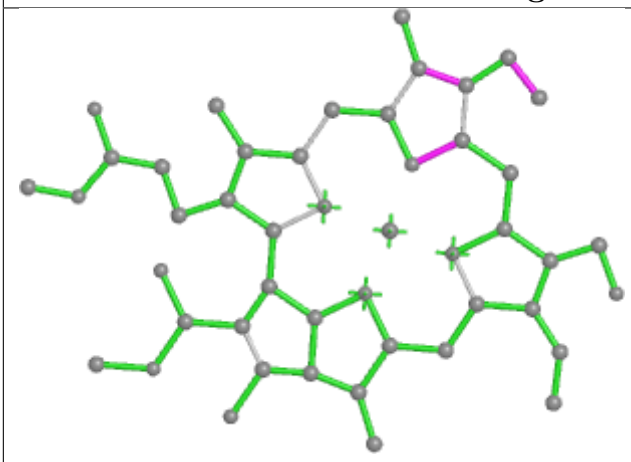


Rings

## Ligand CHL 5 617



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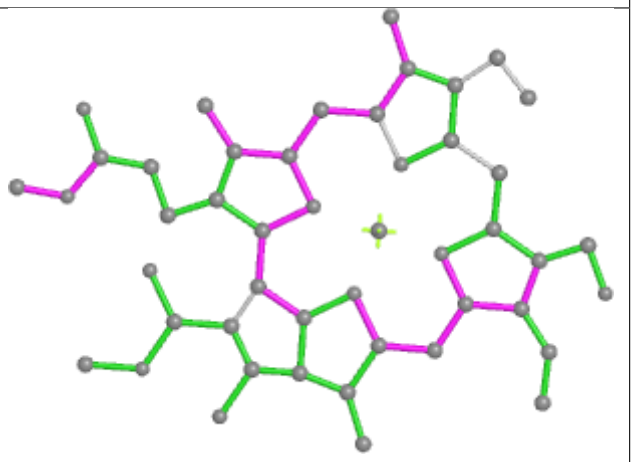
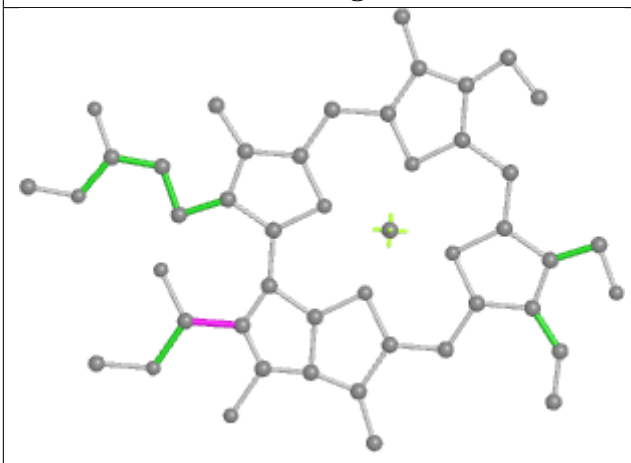


Bond angles



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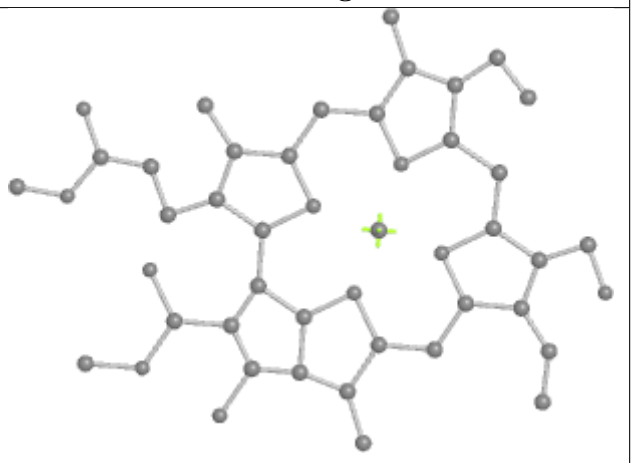
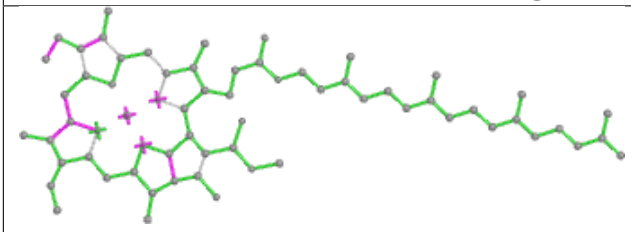
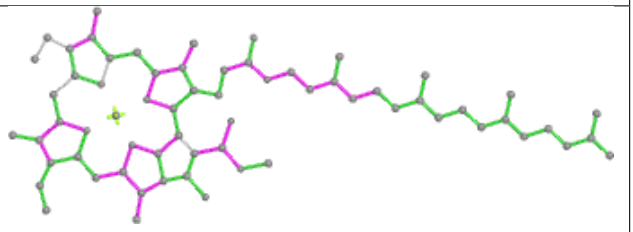


Rings

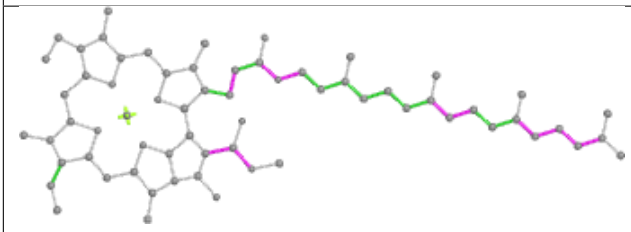
## Ligand CLA 7 604



Bond lengths



Bond angles



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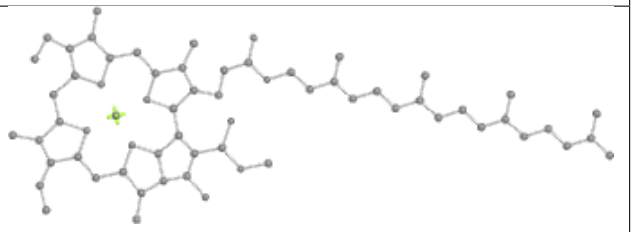
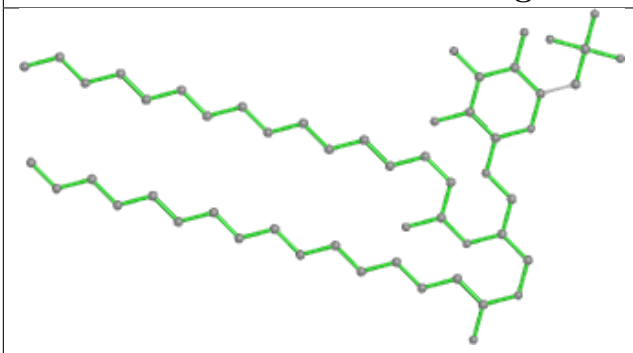
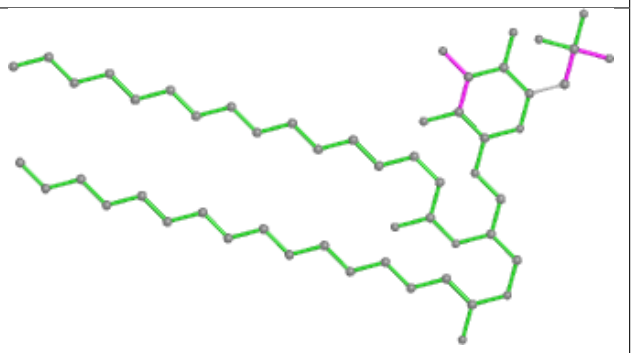


Rings

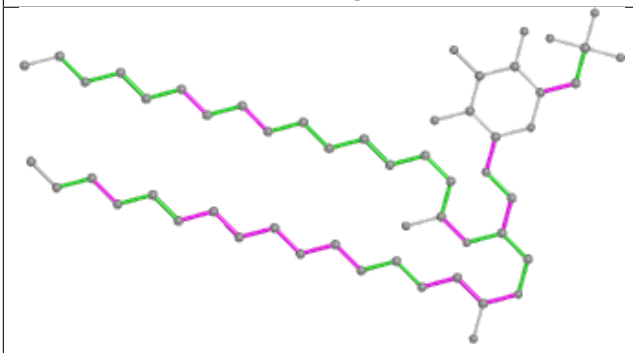
## Ligand SQD A 5005



Bond lengths



Bond angles



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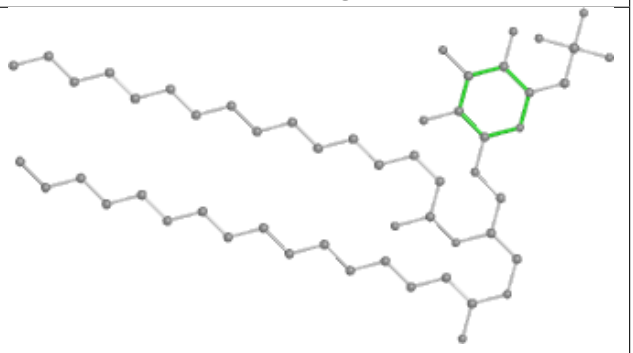
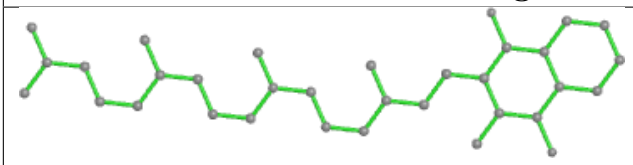
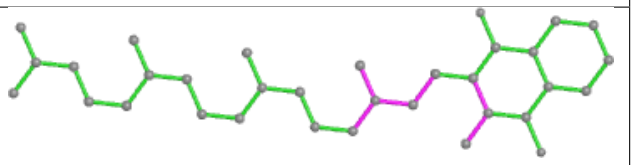


Rings

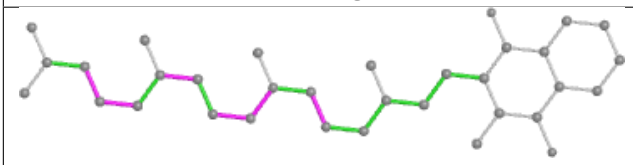
## Ligand PQN B 2002



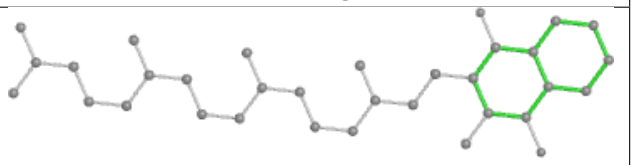
Bond lengths



Bond angles

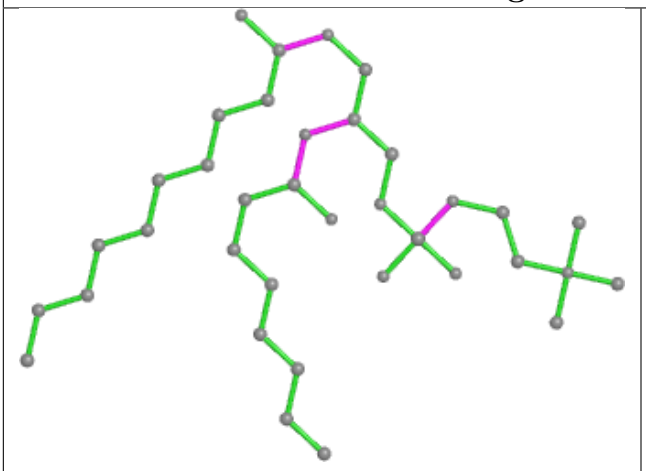


Torsions



Rings

## Ligand PCW K 5002



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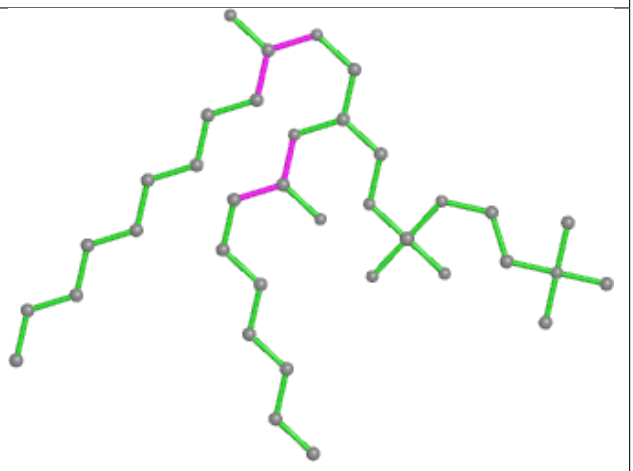

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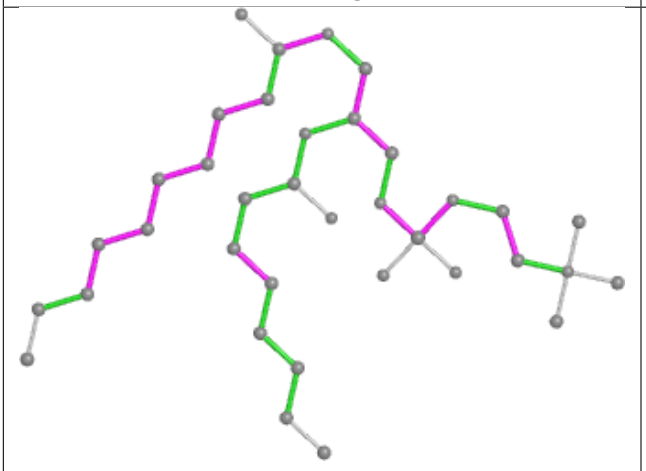

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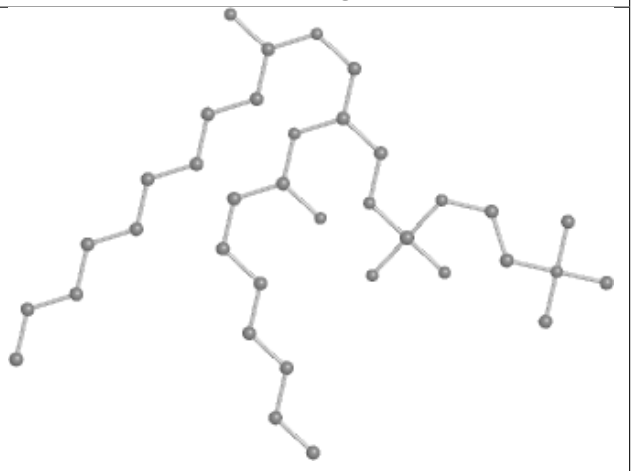
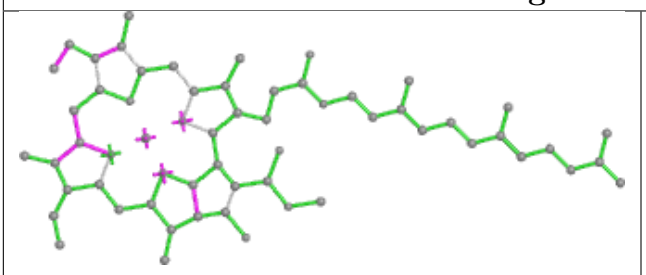


Rings

## Ligand CLA 8 618



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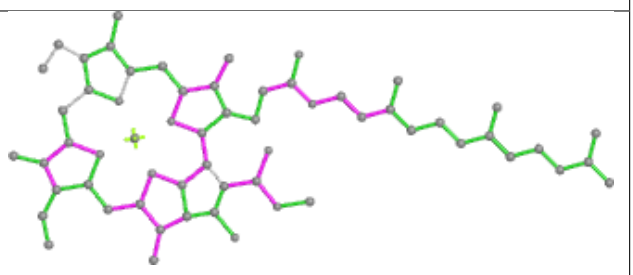

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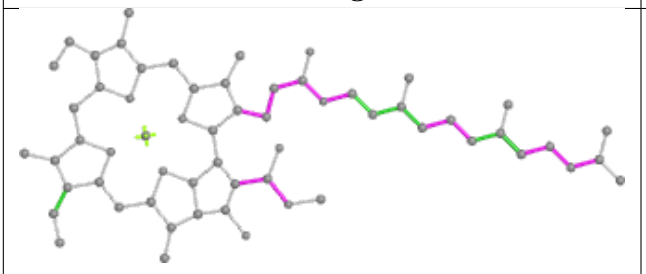

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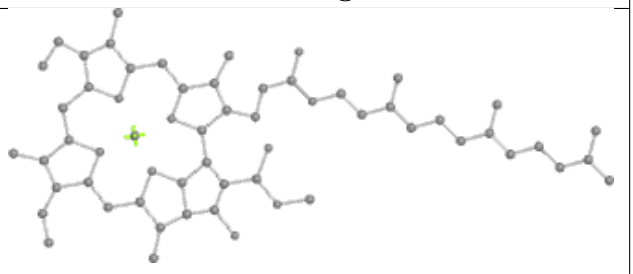
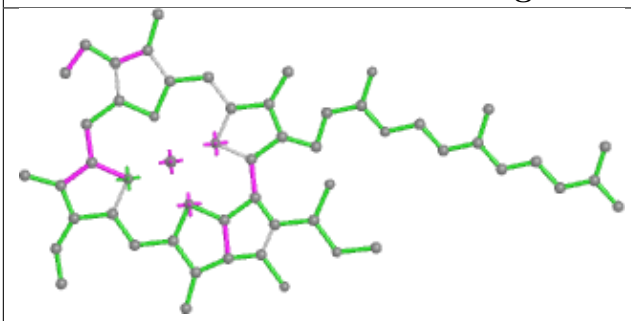


Rings

## Ligand CLA A 1139



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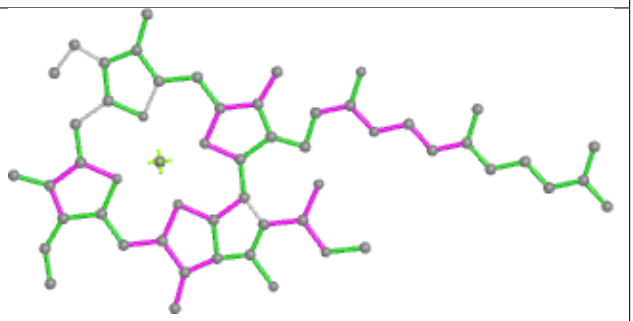

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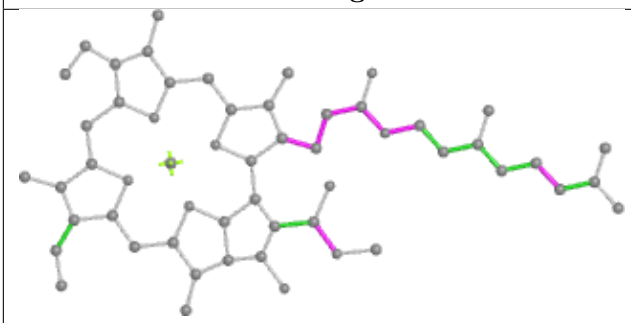

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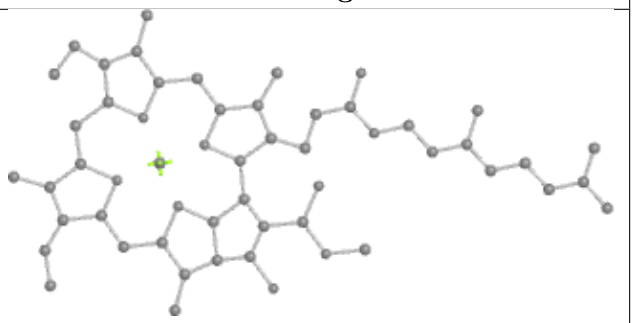
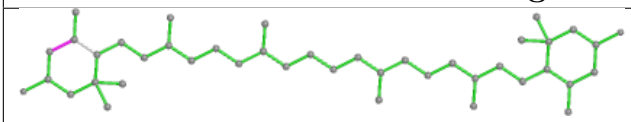


Rings

## Ligand LUT 6 502



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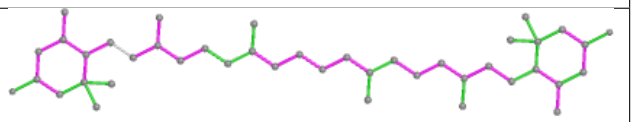
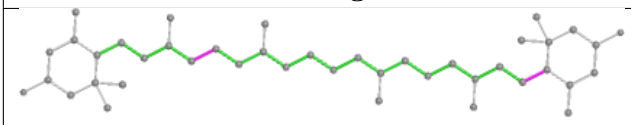


Bond angles



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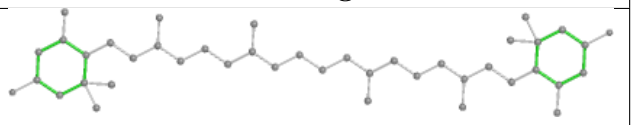
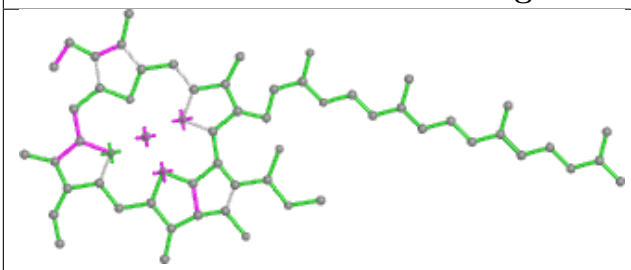


Rings

## Ligand CLA A 1137



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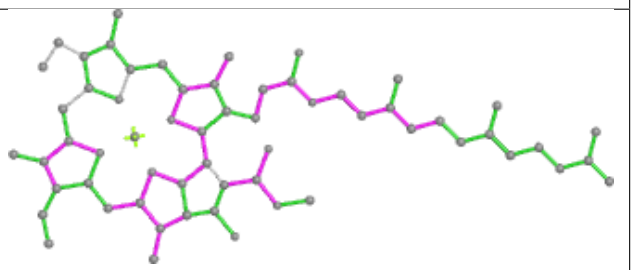

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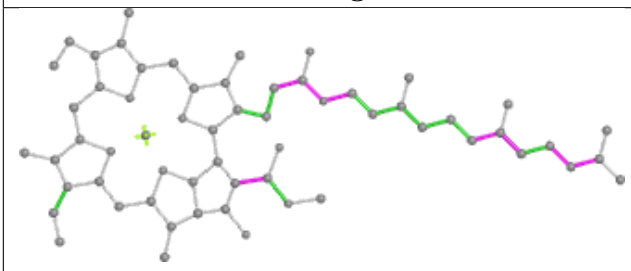

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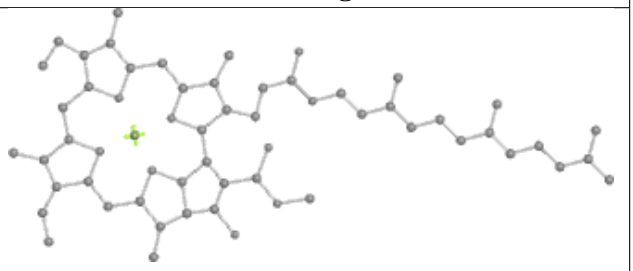
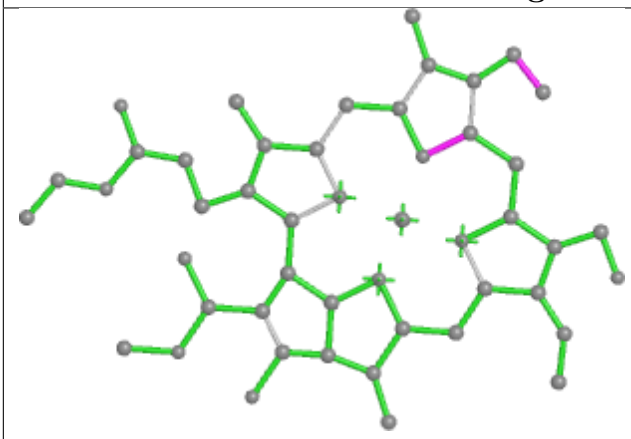


Rings

## Ligand CHL 1 613



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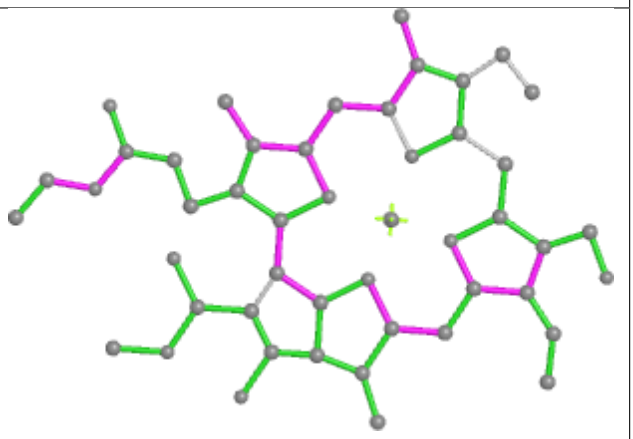

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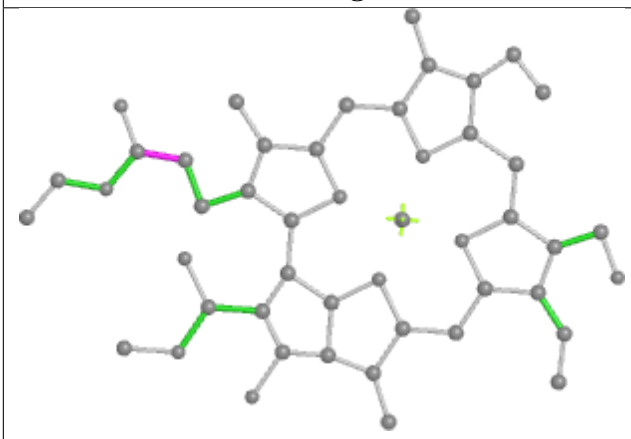

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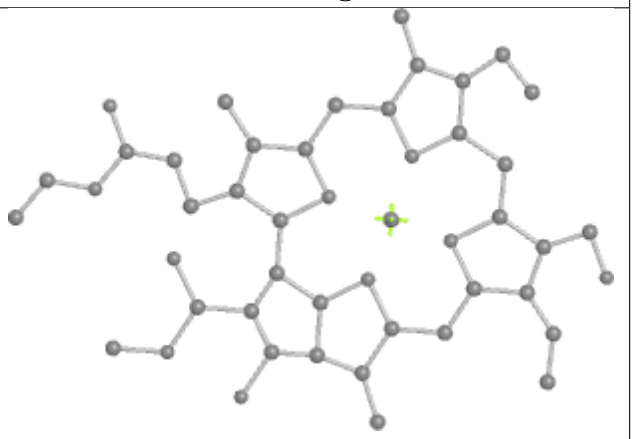

Rings

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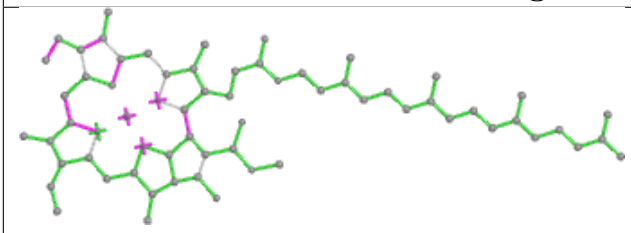

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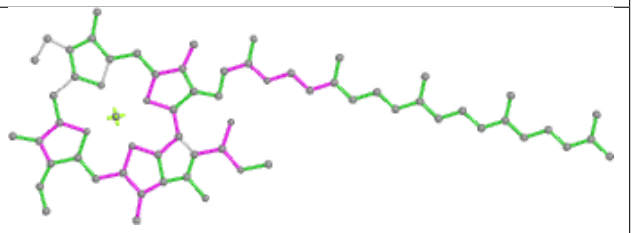

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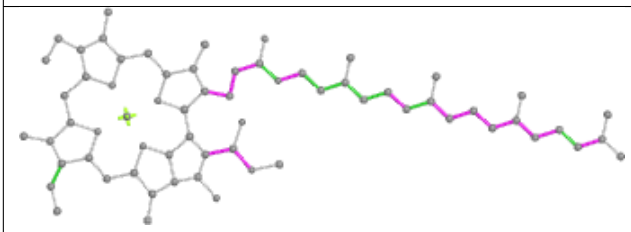
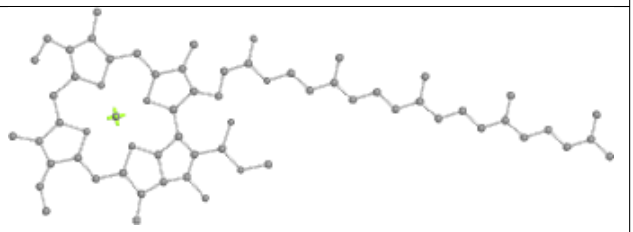
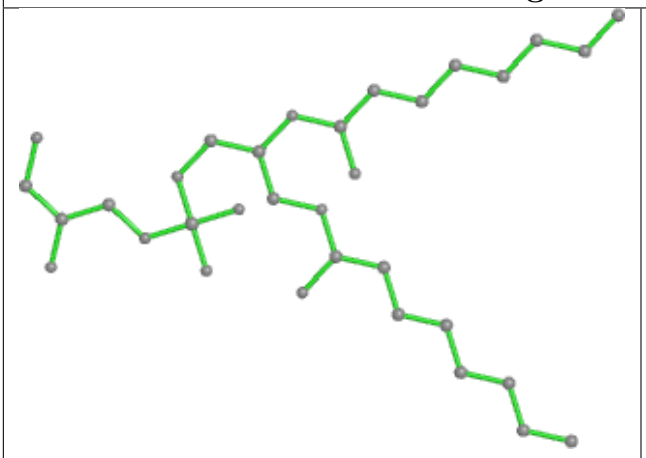


Torsions



Rings

## Ligand LHG 9 801



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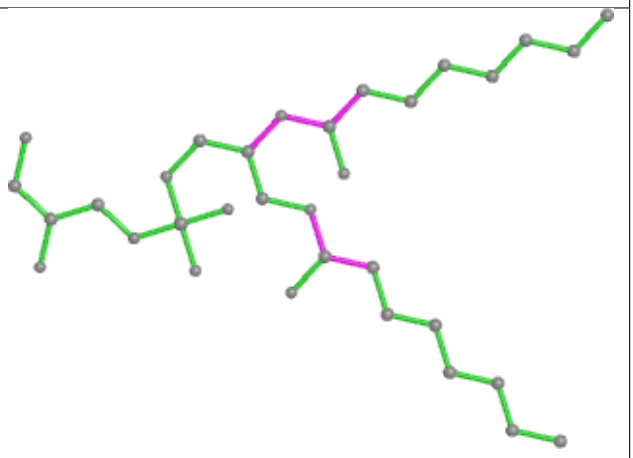
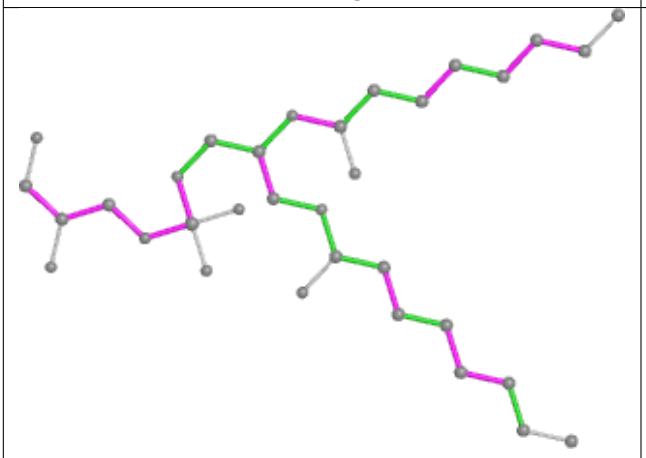


Bond angles



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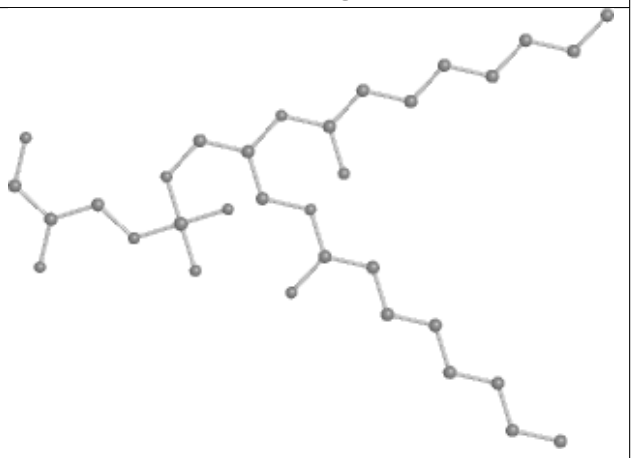

Rings

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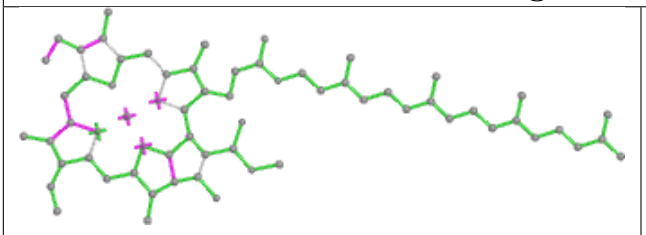

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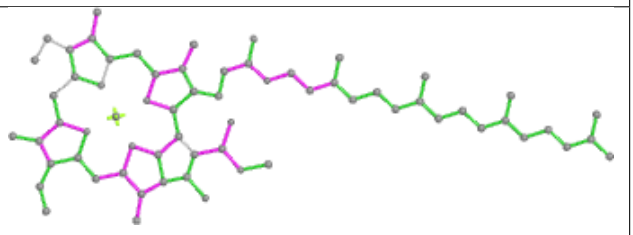
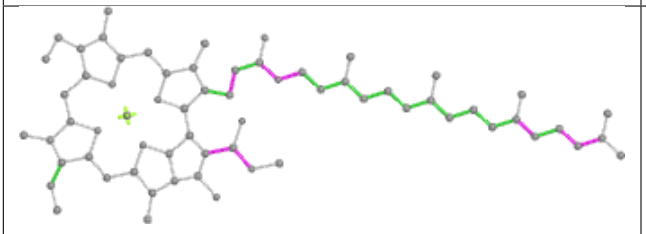


Bond angles



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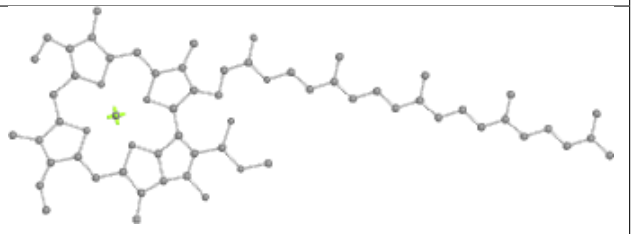
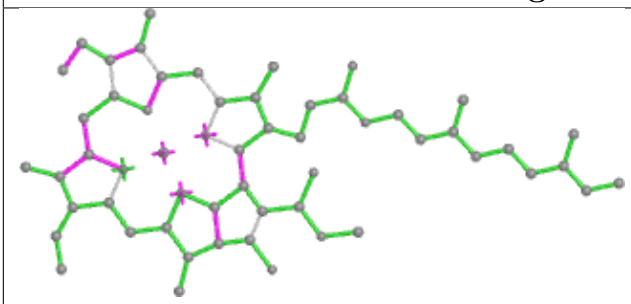


Rings

## Ligand CLA 5 603



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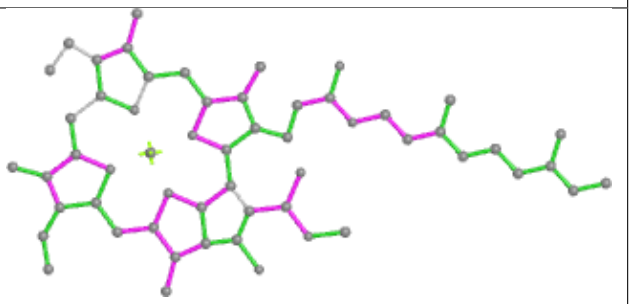
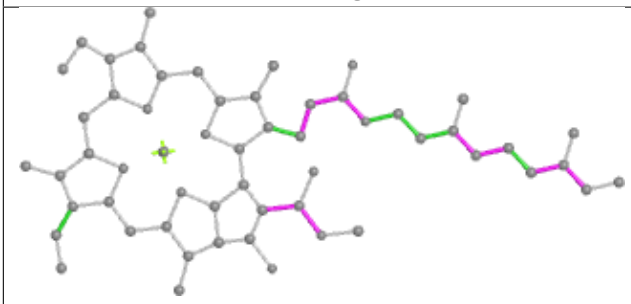


Bond angles



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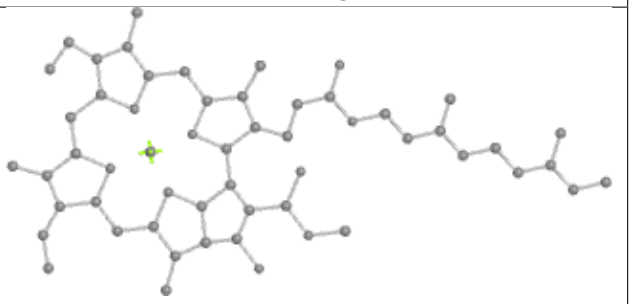
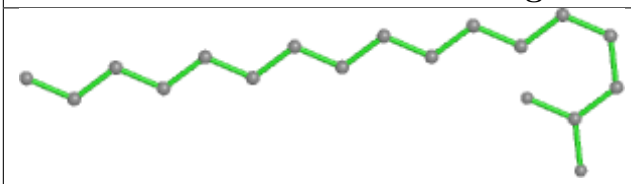


Rings

## Ligand PLM 4 804



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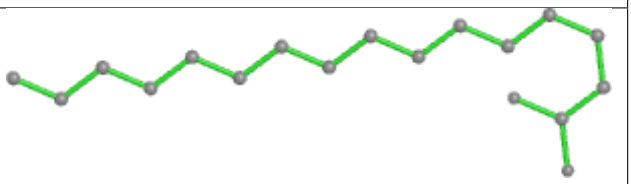
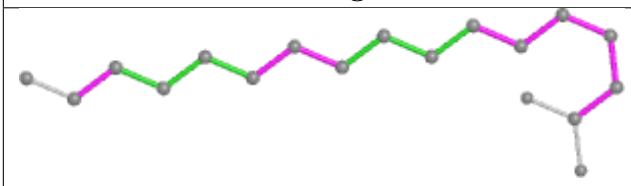
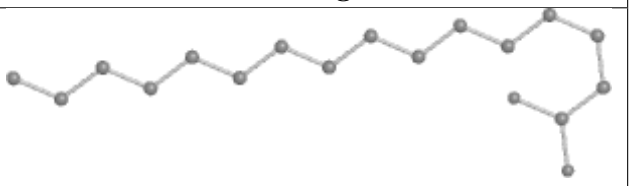


Bond angles

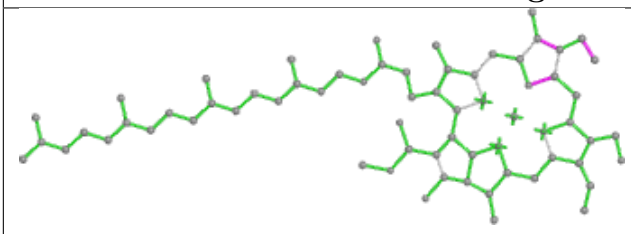


Torsions



Rings

## Ligand CHL 9 603



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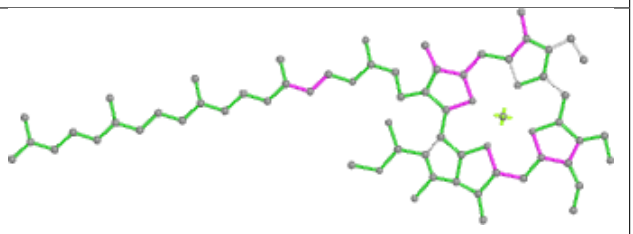
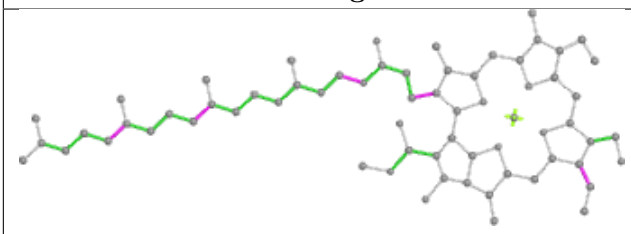


Bond angles



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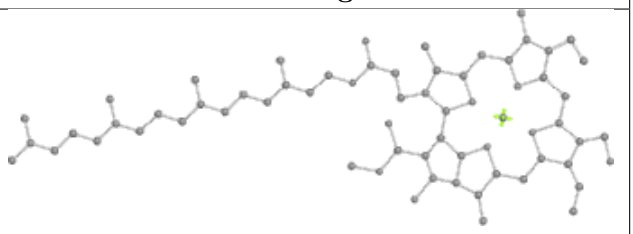
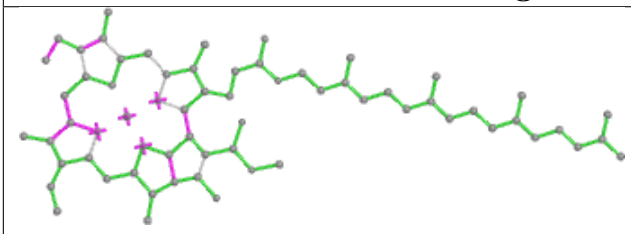
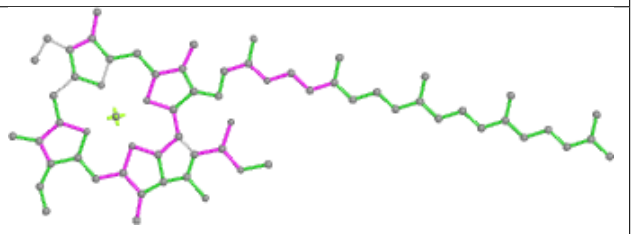


Rings

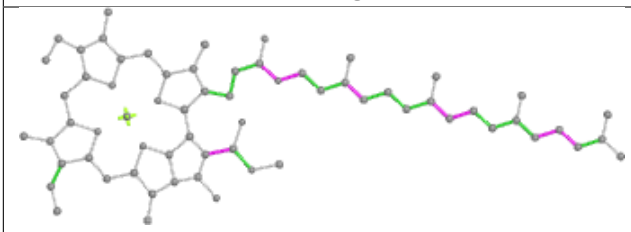
## Ligand CLA A 1123



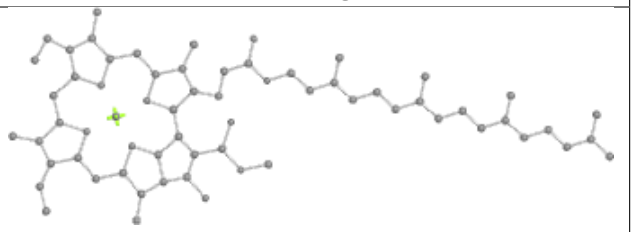
Bond lengths



Bond angles

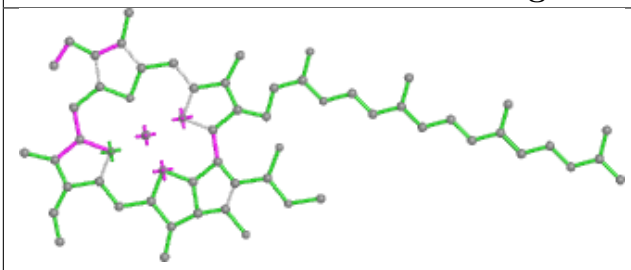


Torsions

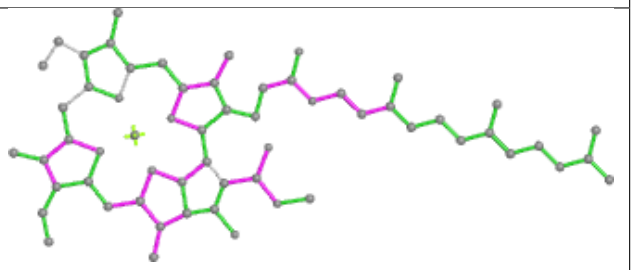


Rings

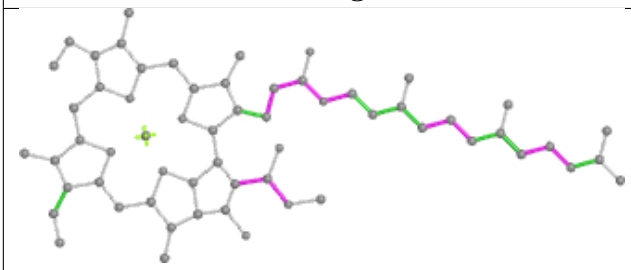
## Ligand CLA 8 609



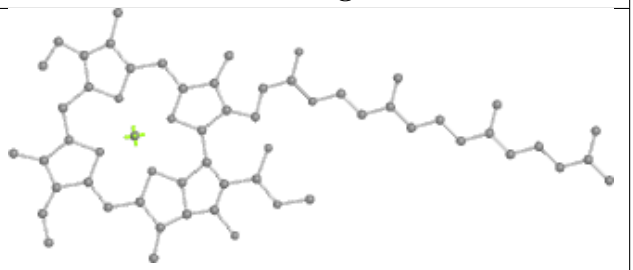
Bond lengths



Bond angles

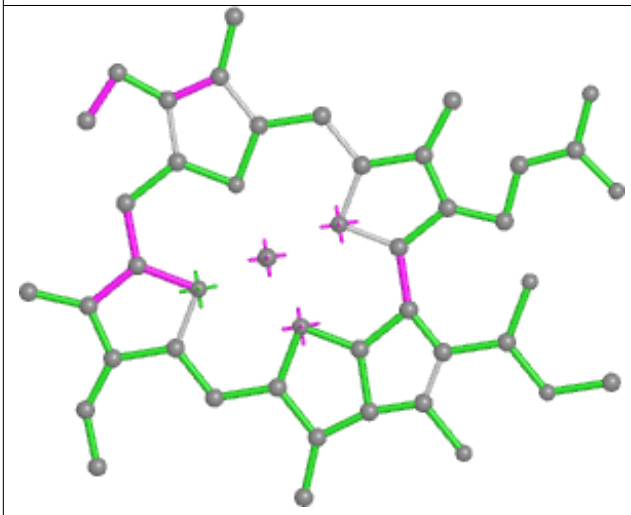


Torsions

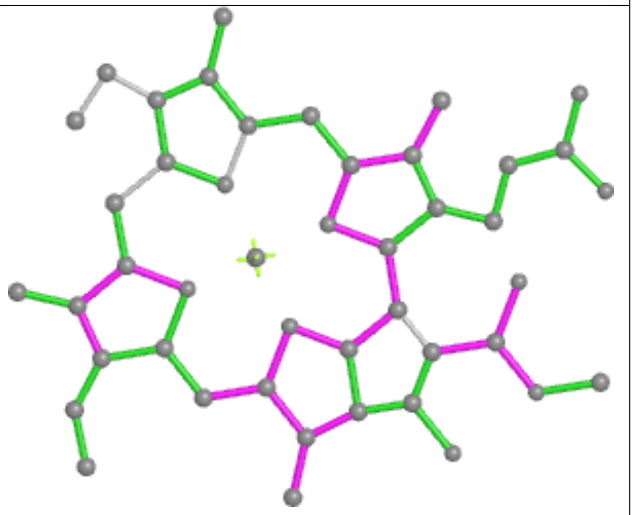


Rings

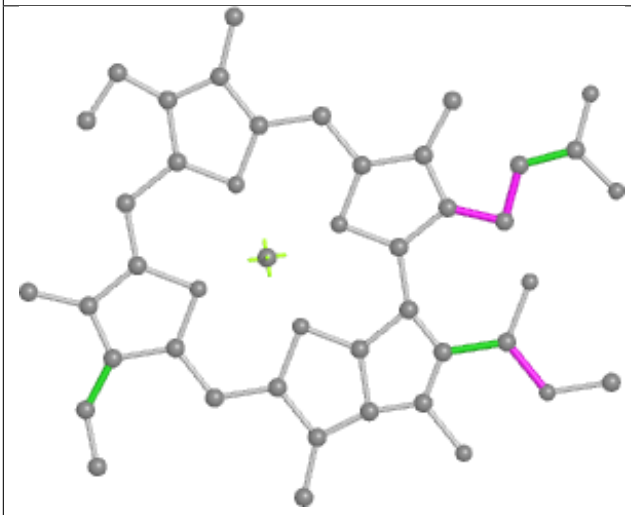
## Ligand CLA G 1603



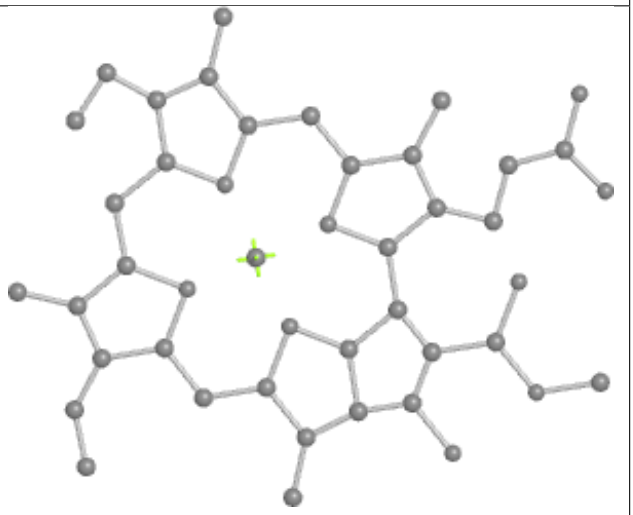
Bond lengths



Bond angles

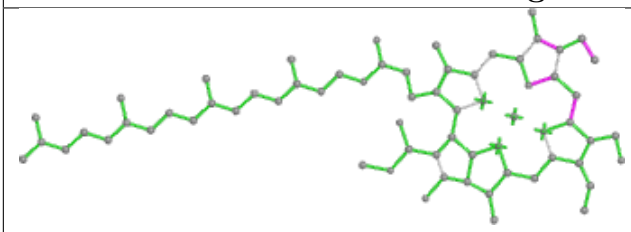


Torsions

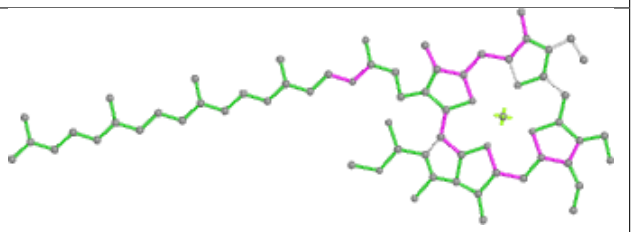


Rings

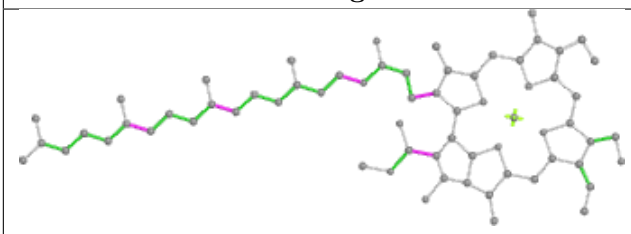
## Ligand CHL 3 604



Bond lengths



Bond angles



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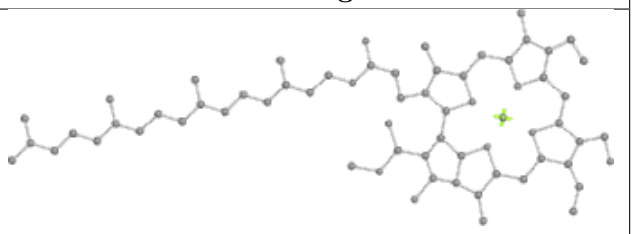
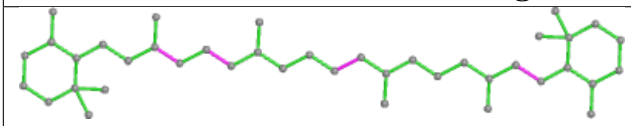
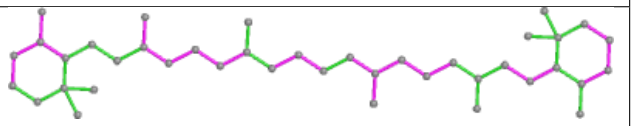


Rings

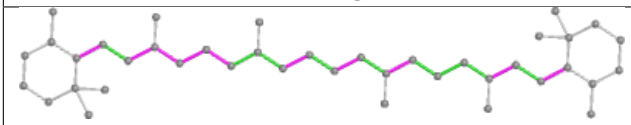
## Ligand BCR B 4002



Bond lengths



Bond angles



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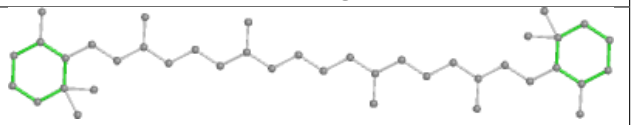
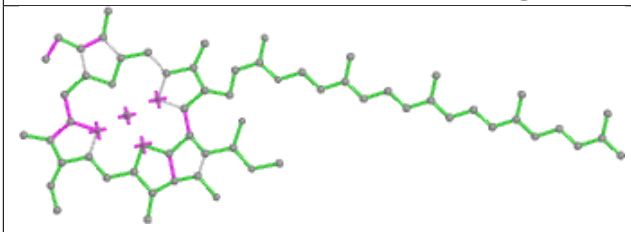
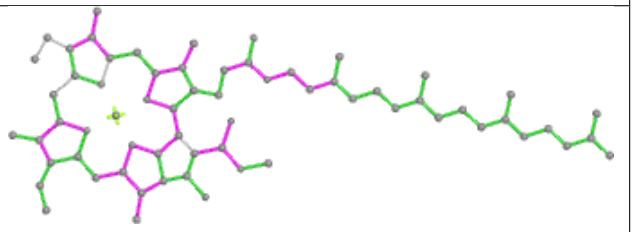


Rings

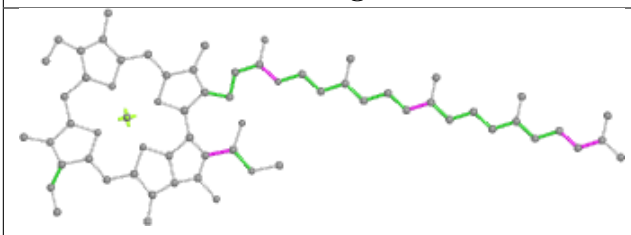
## Ligand CLA B 1221



Bond lengths



Bond angles



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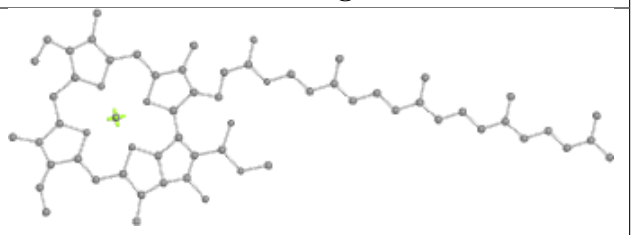
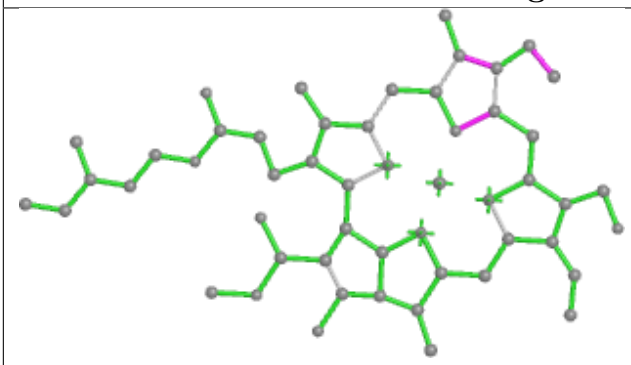
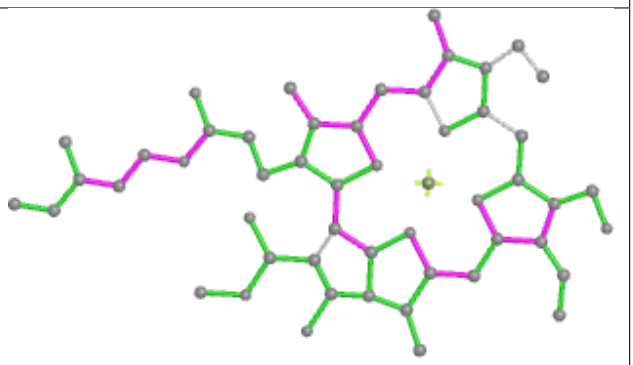


Rings

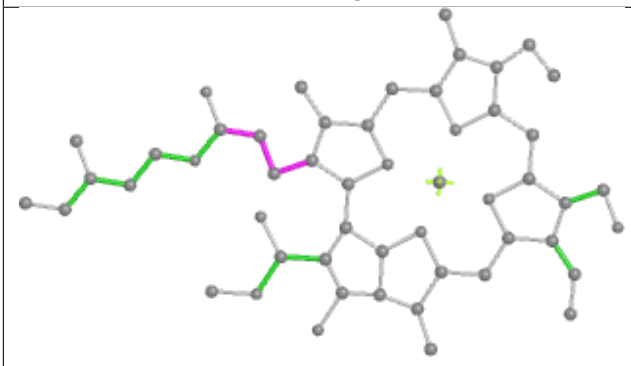
## Ligand CHL 4 613



Bond lengths



Bond angles



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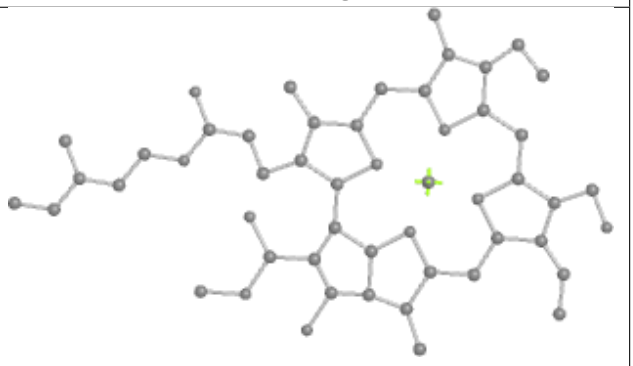
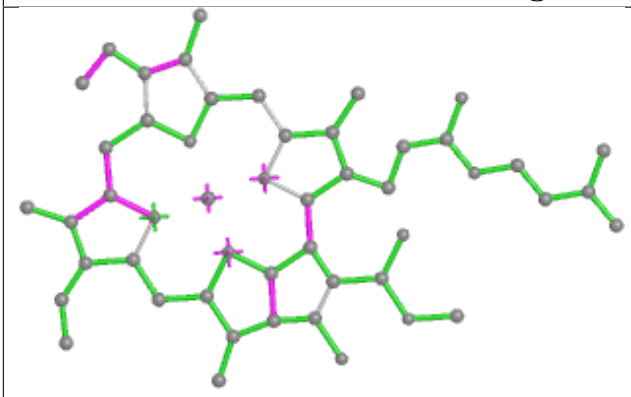
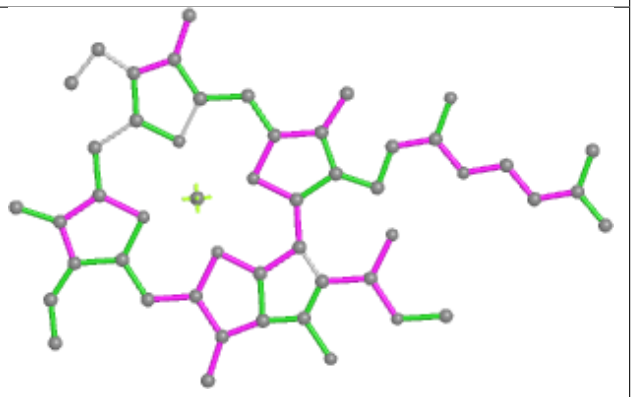


Rings

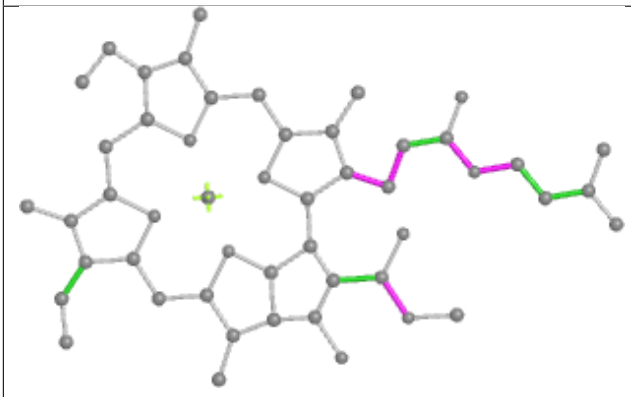
## Ligand CLA a 611



Bond lengths



Bond angles



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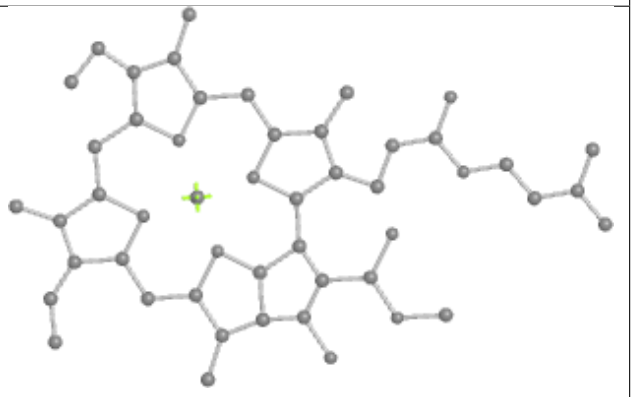
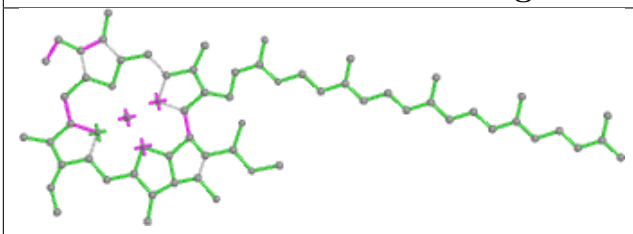
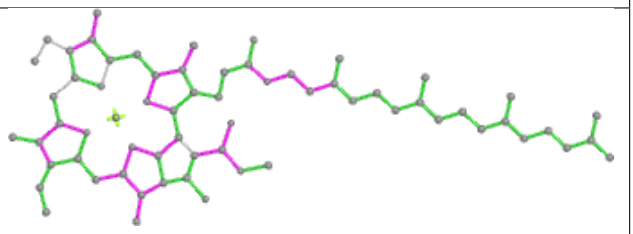


Rings

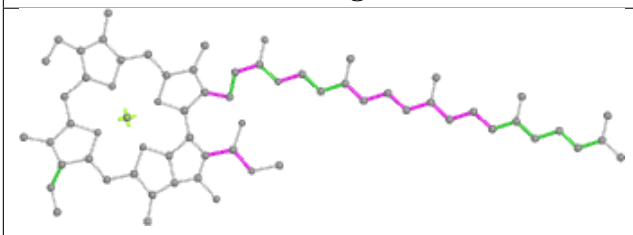
## Ligand CLA A 1103



Bond lengths



Bond angles



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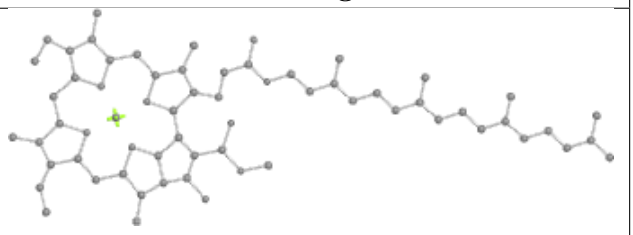
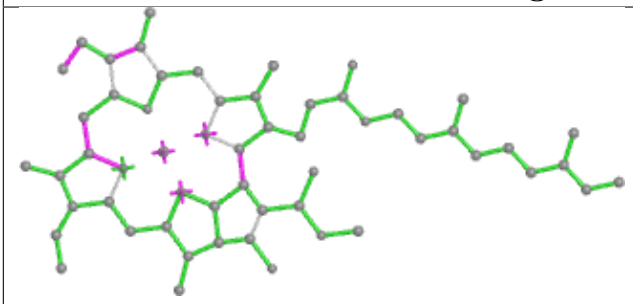
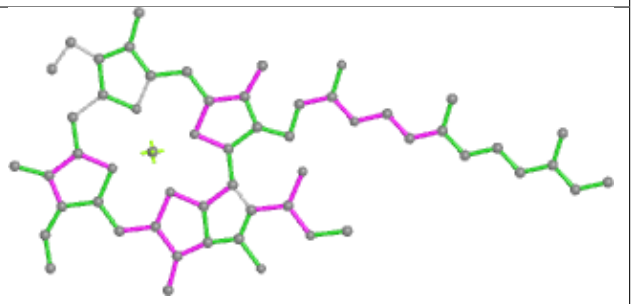


Rings

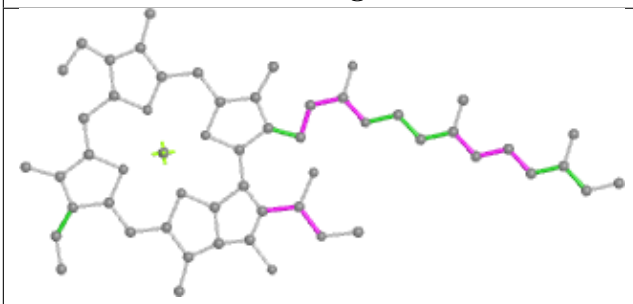
## Ligand CLA 3 616



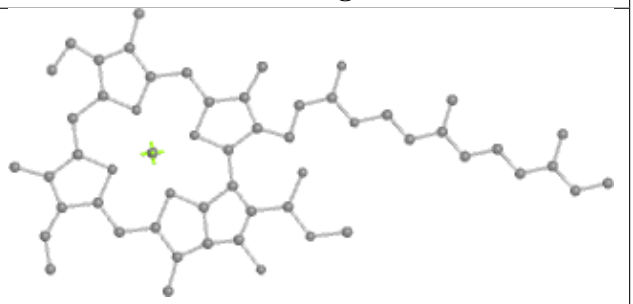
Bond lengths



Bond angles

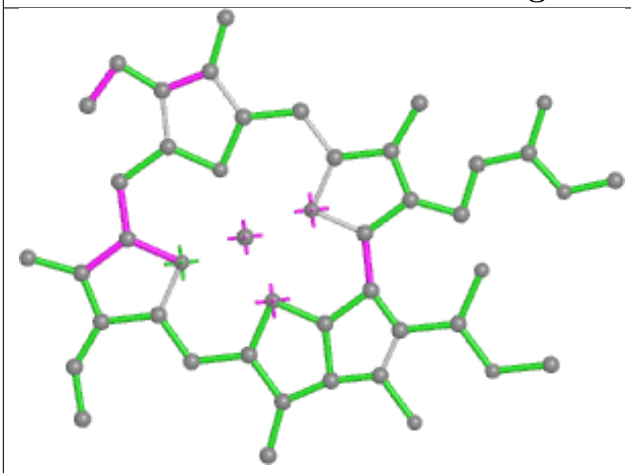


Torsions

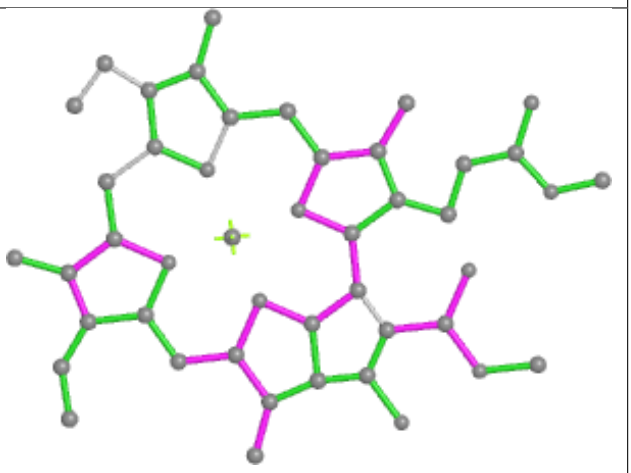


Rings

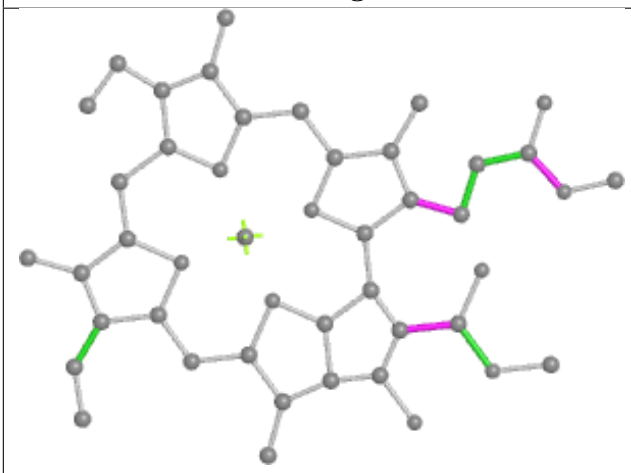
**Ligand CLA 8 607**



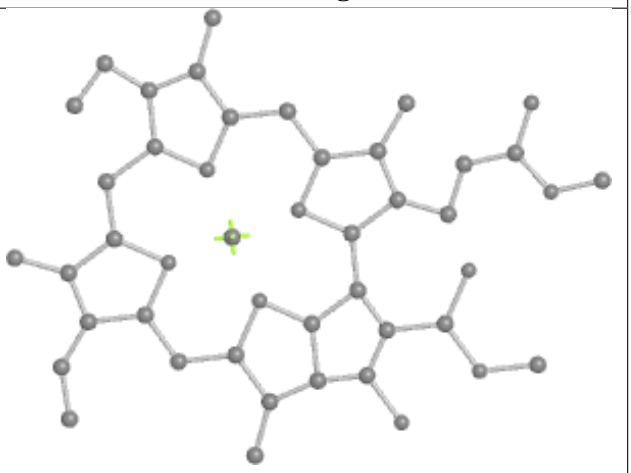
**Bond lengths**



**Bond angles**

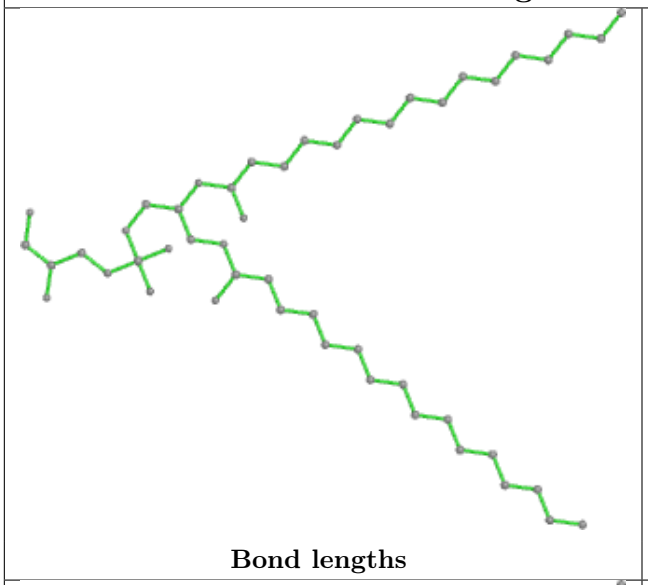


**Torsions**

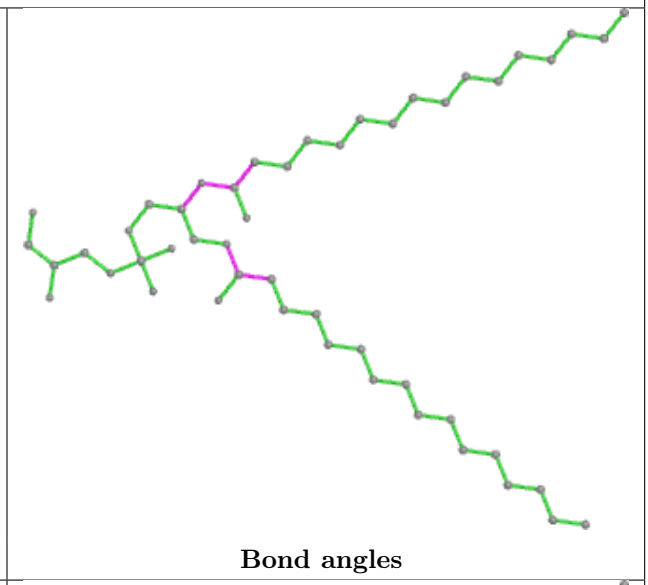


**Rings**

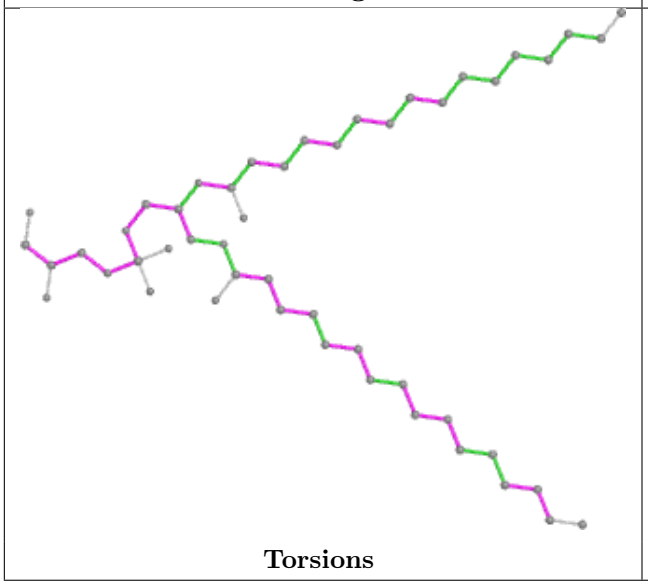
**Ligand LHG B 5002**



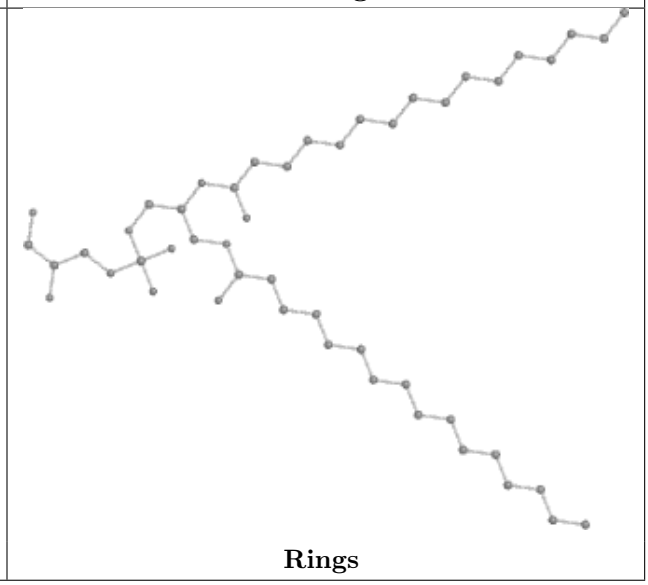
**Bond lengths**



**Bond angles**

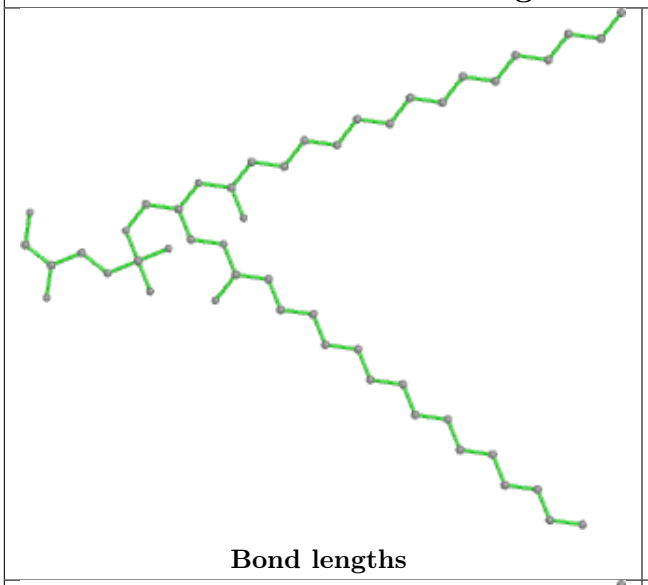


**Torsions**

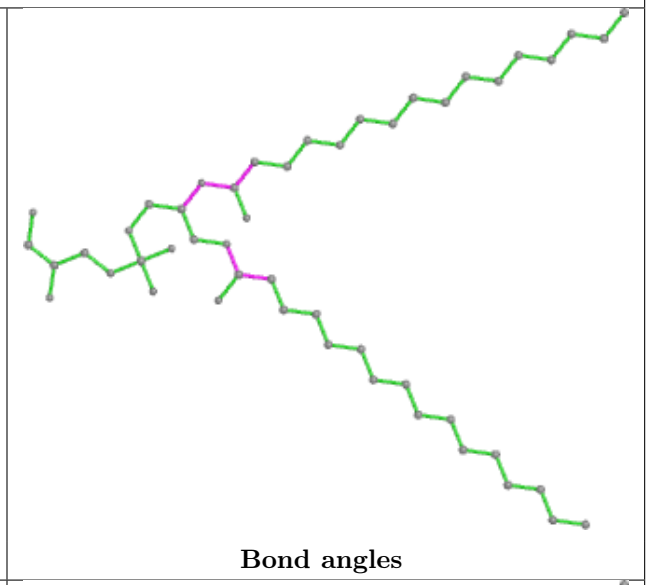


**Rings**

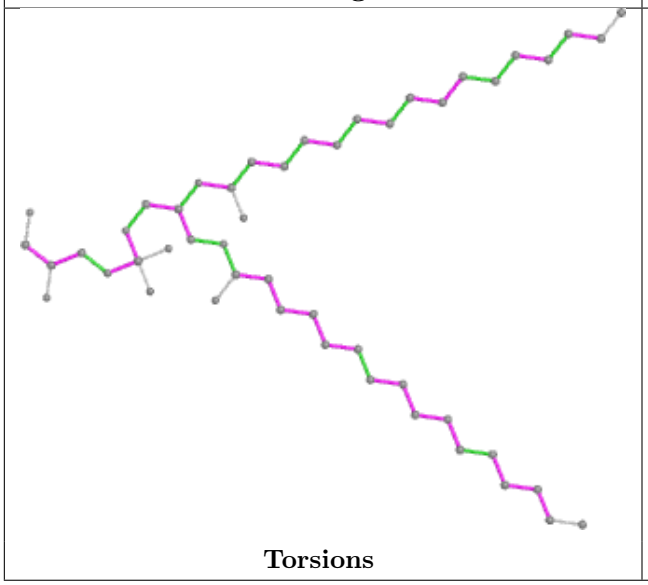
**Ligand LHG B 5001**



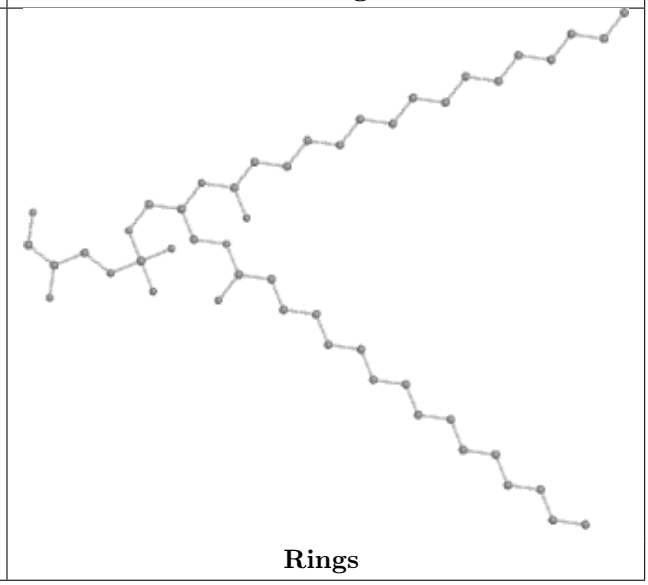
**Bond lengths**



**Bond angles**

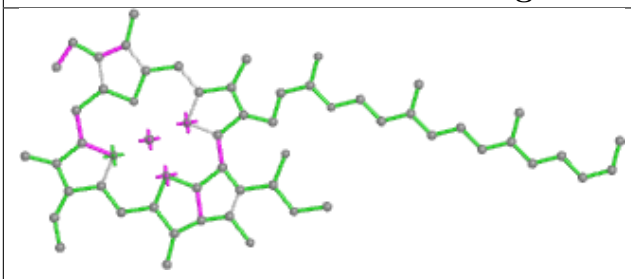


**Torsions**

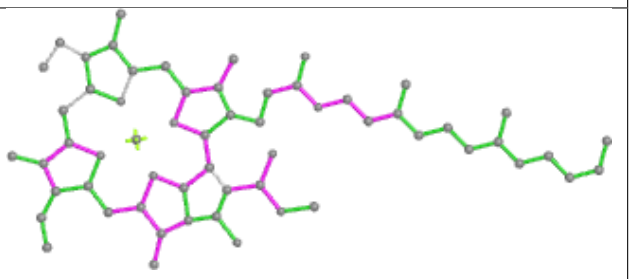


**Rings**

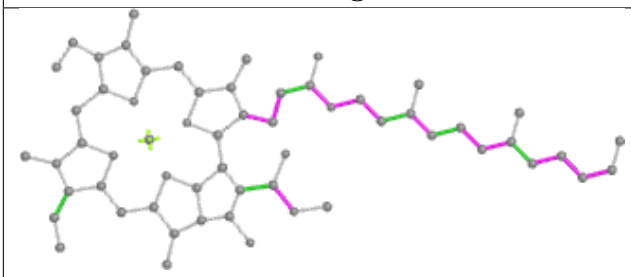
## Ligand CLA B 1214



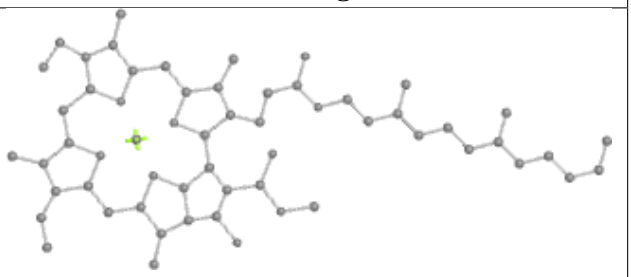
Bond lengths



Bond angles

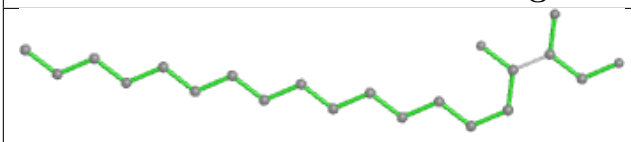


Torsions

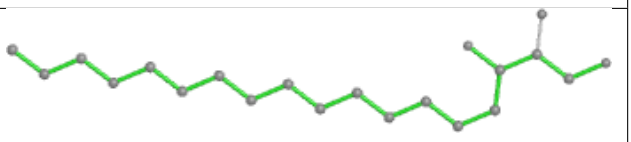


Rings

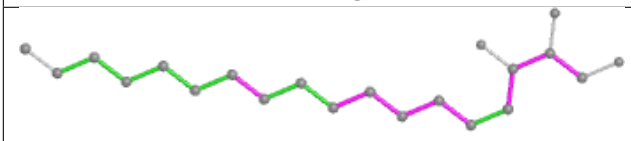
## Ligand SPH 9 804



Bond lengths



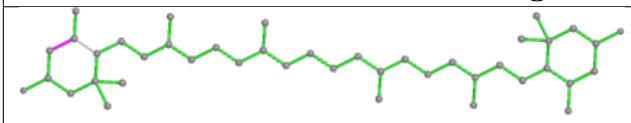
Bond angles



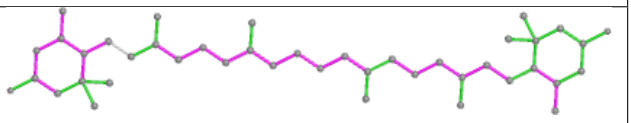
Torsions

Rings

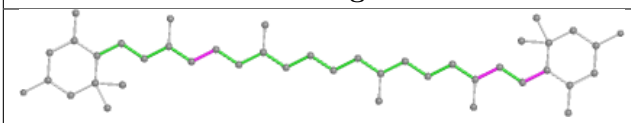
## Ligand LUT 4 502



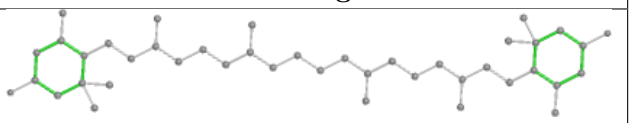
Bond lengths



Bond angles



Torsions



Rings

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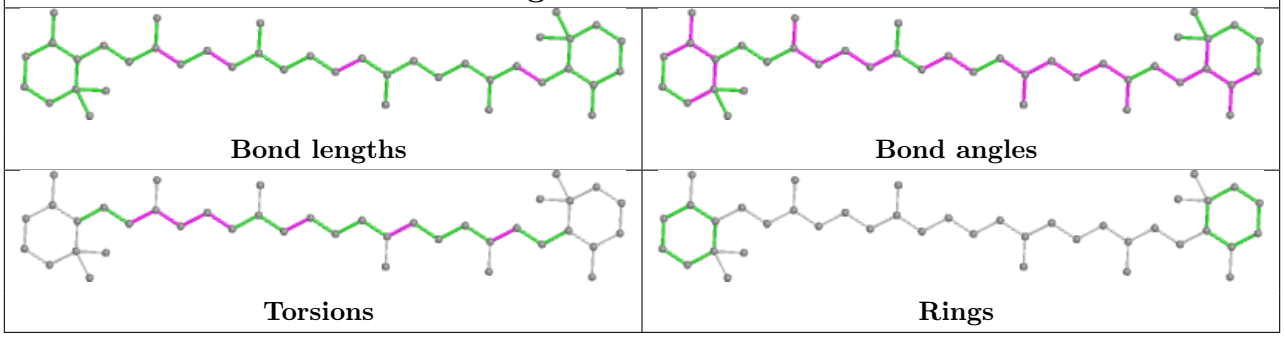
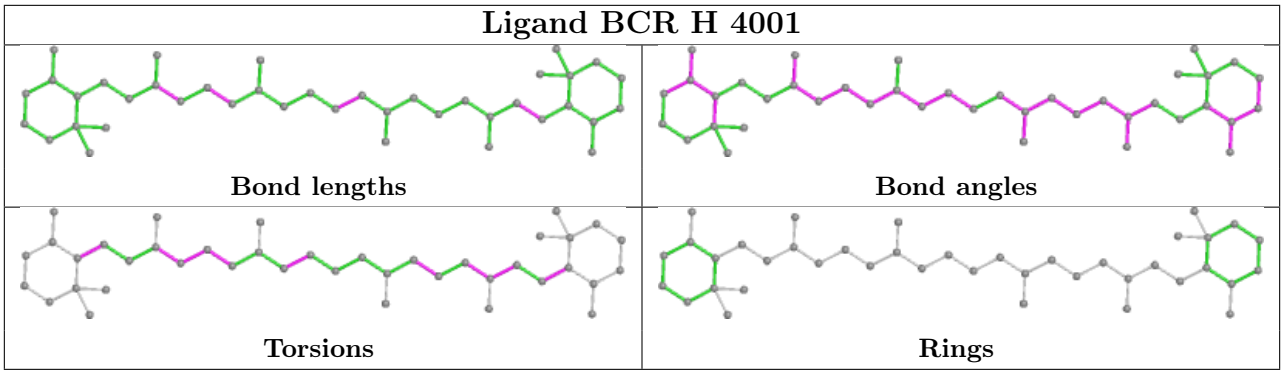
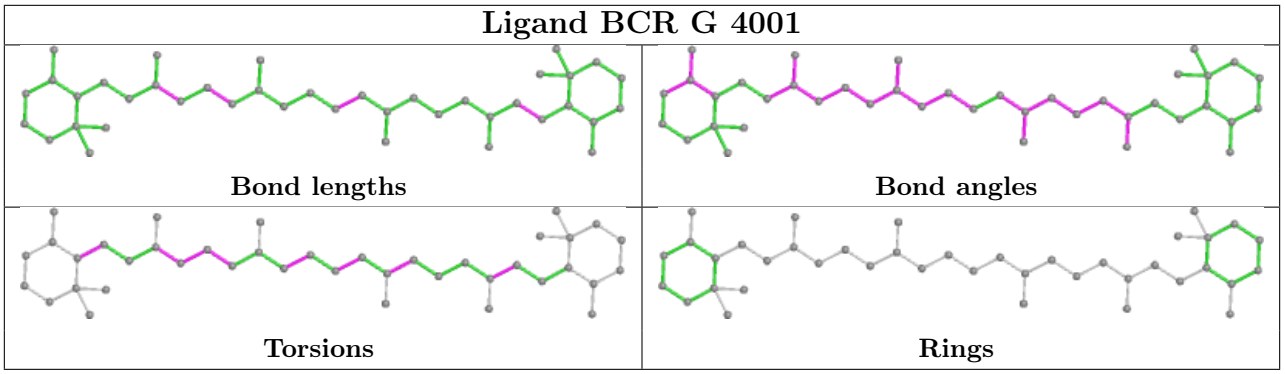



## Ligand BCR H 4001




## Ligand BCR G 4001

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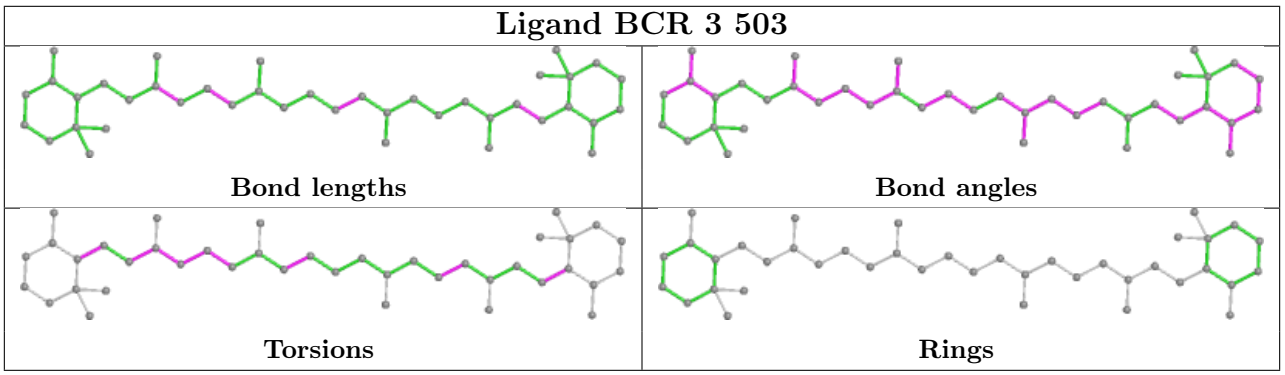
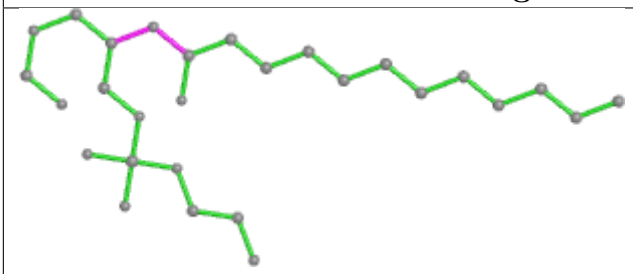
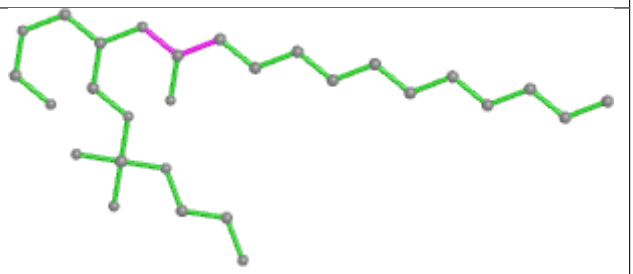


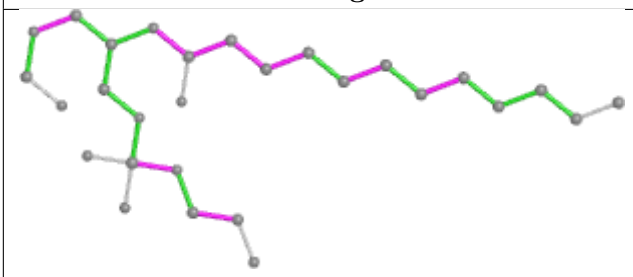
## Ligand PTY G 5003



Bond lengths



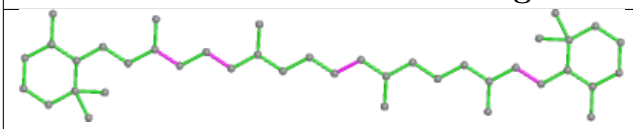
Bond angles



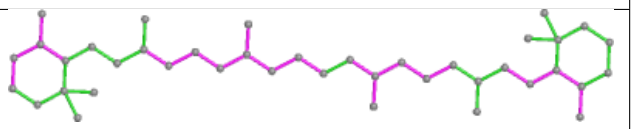
Torsions

Rings

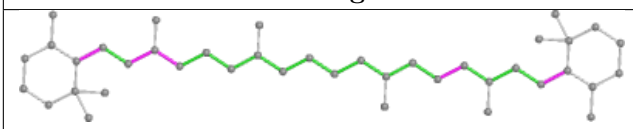
## Ligand BCR B 4004



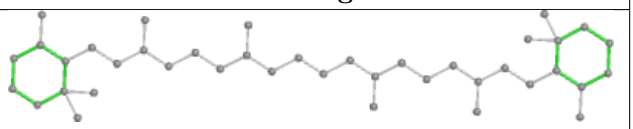
Bond lengths



Bond angles

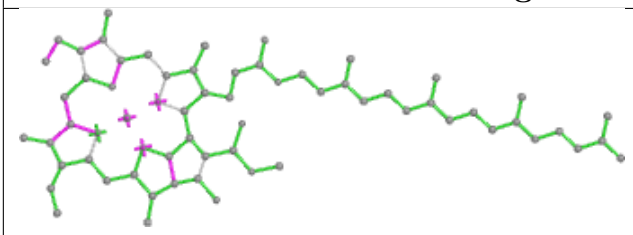


Torsions

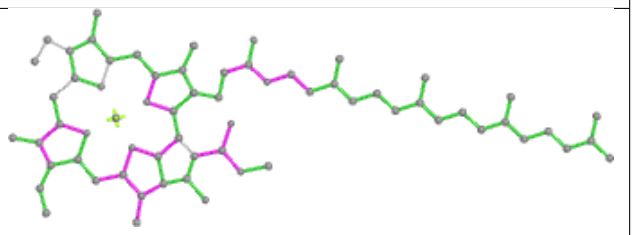


Rings

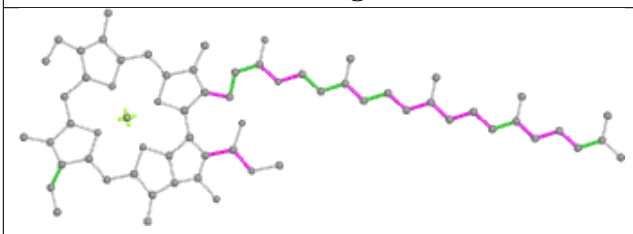
## Ligand CLA A 1133



Bond lengths



Bond angles



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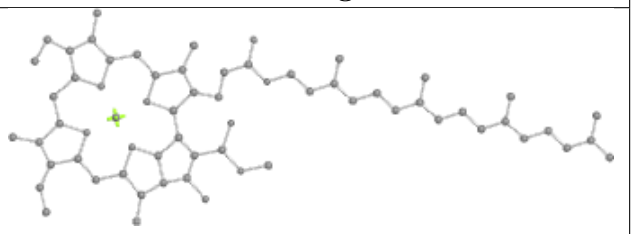
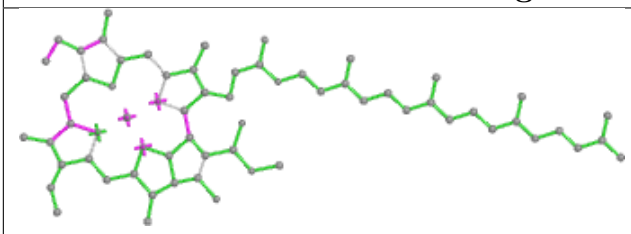
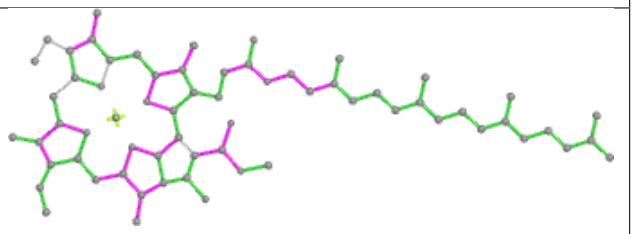


Rings

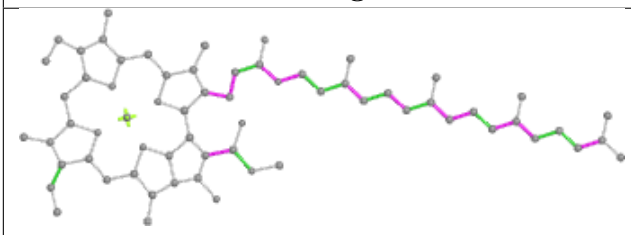
## Ligand CLA B 1235



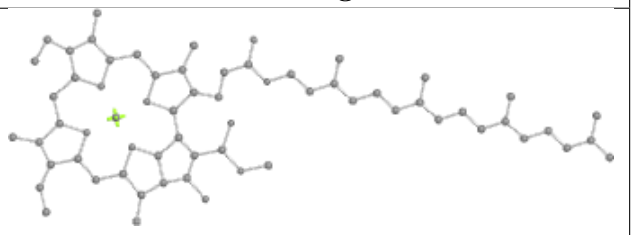
Bond lengths



Bond angles

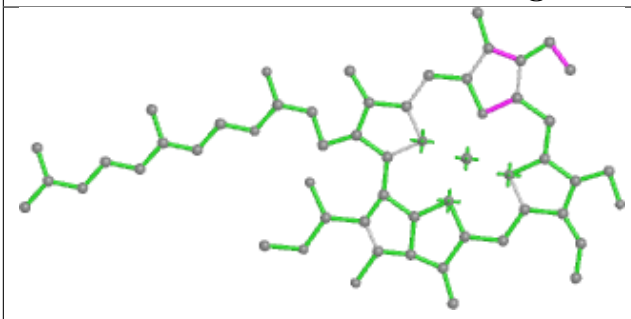


Torsions



Rings

## Ligand CHL 8 610



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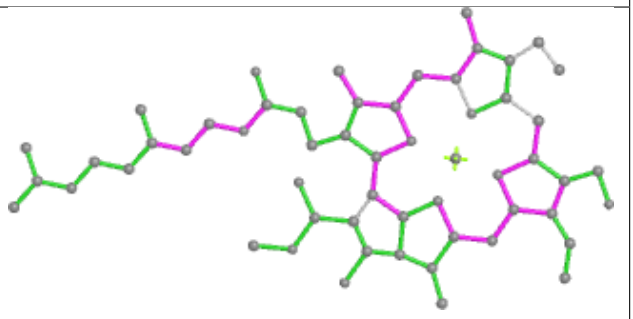
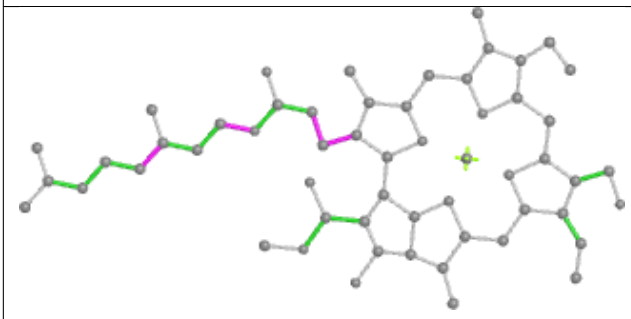
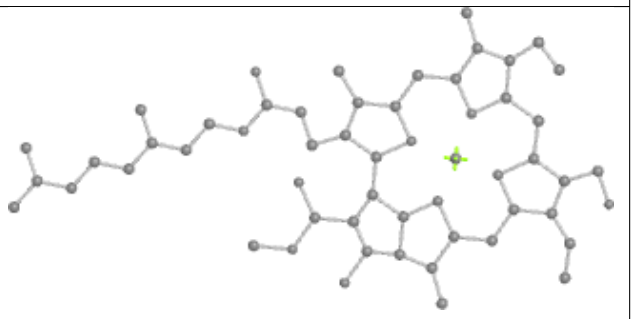


Bond angles

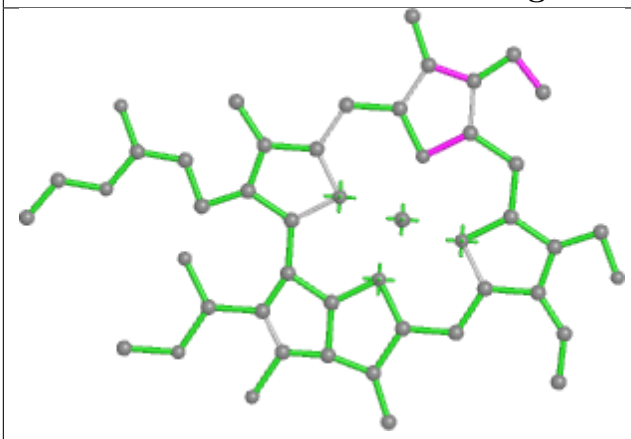


Torsions

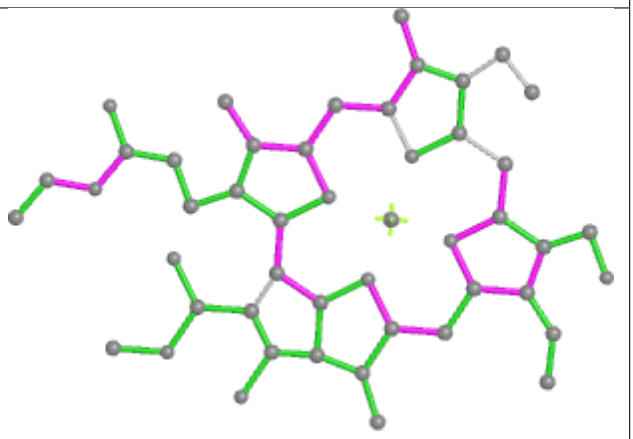


Rings

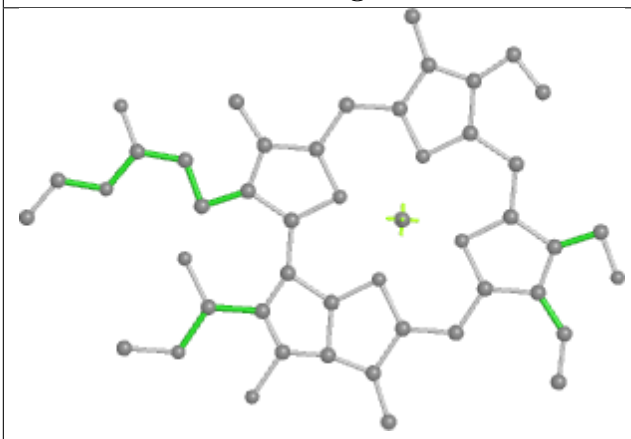
## Ligand CHL a 610



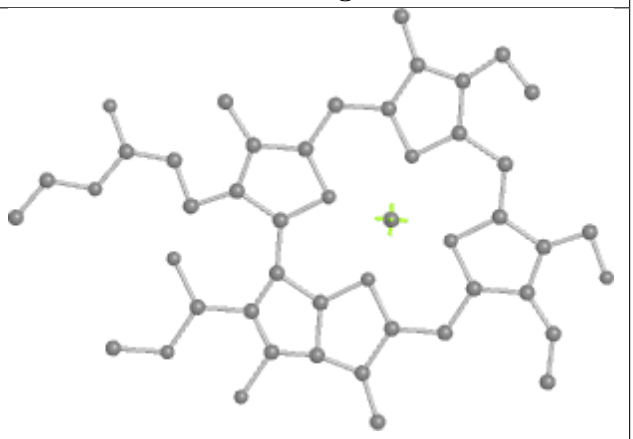
Bond lengths



Bond angles

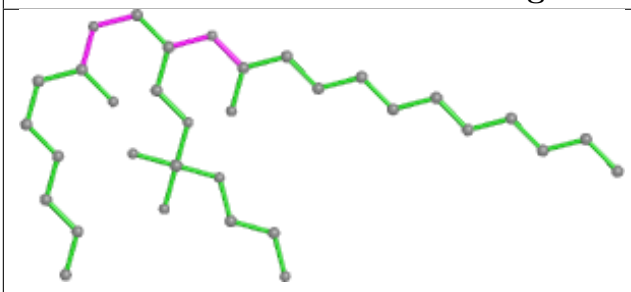


Torsions



Rings

## Ligand PTY 7 804



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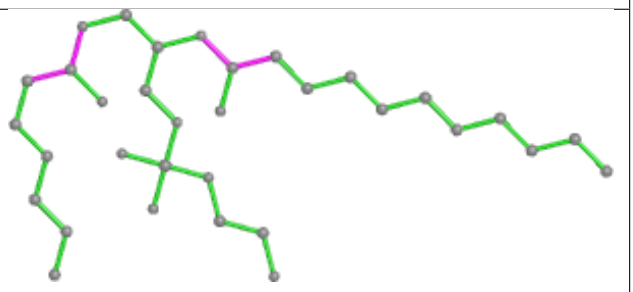
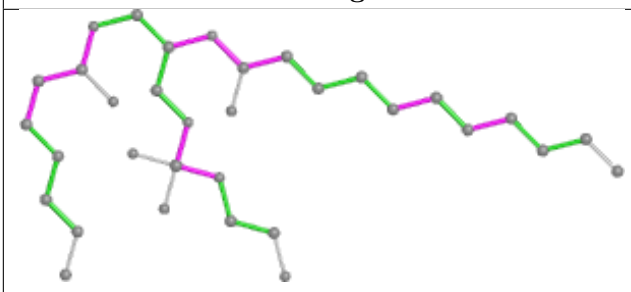


Bond angles



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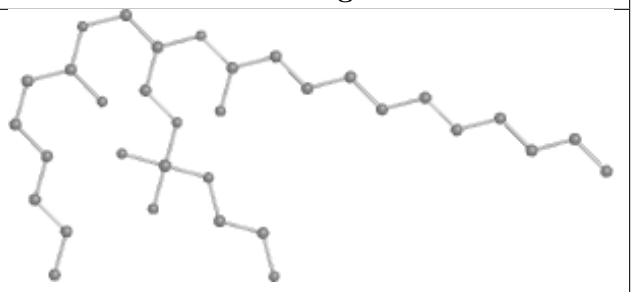
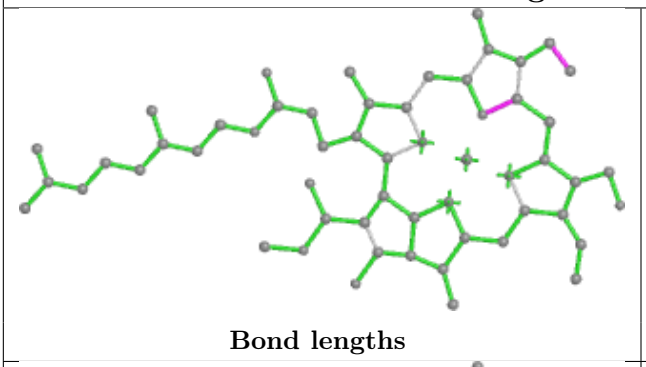
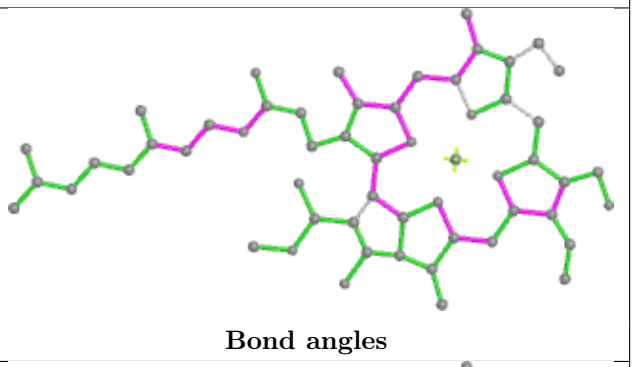


Rings

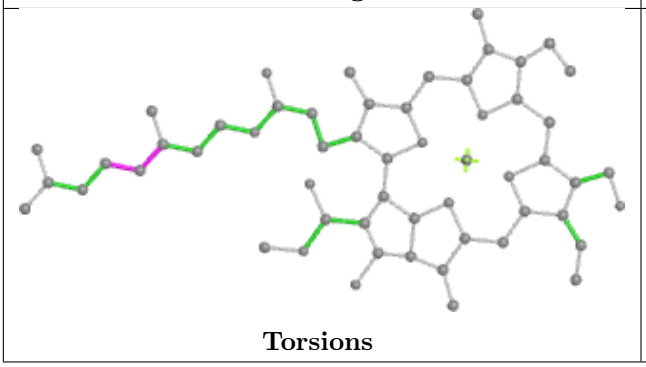
## Ligand CHL 5 613



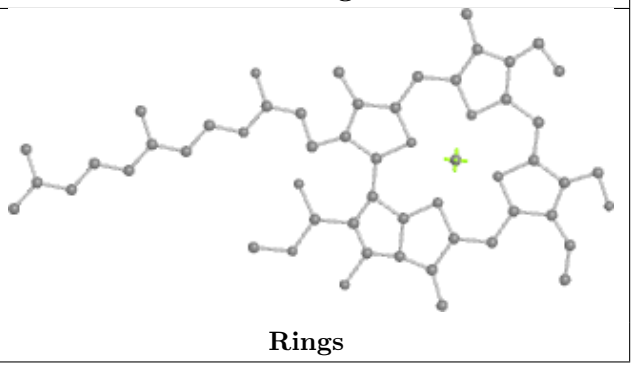
Bond lengths



Bond angles

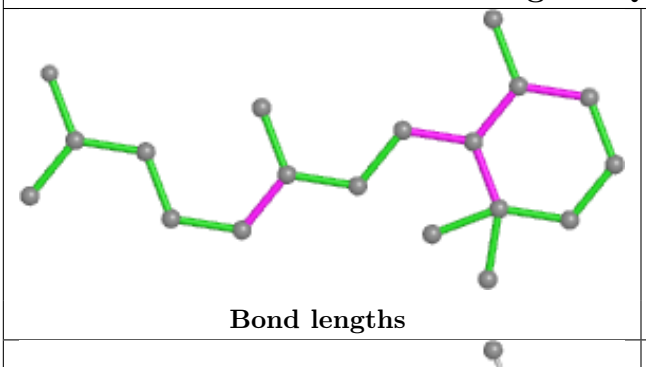


Torsions

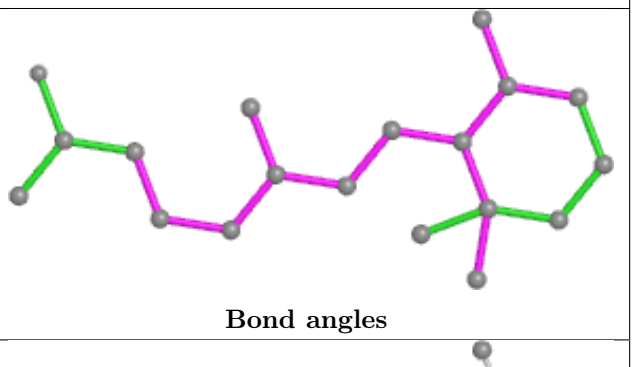


Rings

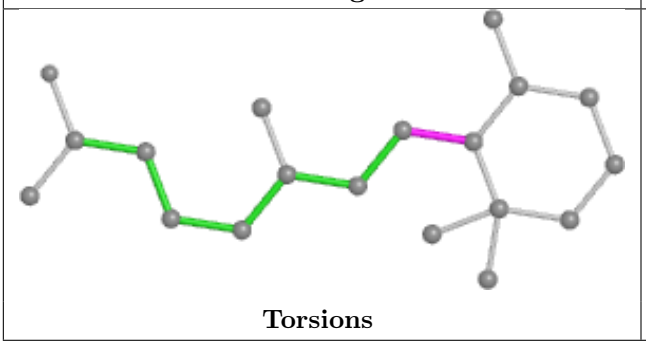
## Ligand QTB a 504



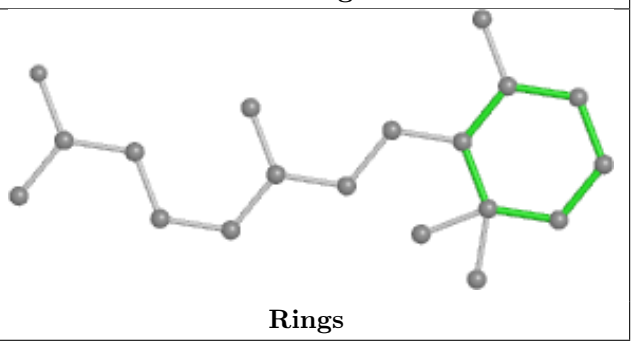
Bond lengths



Bond angles

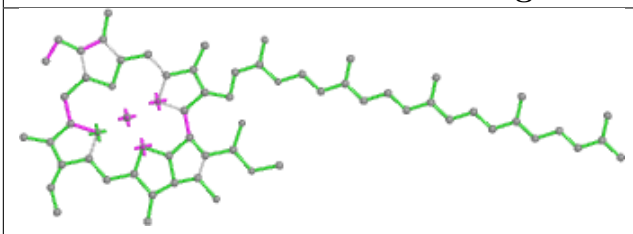


Torsions

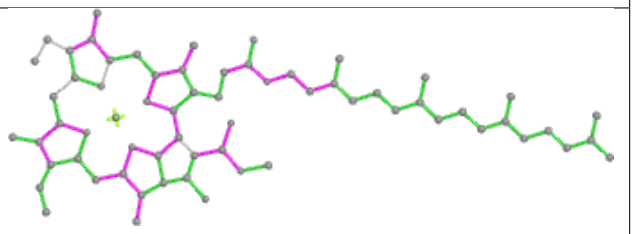


Rings

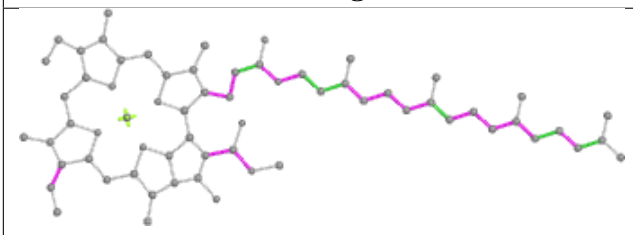
## Ligand CLA B 1206



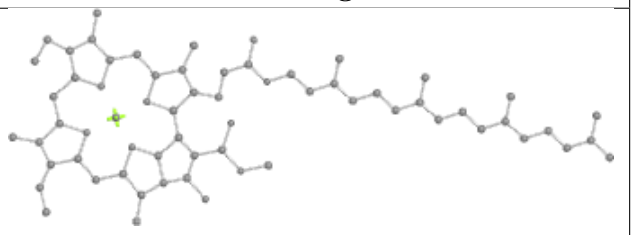
Bond lengths



Bond angles

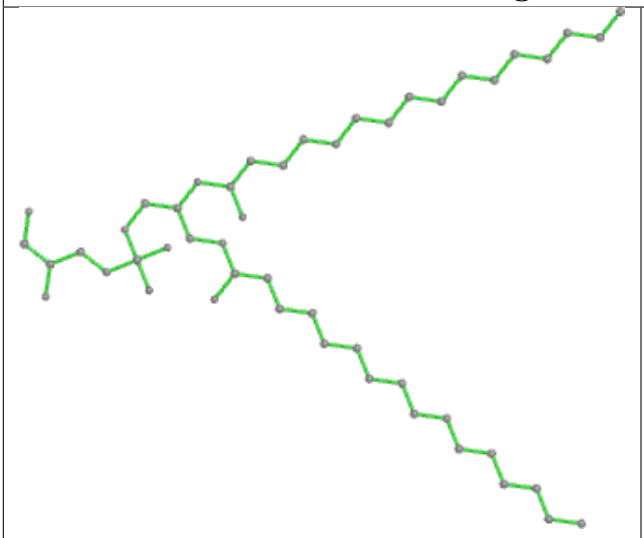


Torsions

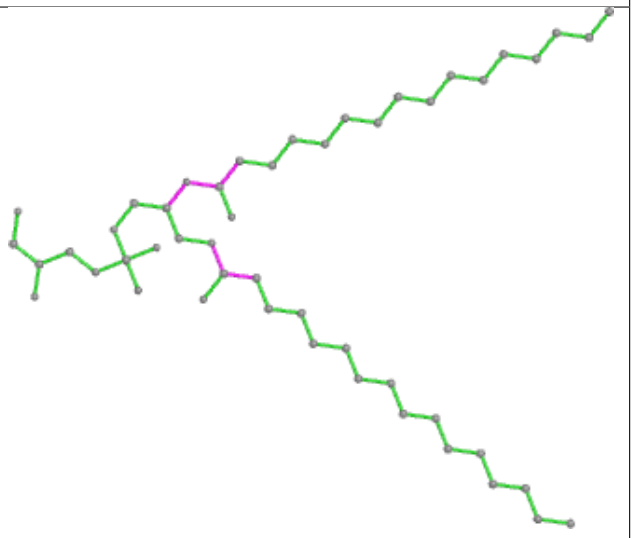


Rings

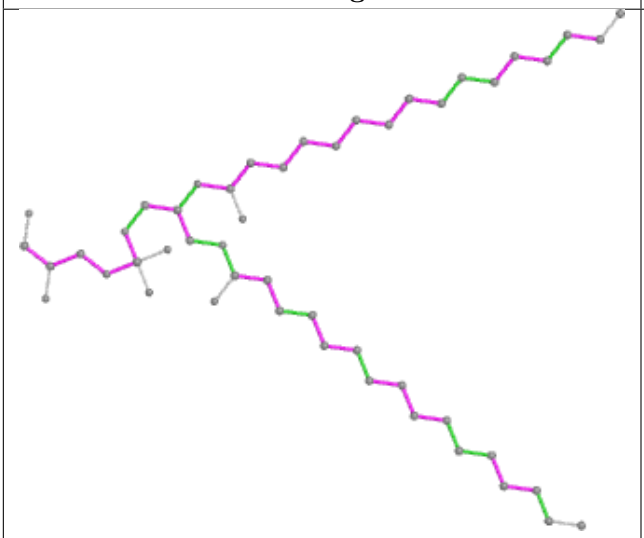
## Ligand LHG A 5002



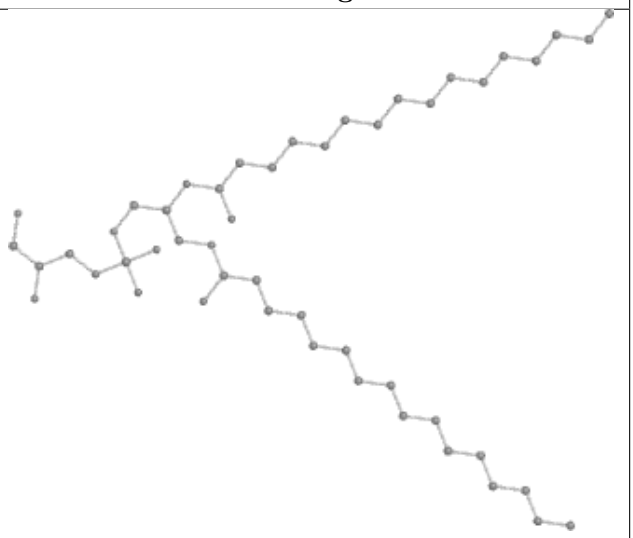
Bond lengths



Bond angles

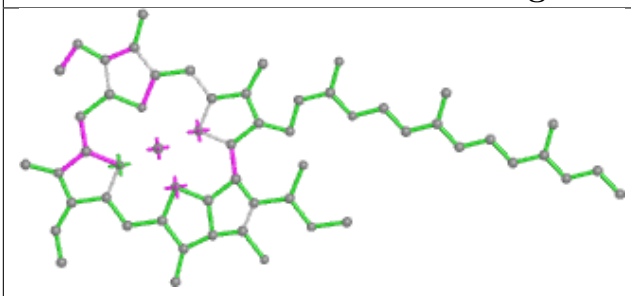


Torsions

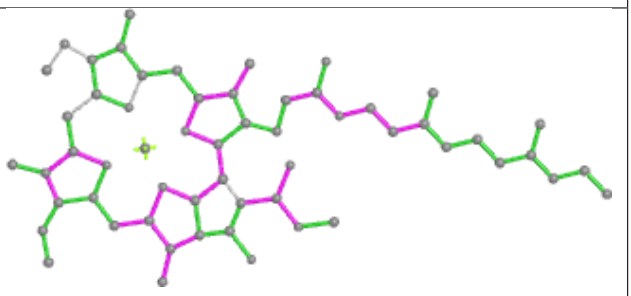


Rings

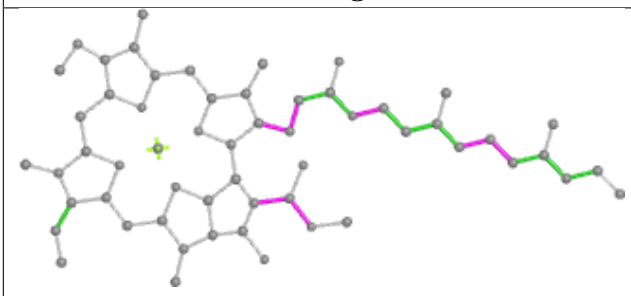
## Ligand CLA a 612



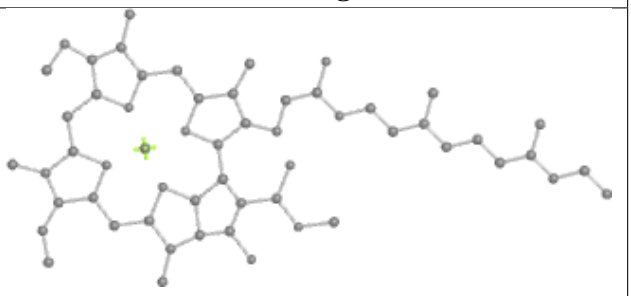
Bond lengths



Bond angles

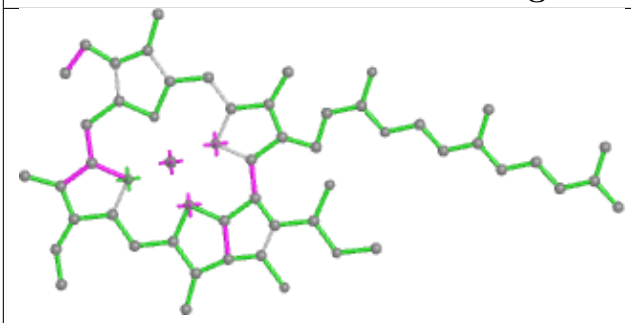


Torsions



Rings

## Ligand CLA a 605



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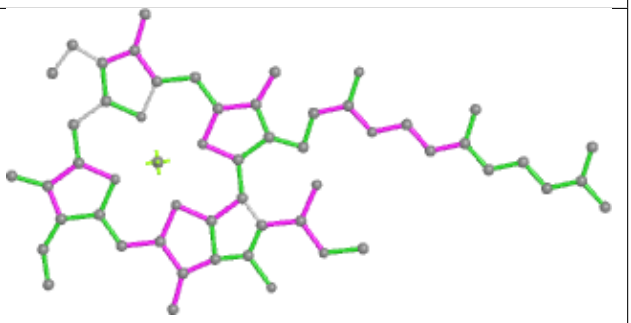

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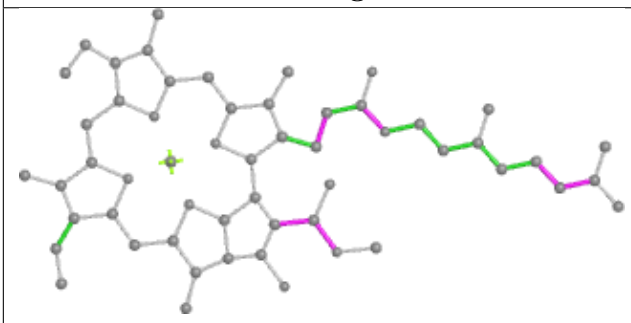

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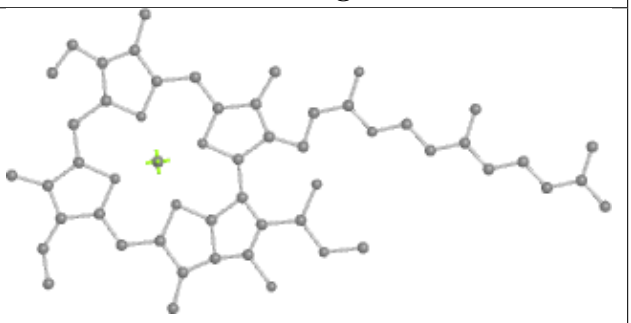
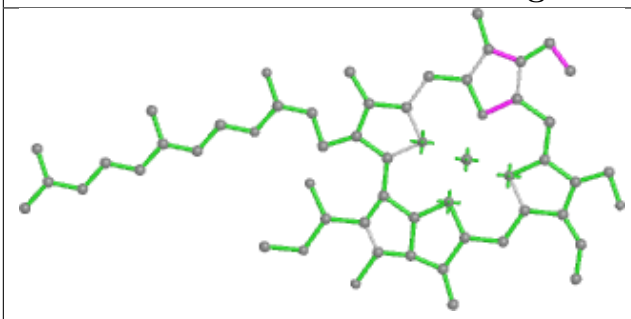


Rings

## Ligand CHL 1 611



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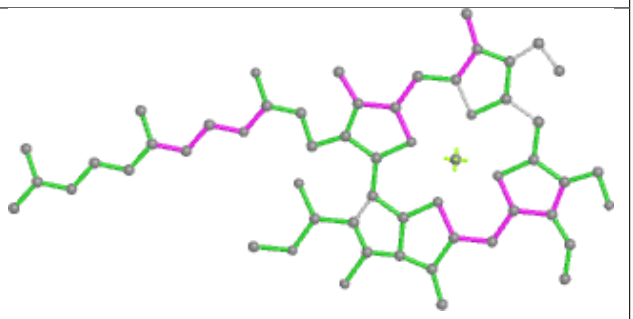

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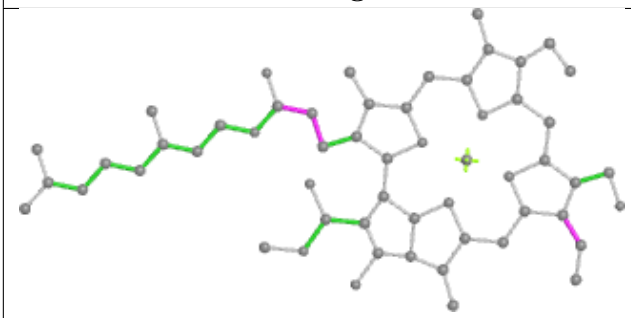

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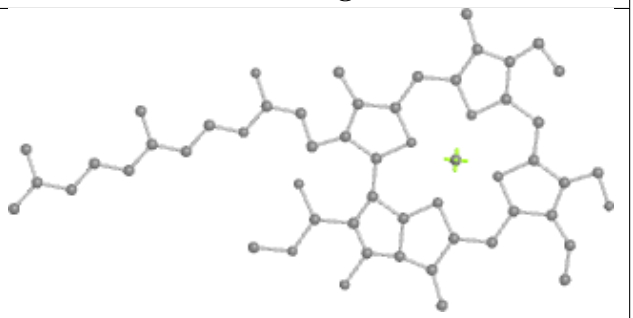

Rings

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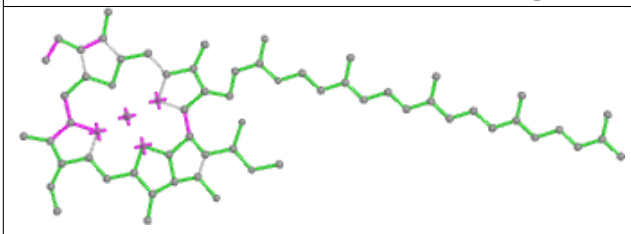

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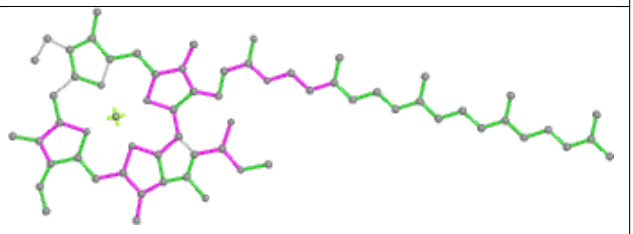

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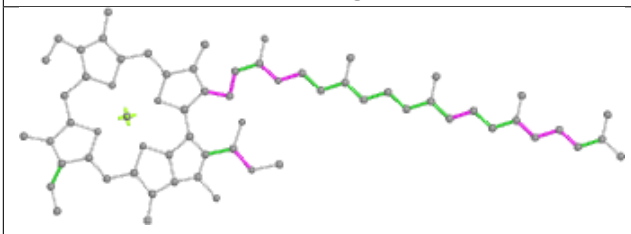

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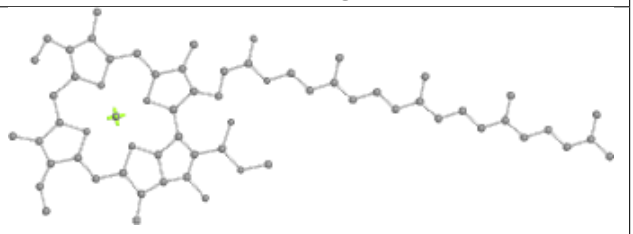
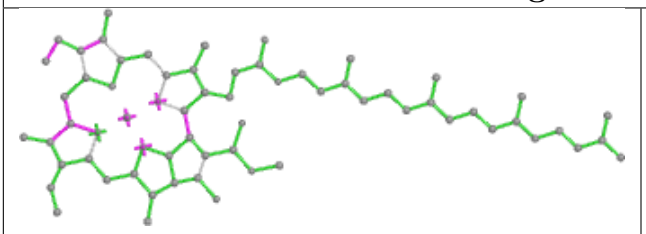


Rings

## Ligand CLA 6 615



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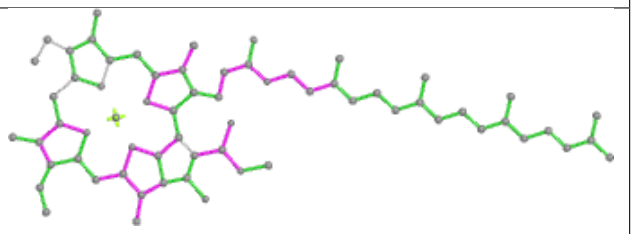
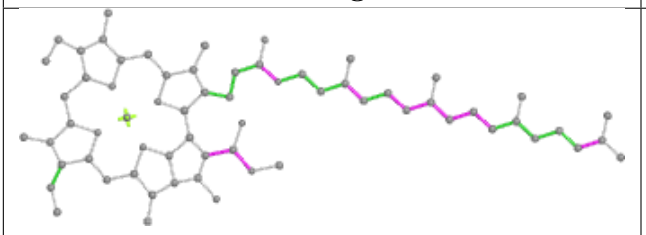


Bond angles



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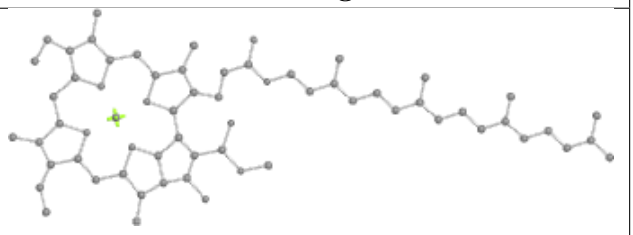
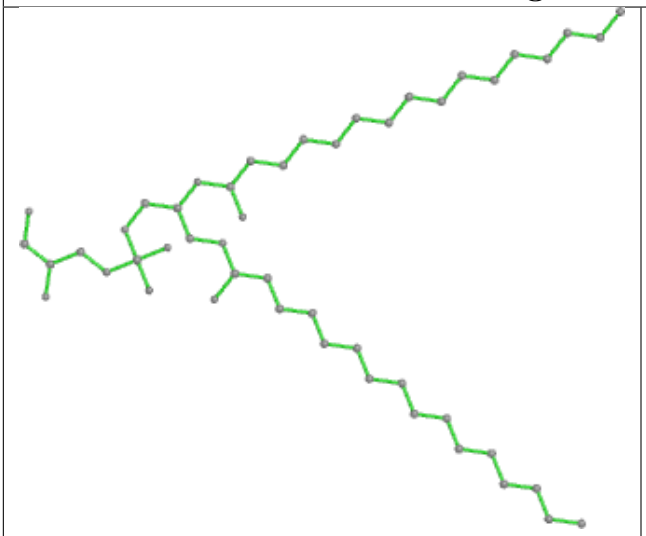


Rings

## Ligand LHG 5 801



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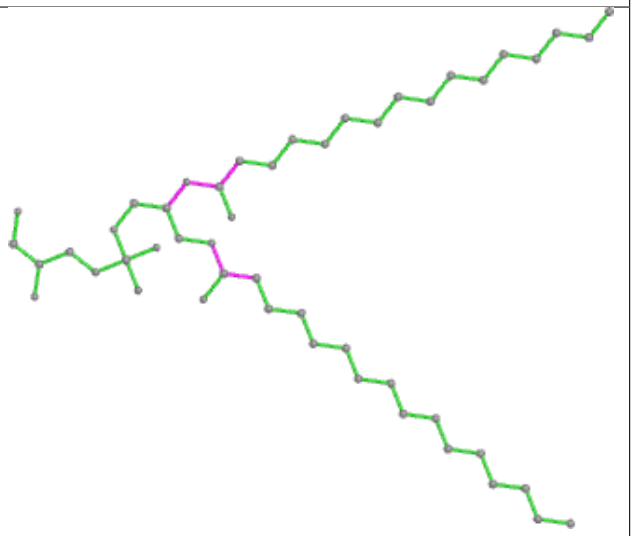

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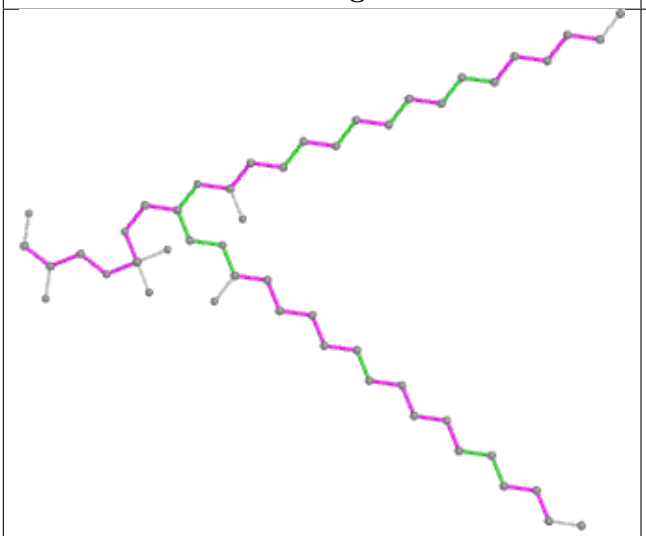

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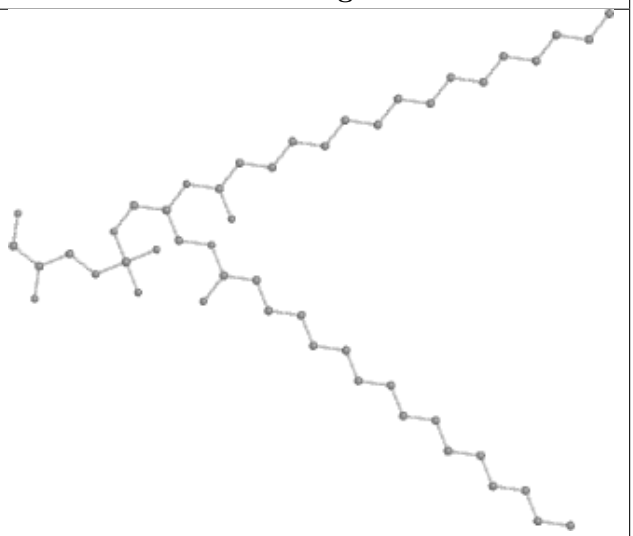
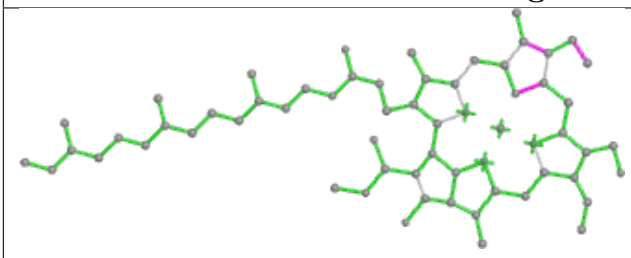


Rings

## Ligand CHL 7 609



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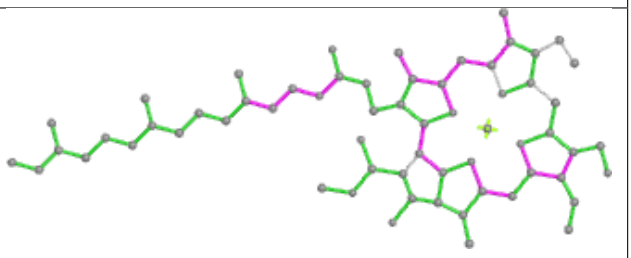
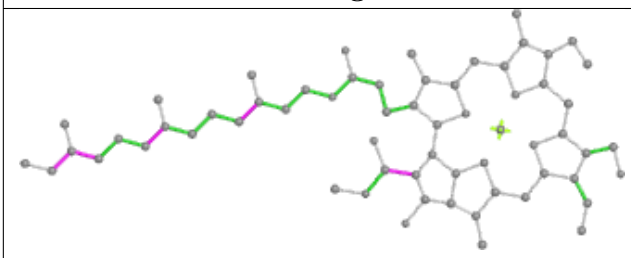


Bond angles



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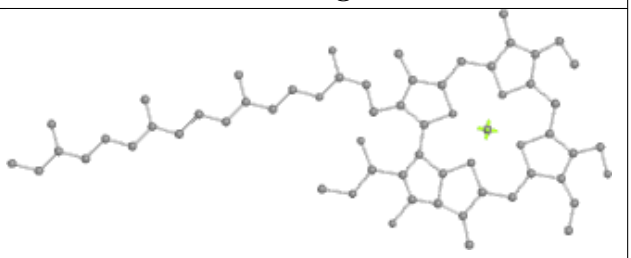
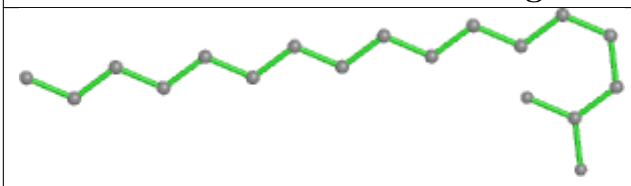


Rings

## Ligand PLM 8 807



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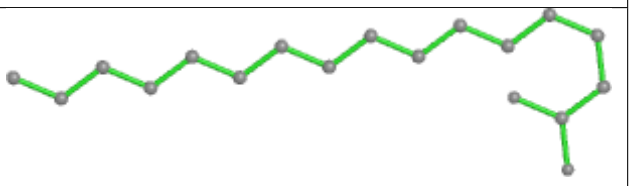

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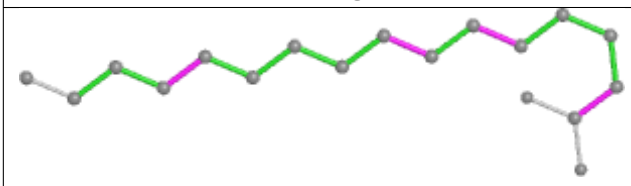

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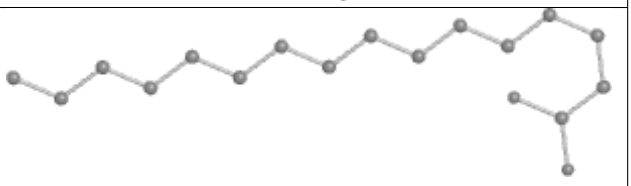
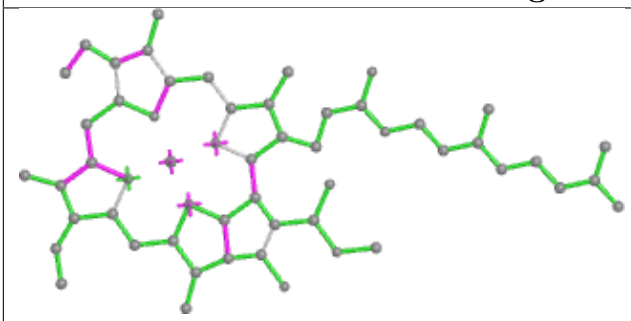


Rings

## Ligand CLA 6 608



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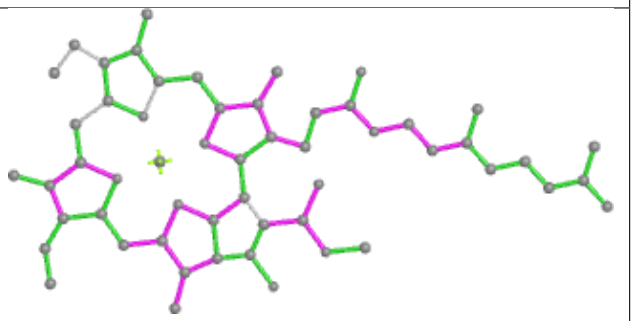
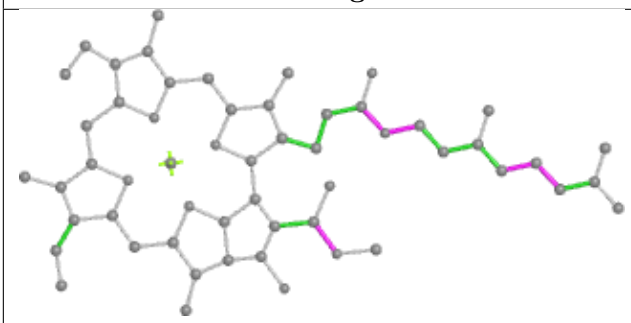


Bond angles



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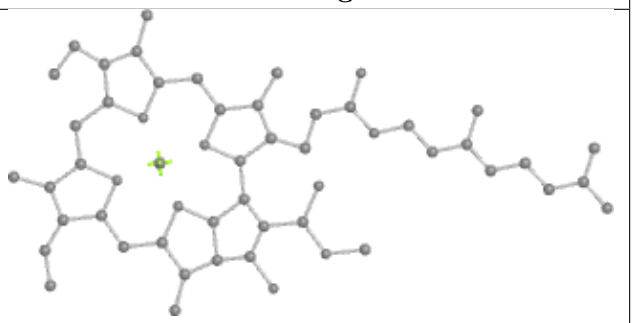
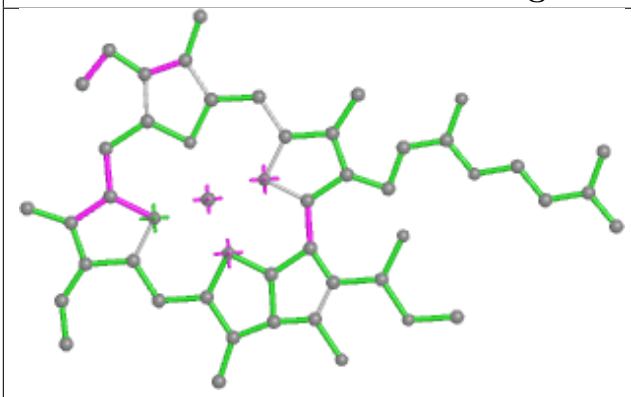
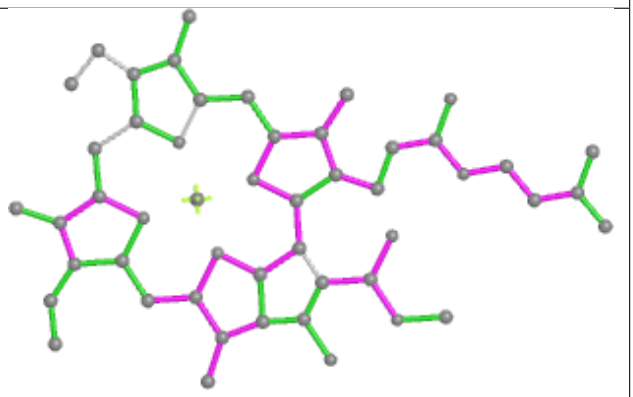


Rings

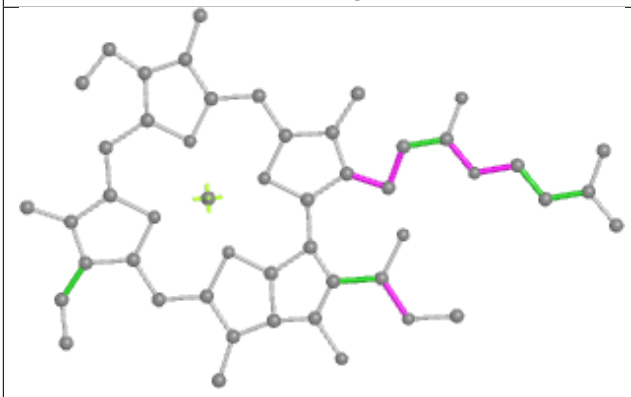
## Ligand CLA a 602



Bond lengths



Bond angles



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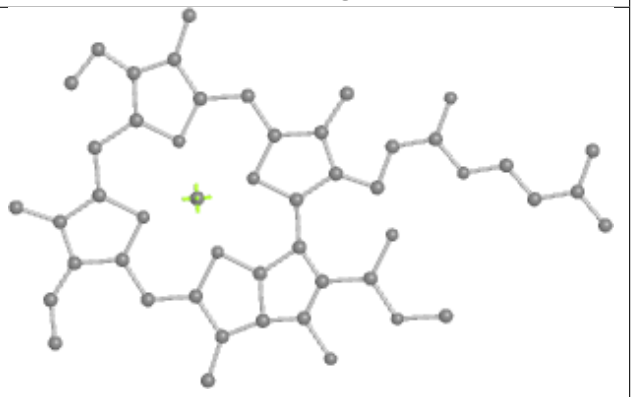

Rings

| Ligand CLA B 1236 | |
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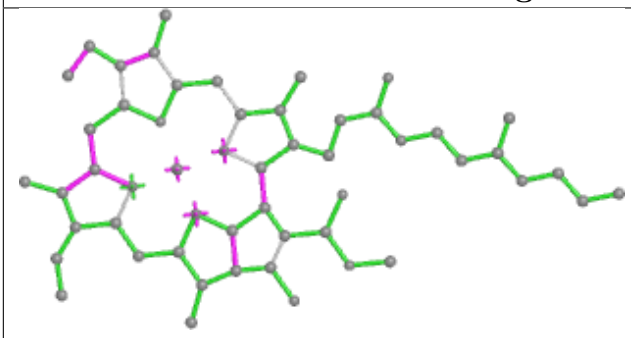
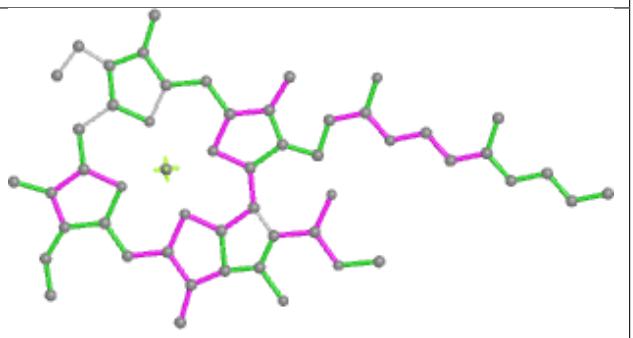
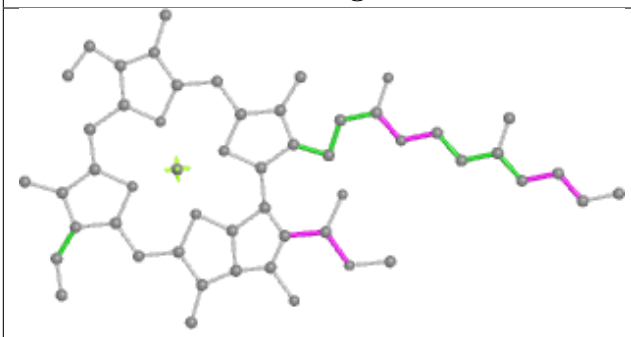
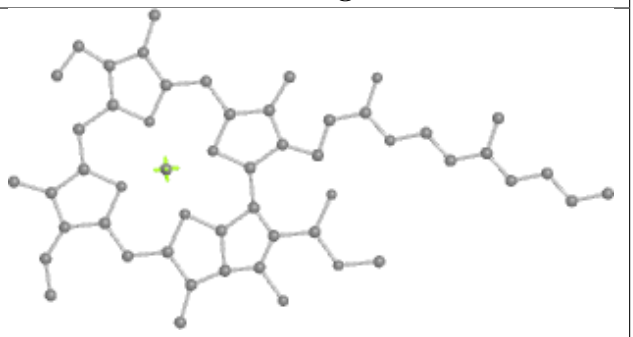
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA B 1208 | |
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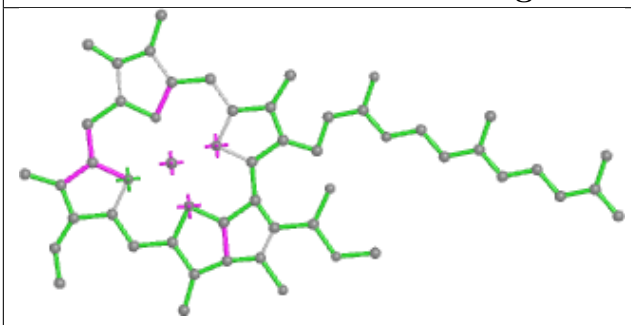
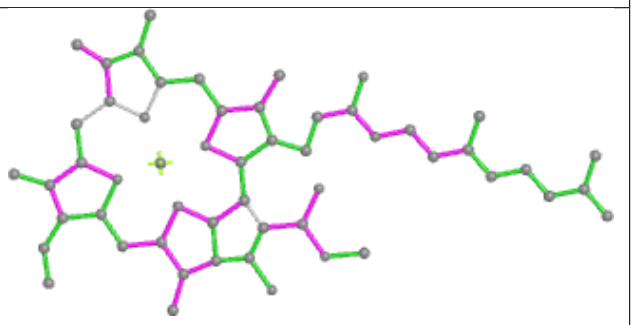
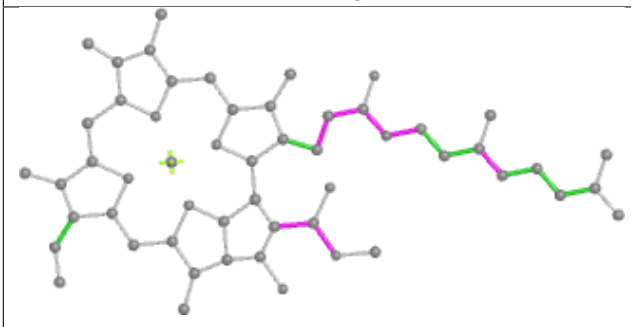
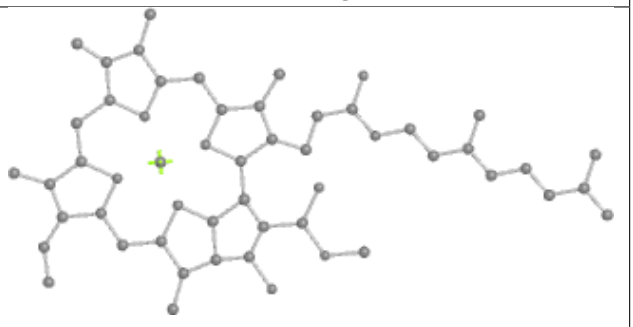
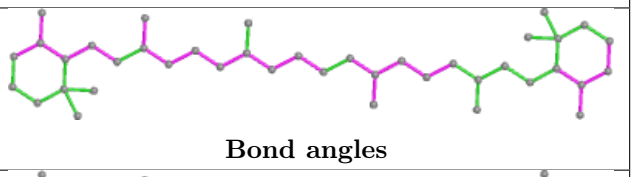
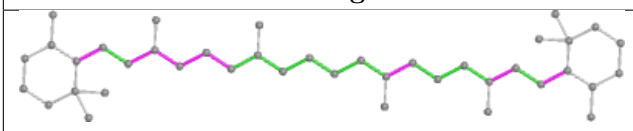
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## Ligand BCR 6 504

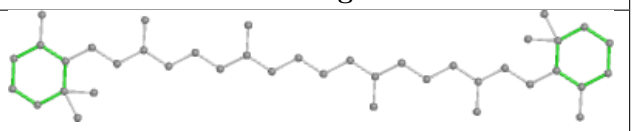
Bond lengths



Bond angles

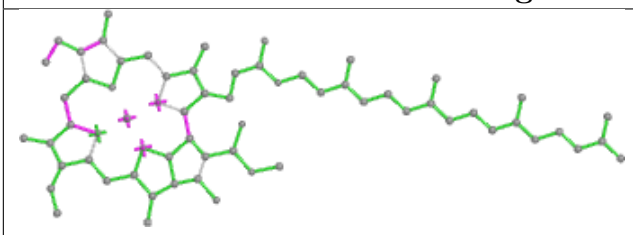


Torsions

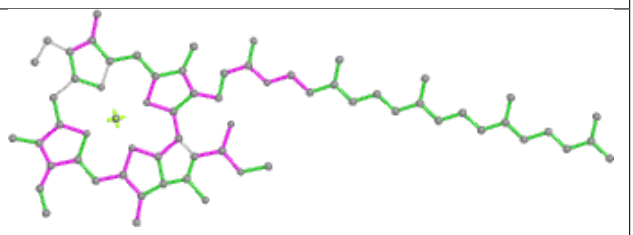


Rings

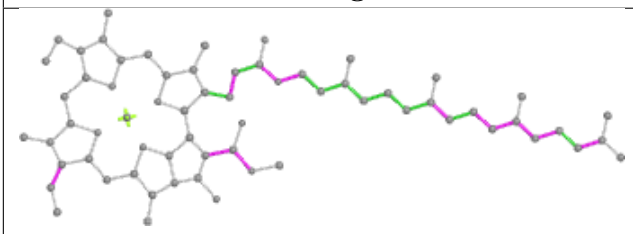
## Ligand CLA B 1023



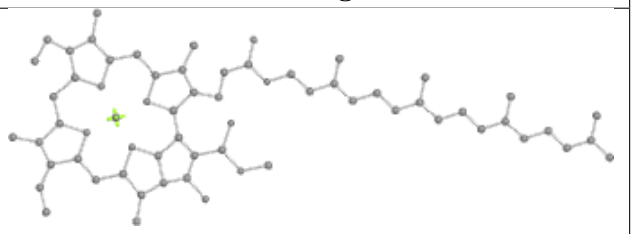
Bond lengths



Bond angles

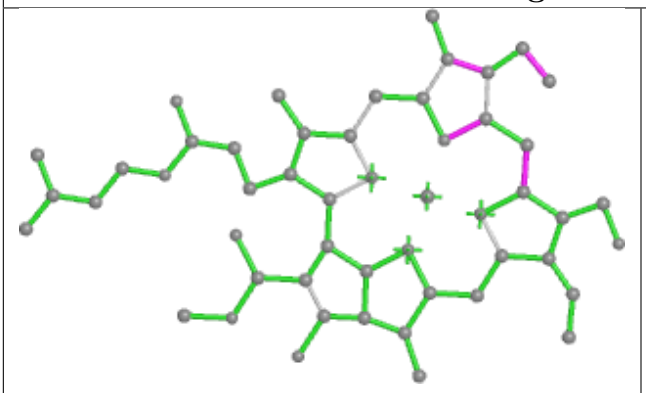


Torsions

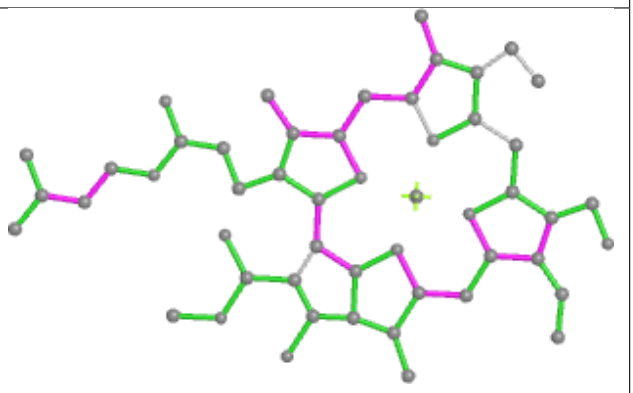


Rings

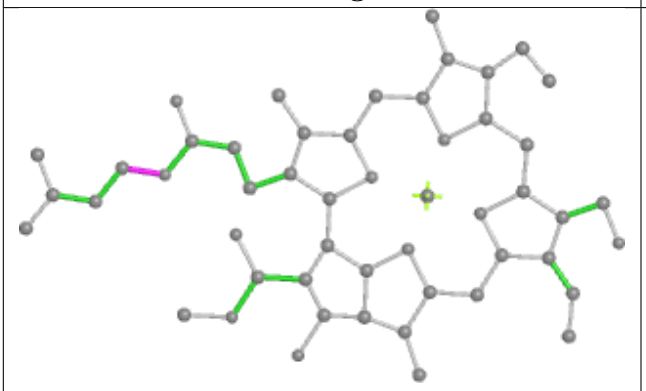
## Ligand CHL 5 611



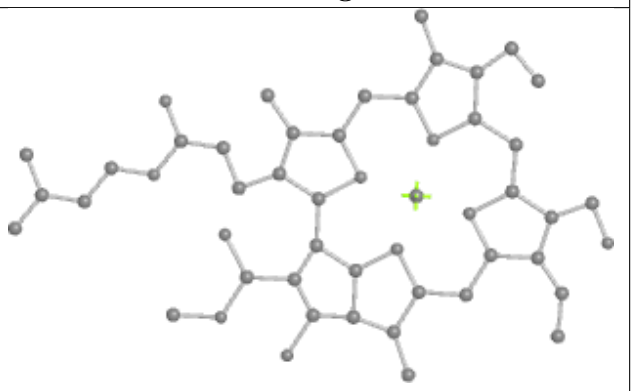
Bond lengths



Bond angles

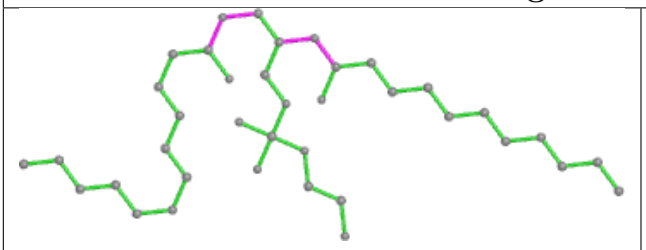


Torsions



Rings

## Ligand PTY 3 802



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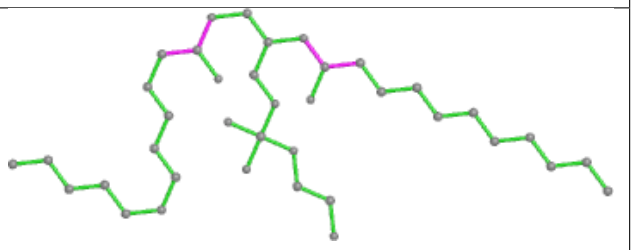

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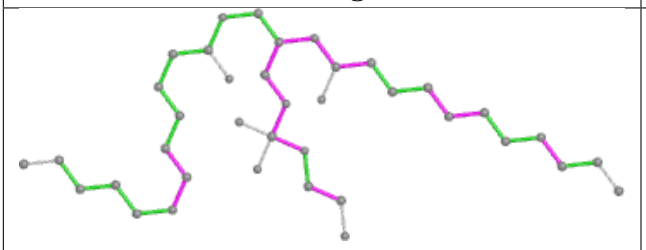

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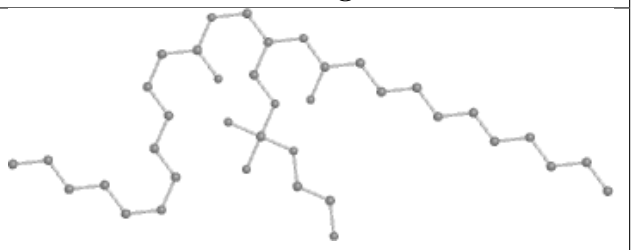
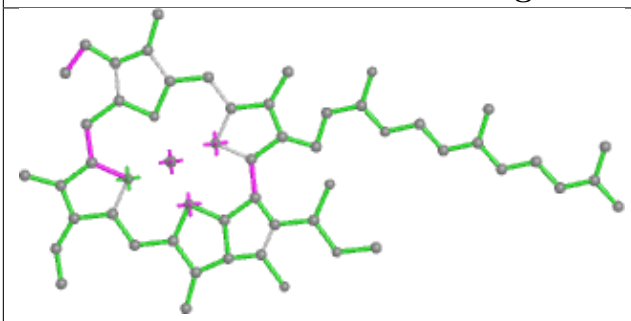


Rings

## Ligand CLA A 1112



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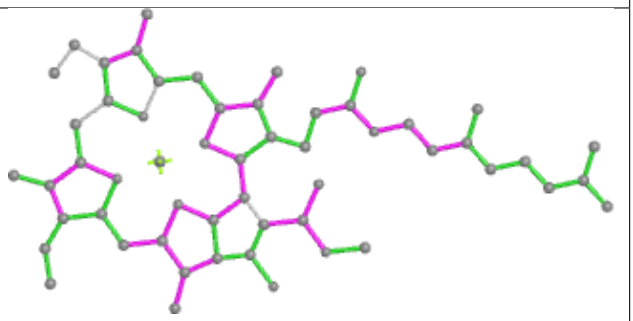
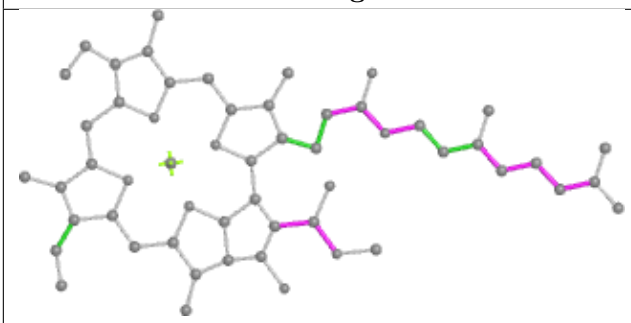


Bond angles



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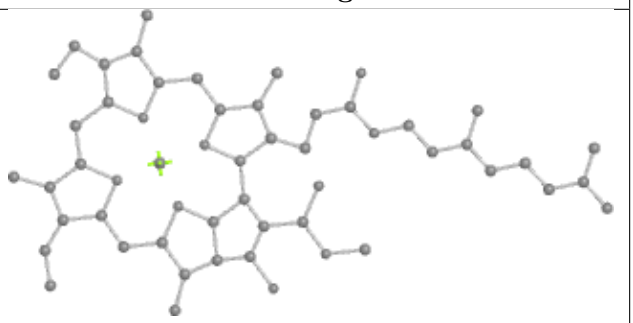
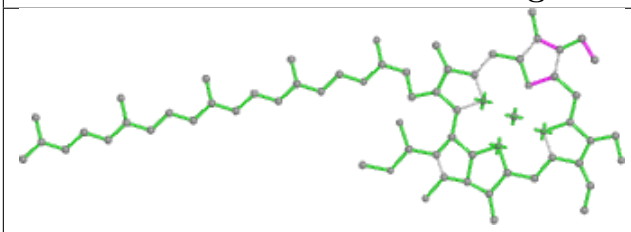


Rings

## Ligand CHL 1 609



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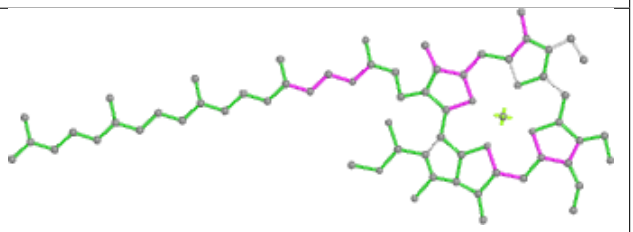
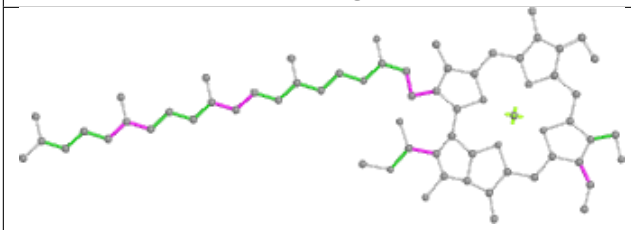


Bond angles



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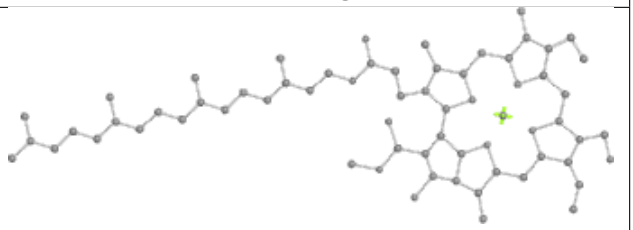
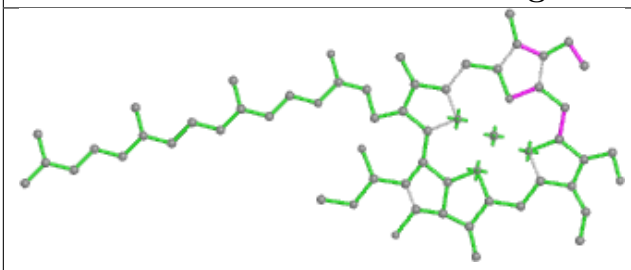


Rings

## Ligand CHL a 604



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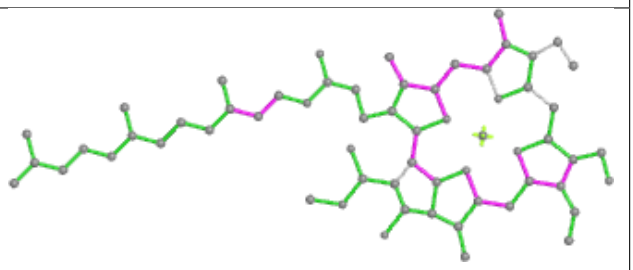
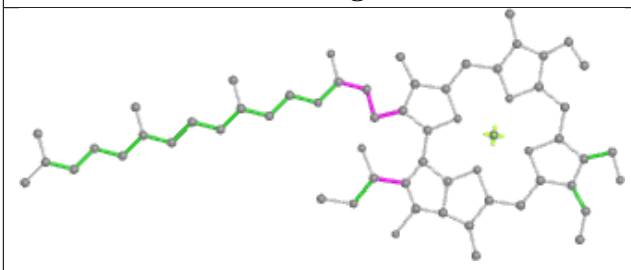


Bond angles



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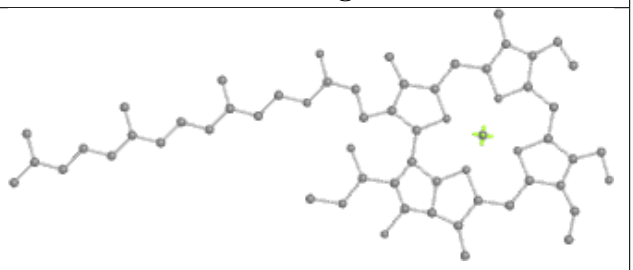
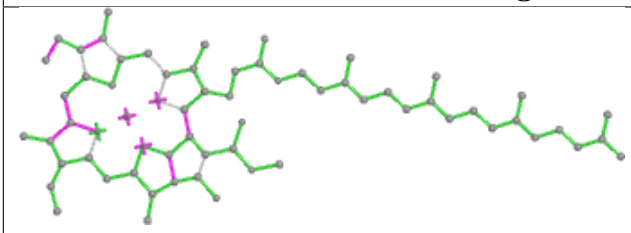
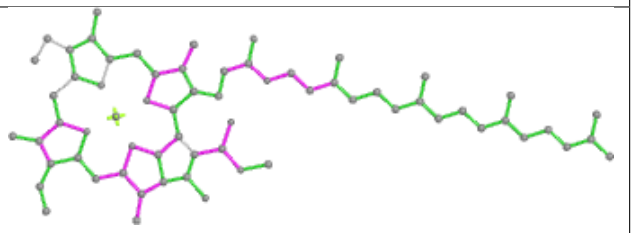


Rings

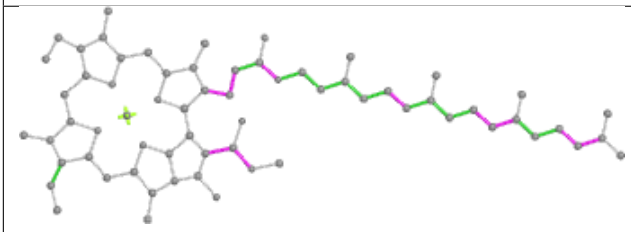
## Ligand CLA B 1202



Bond lengths



Bond angles



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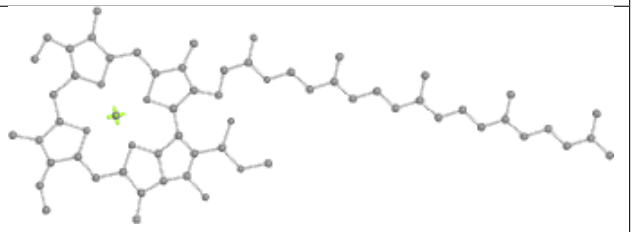
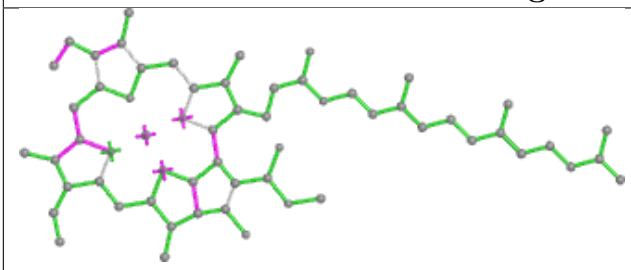


Rings

## Ligand CLA 2 605



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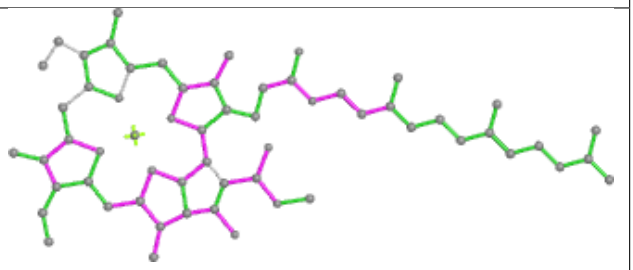
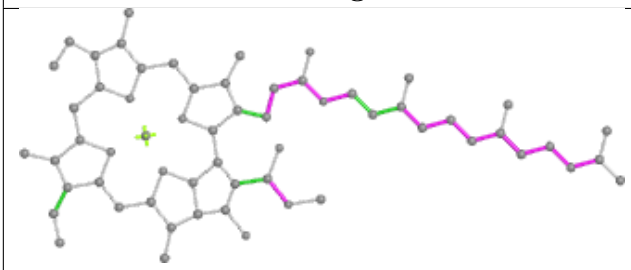


Bond angles



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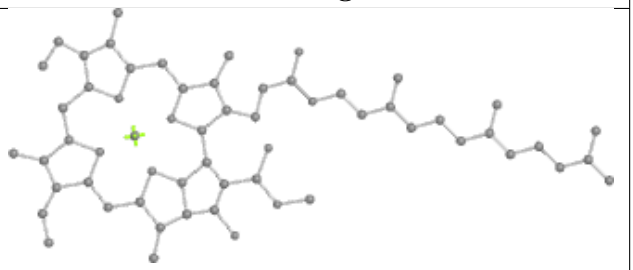
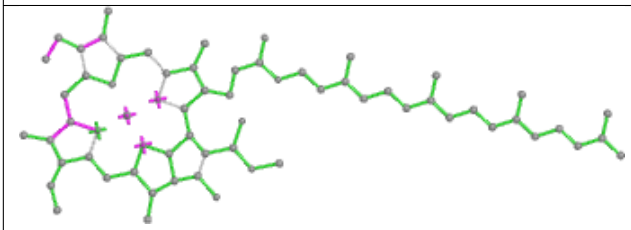
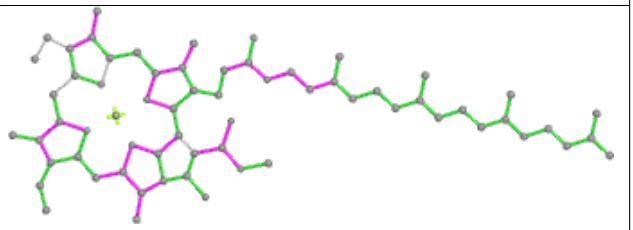


Rings

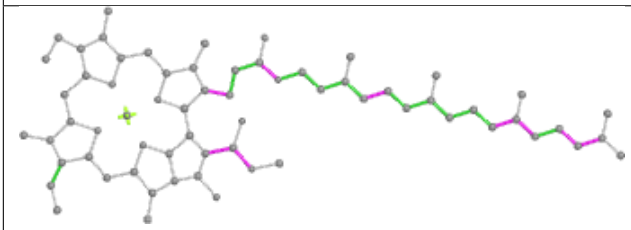
## Ligand CLA 3 601



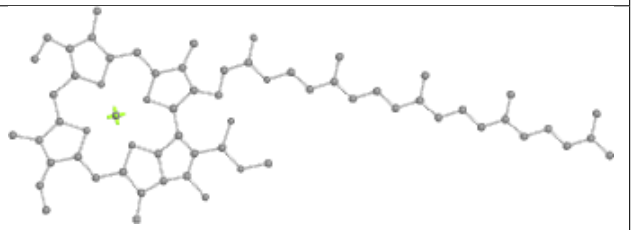
Bond lengths



Bond angles

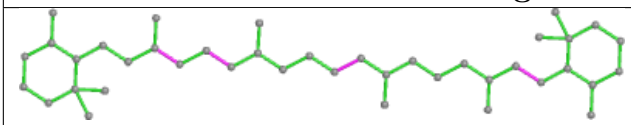


Torsions

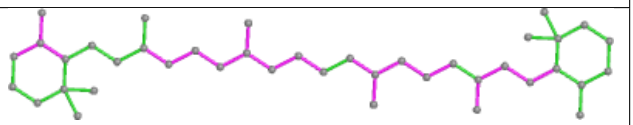


Rings

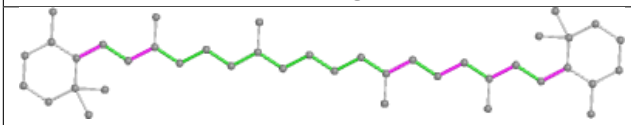
## Ligand BCR B 4001



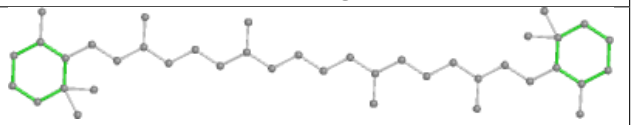
Bond lengths



Bond angles

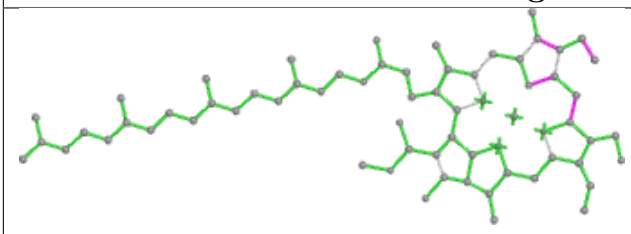


Torsions



Rings

## Ligand CHL 3 603



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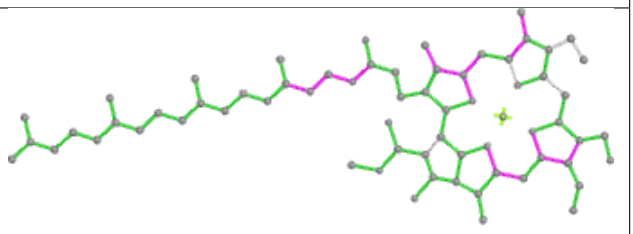
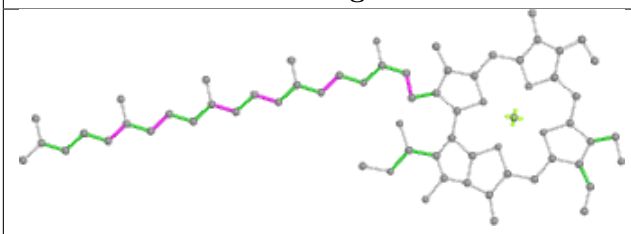


Bond angles



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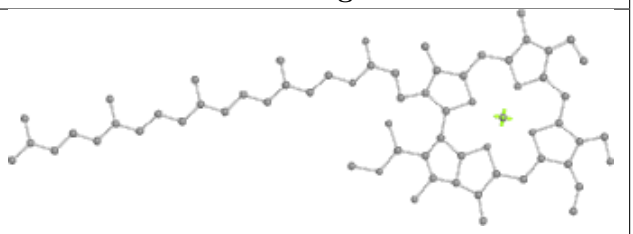
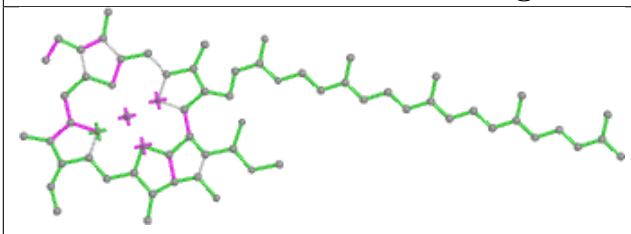
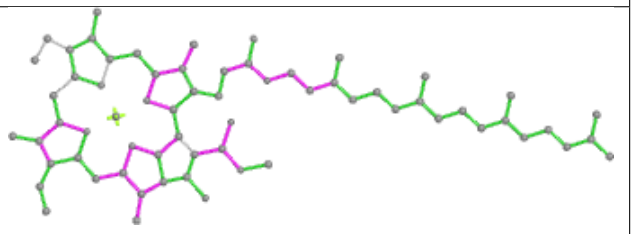


Rings

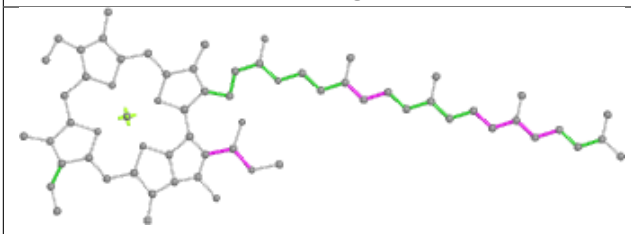
## Ligand CLA B 1205



Bond lengths



Bond angles



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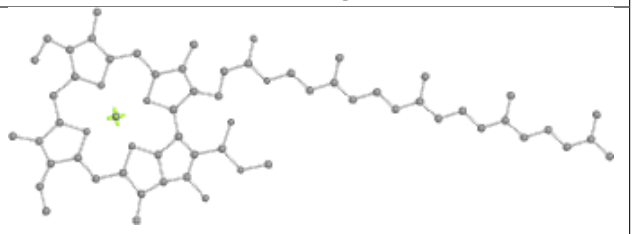
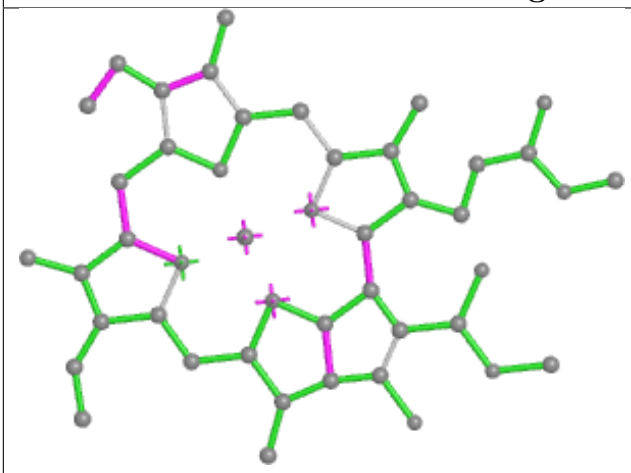
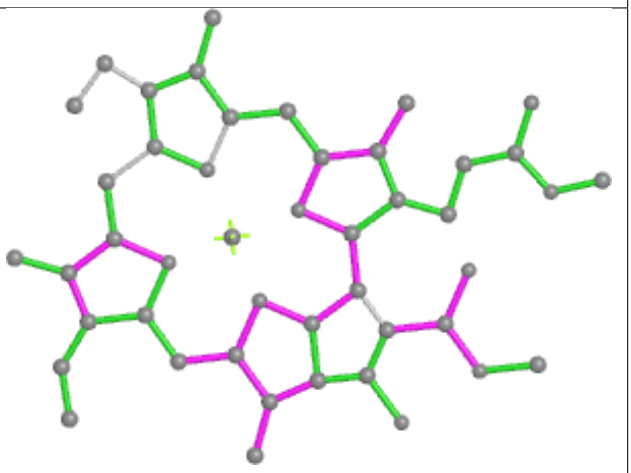


Rings

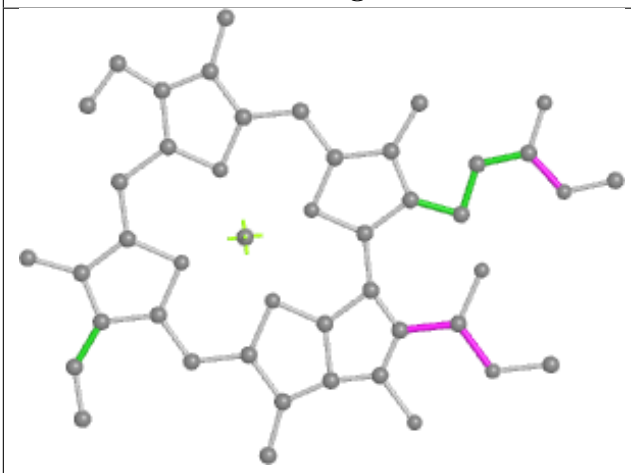
## Ligand CLA 4 605



Bond lengths



Bond angles



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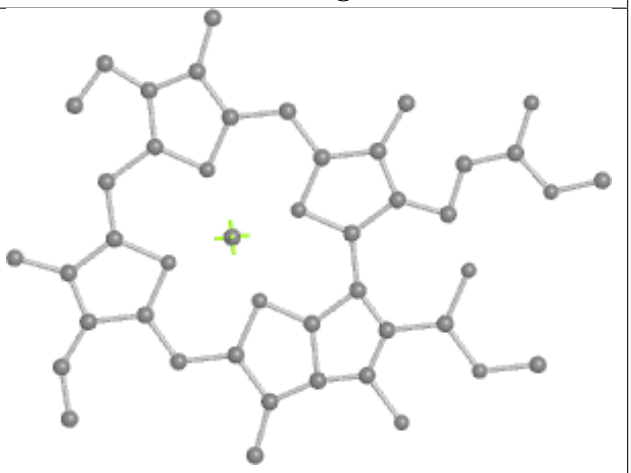
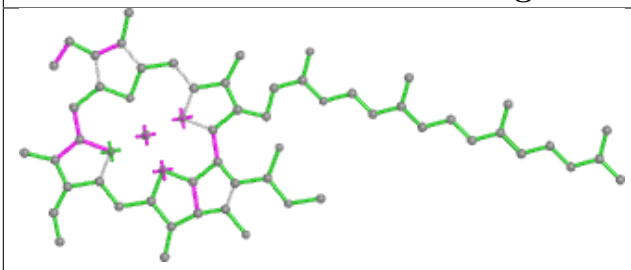


Rings

## Ligand CLA A 1116



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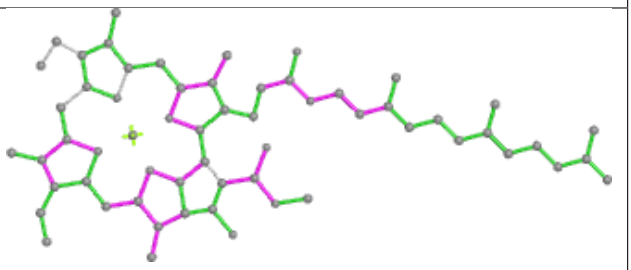
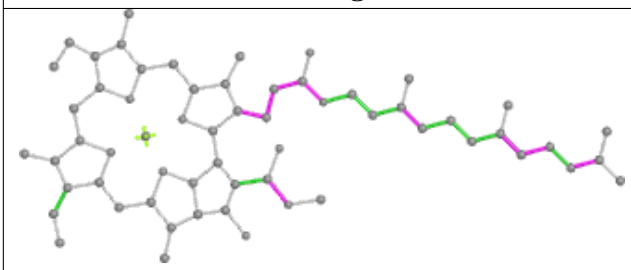


Bond angles



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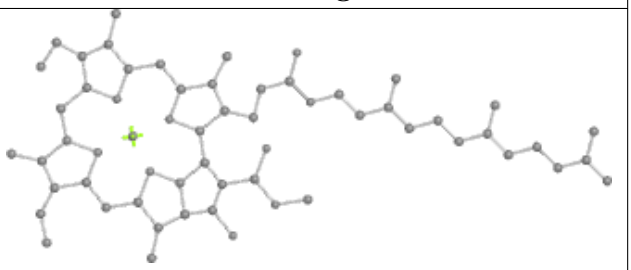
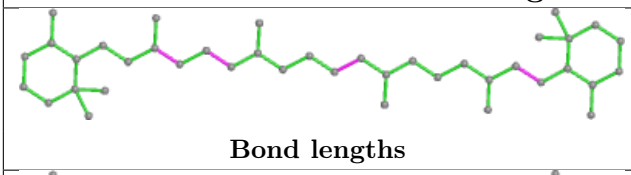
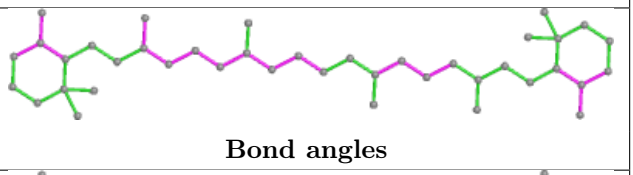


Rings

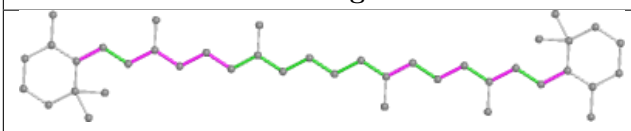
## Ligand BCR 4 503



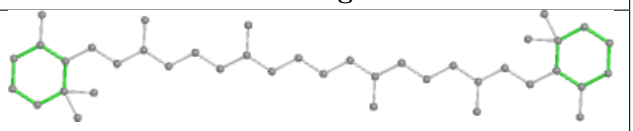
Bond lengths



Bond angles

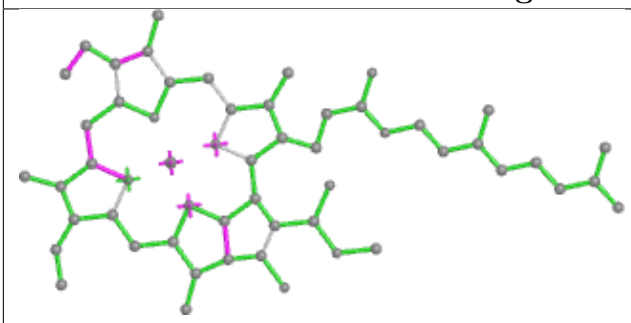


Torsions

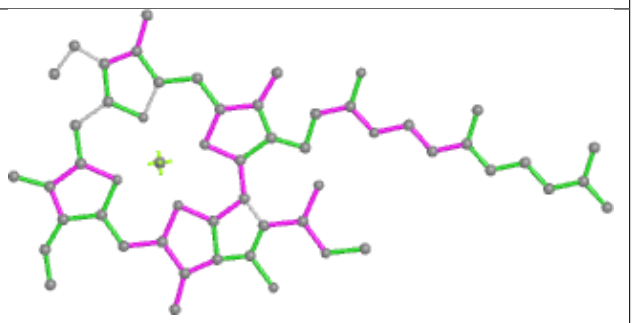


Rings

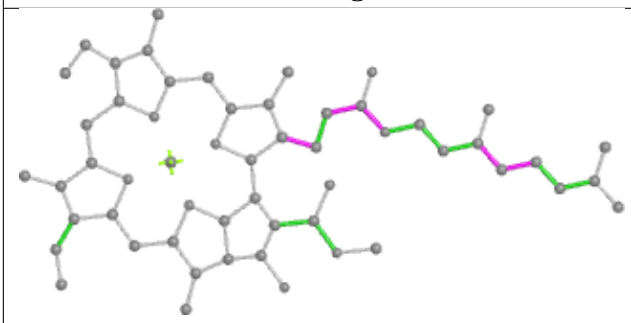
## Ligand CLA B 1218



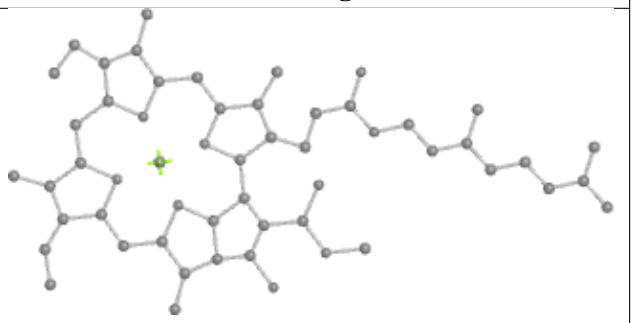
Bond lengths



Bond angles

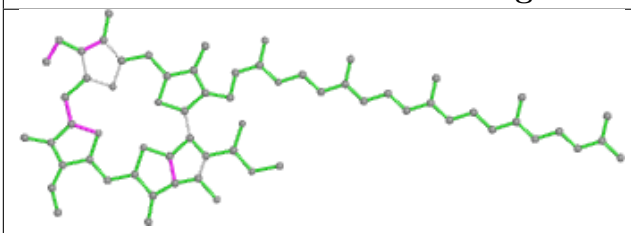


Torsions

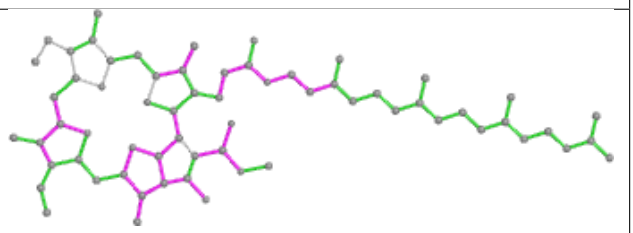


Rings

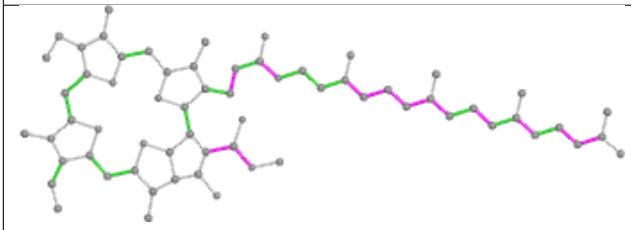
## Ligand CLA B 1234



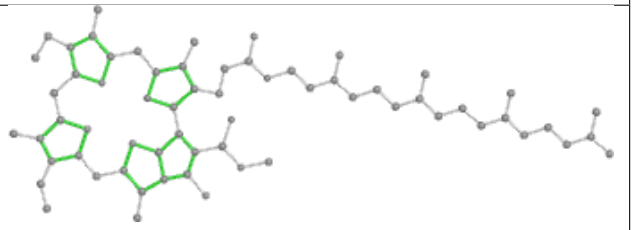
Bond lengths



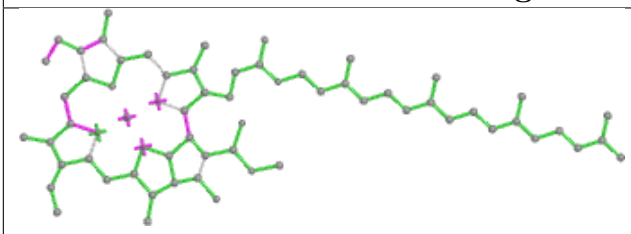
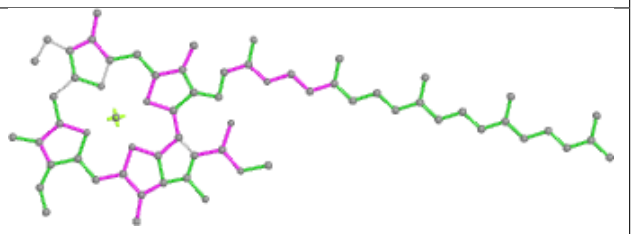
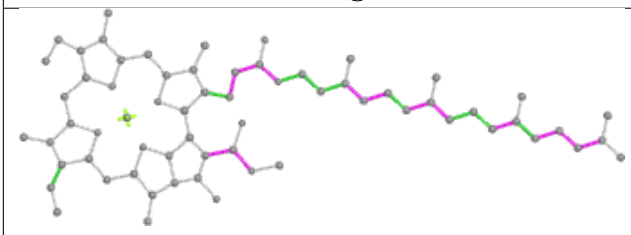
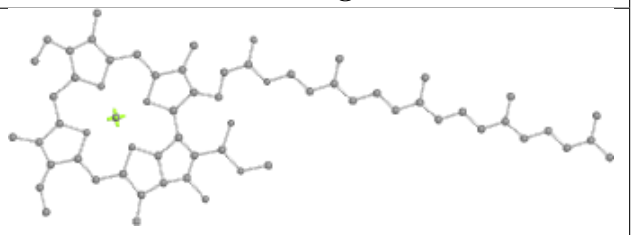
Bond angles

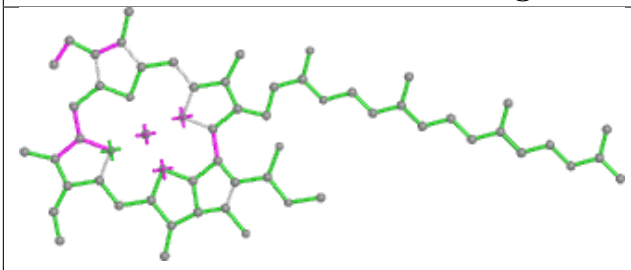
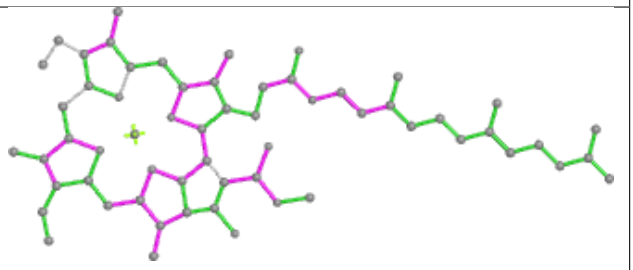
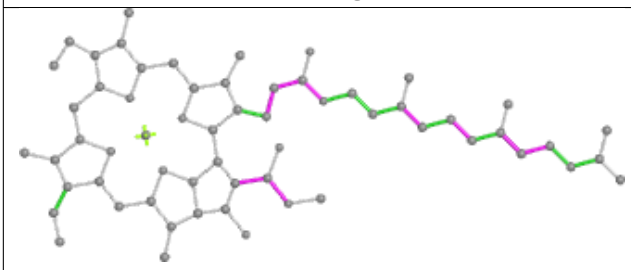
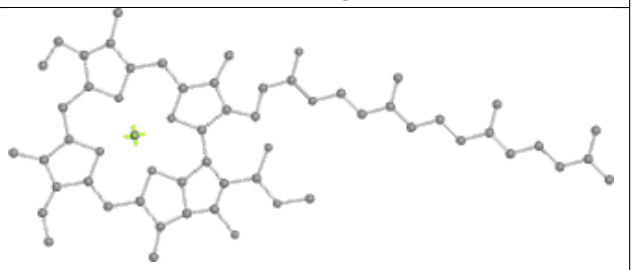


Torsions

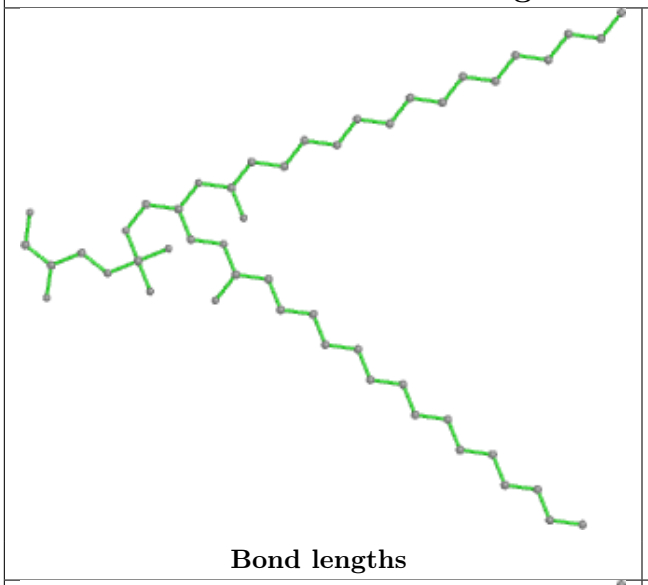


Rings

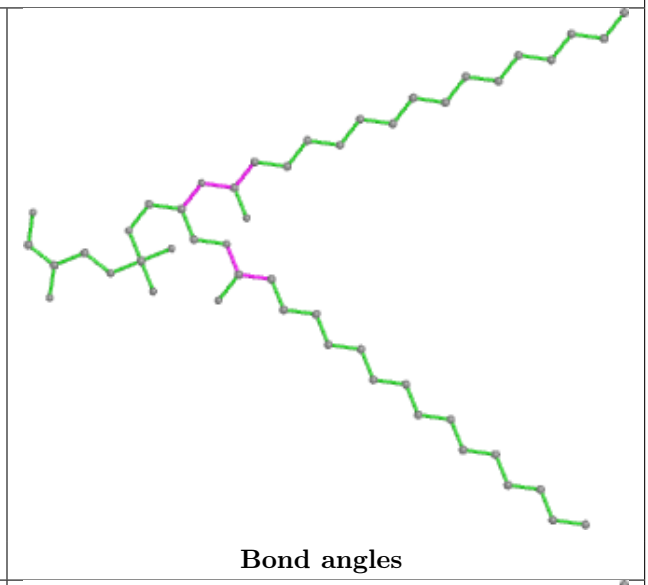
| Ligand CLA A 1111 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA G 1602 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

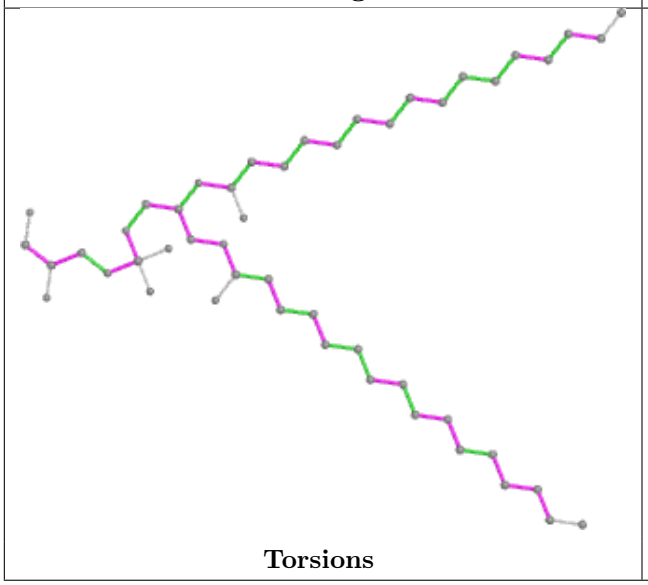
**Ligand LHG A 5001**



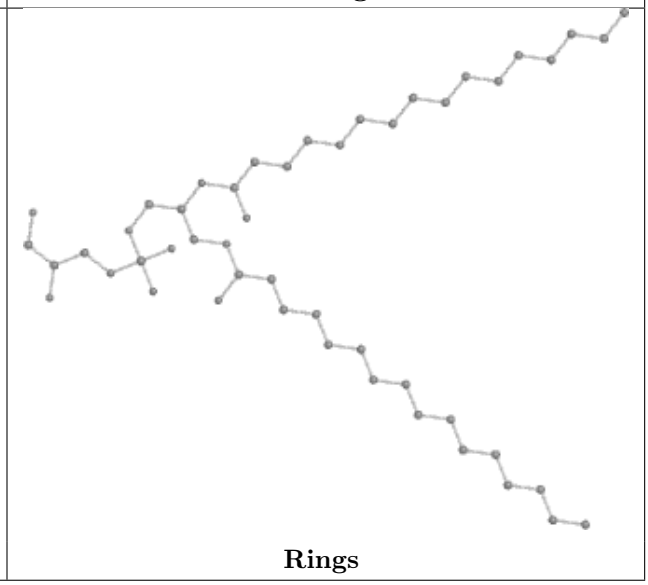
**Bond lengths**



**Bond angles**

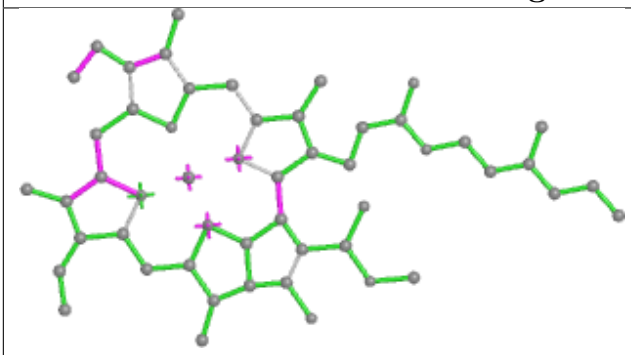


**Torsions**

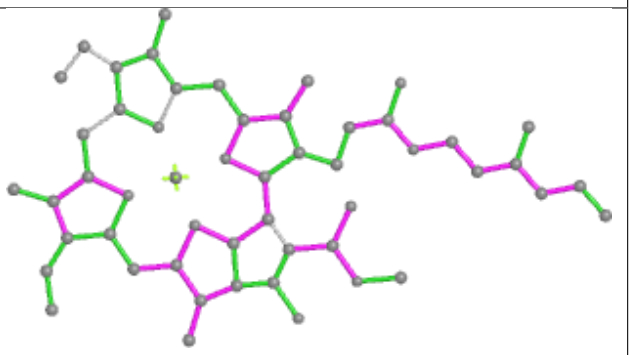


**Rings**

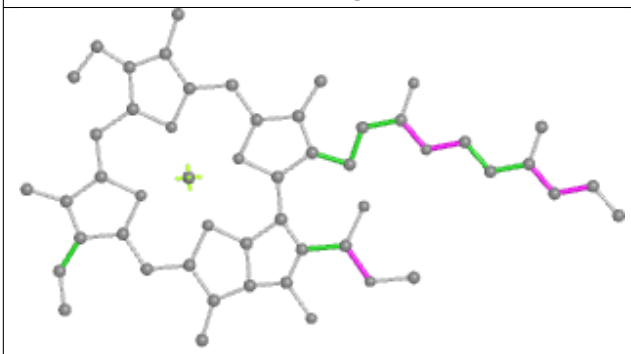
## Ligand CLA 4 602



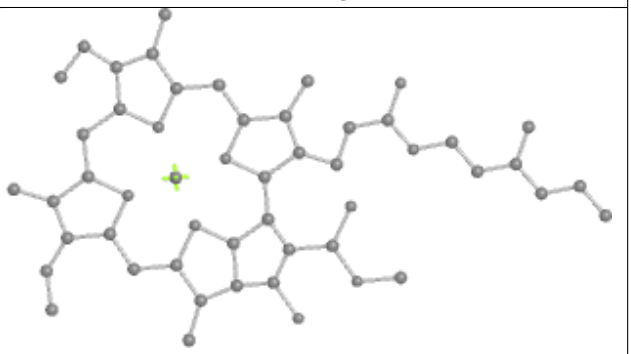
Bond lengths



Bond angles

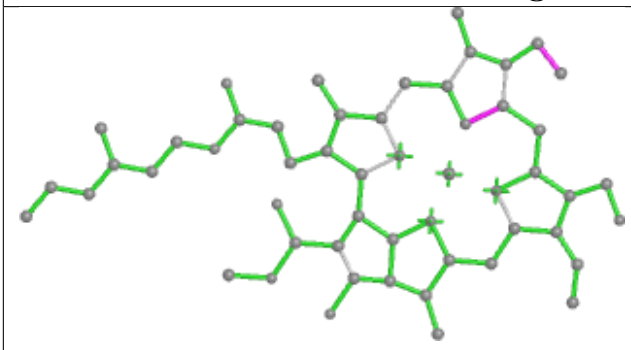


Torsions

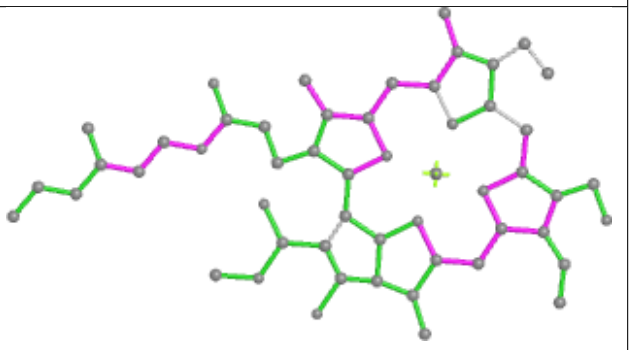


Rings

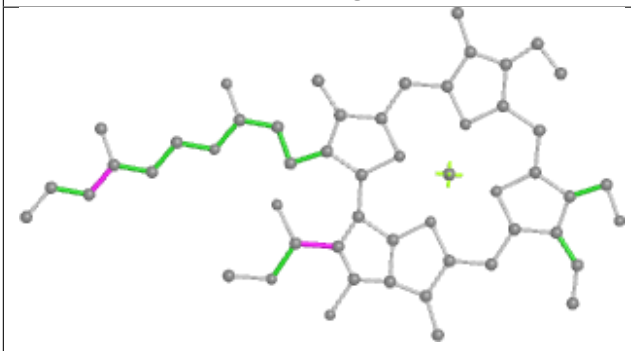
## Ligand CHL a 609



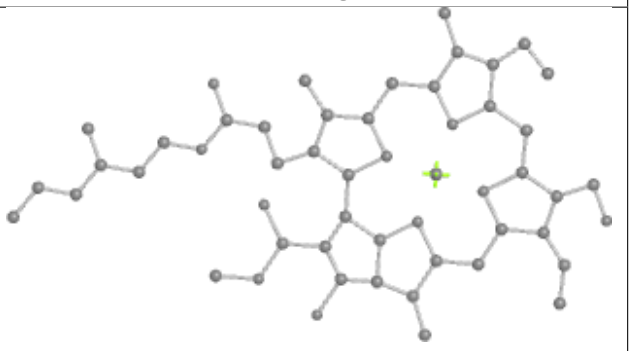
Bond lengths



Bond angles

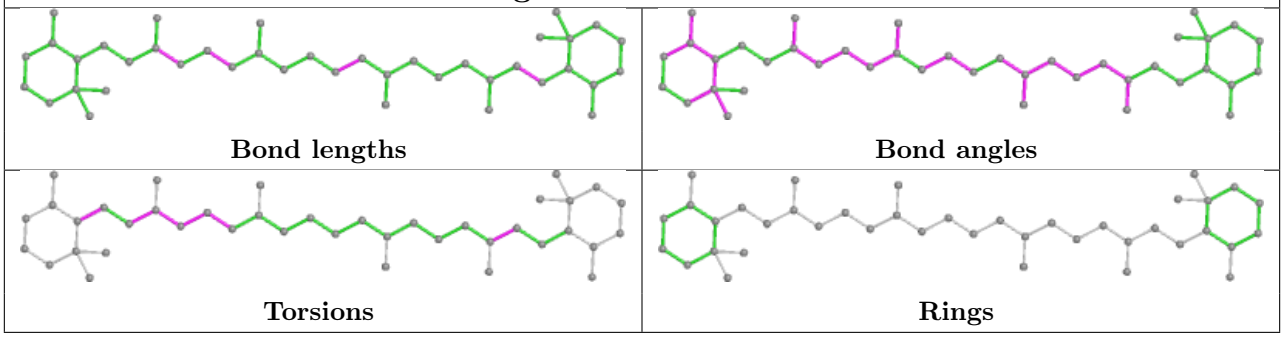


Torsions

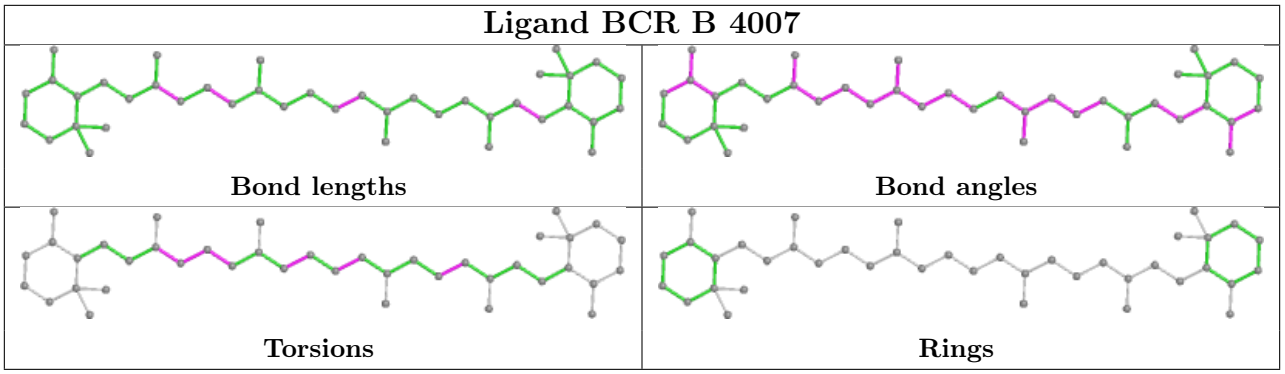


Rings

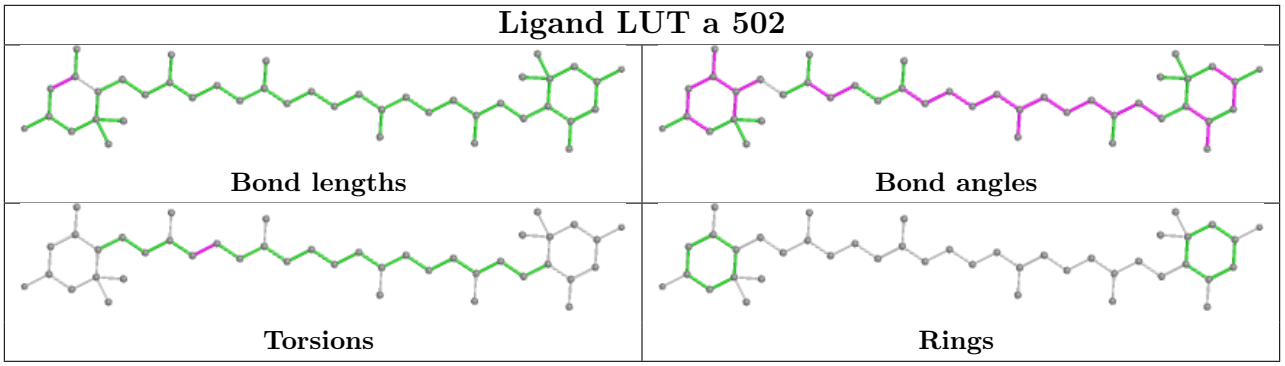
## Ligand BCR K 4001



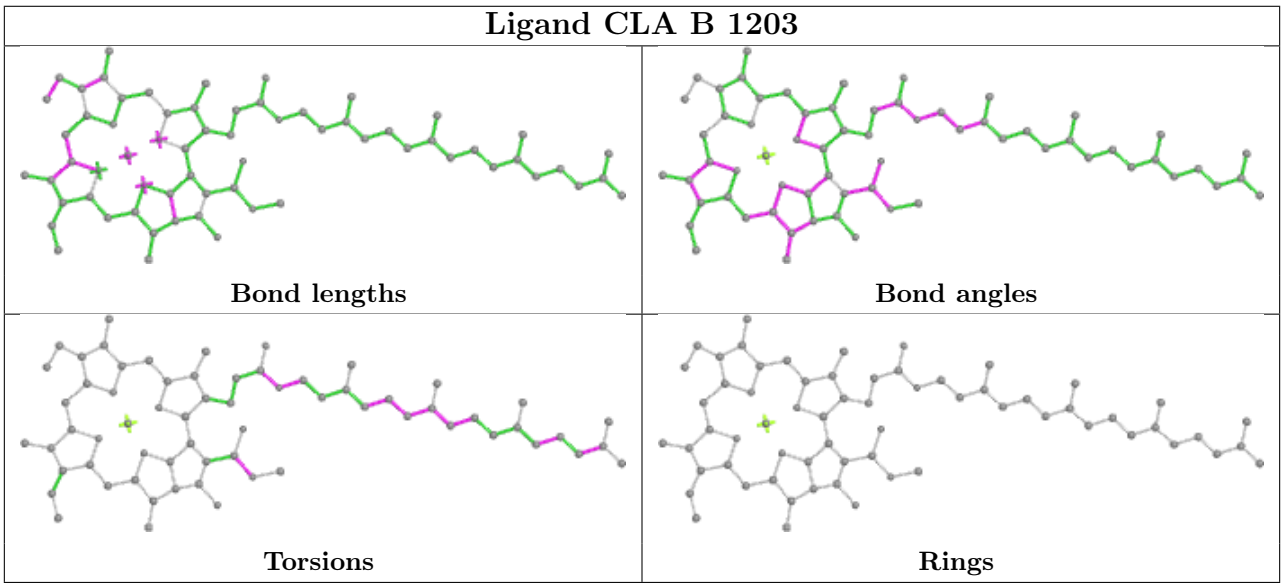

## Ligand BCR B 4007



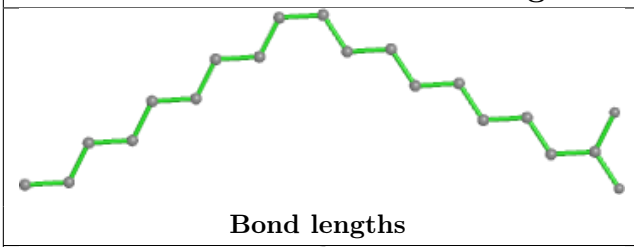

## Ligand LUT a 502



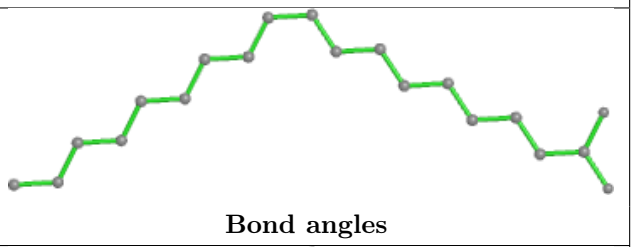

## Ligand CLA B 1203



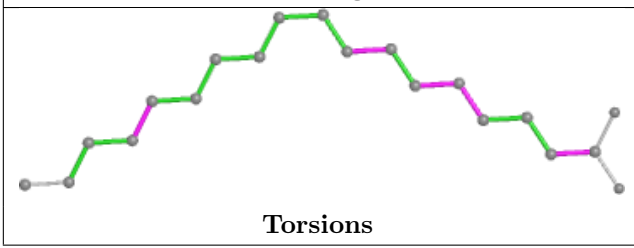
## Ligand OLA 1 803



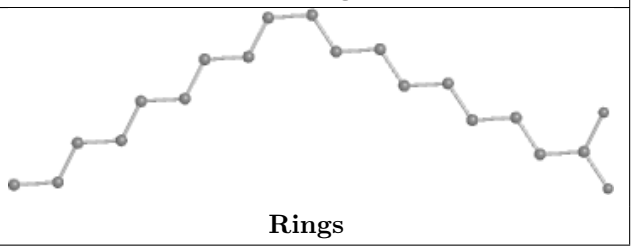
Bond lengths



Bond angles

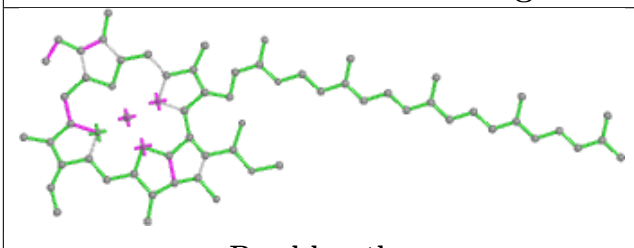


Torsions

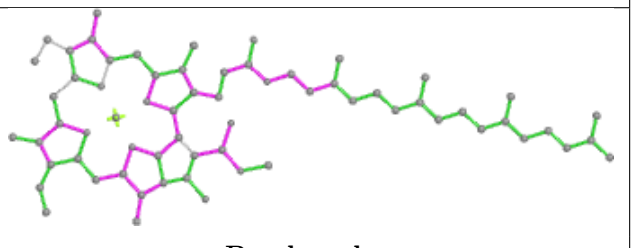


Rings

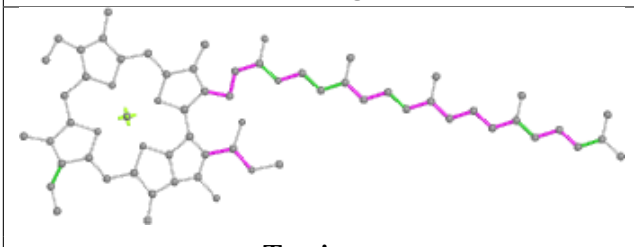
## Ligand CLA B 1216



Bond lengths



Bond angles



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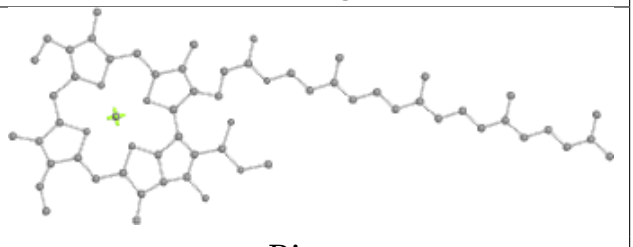
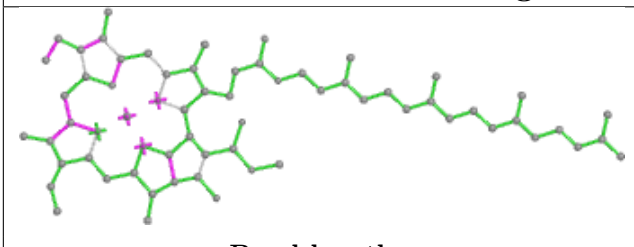
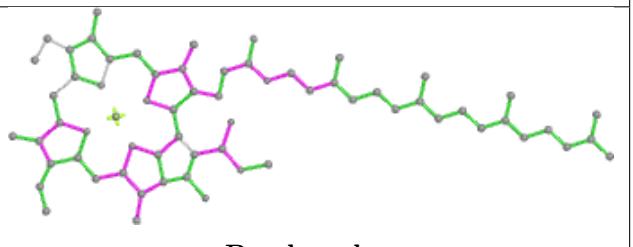


Rings

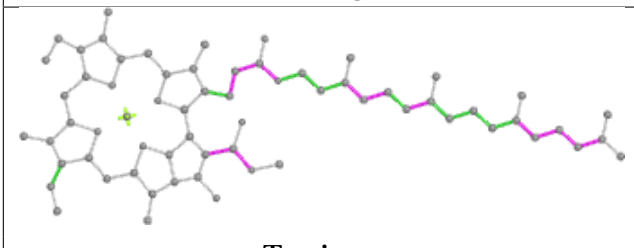
## Ligand CLA B 1204



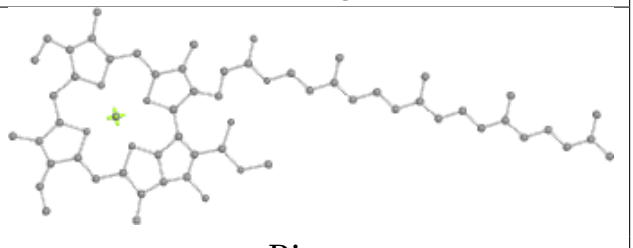
Bond lengths



Bond angles

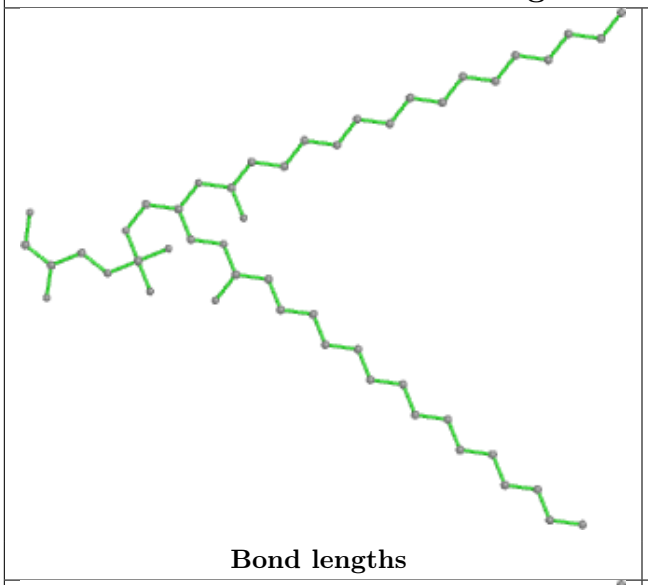


Torsions

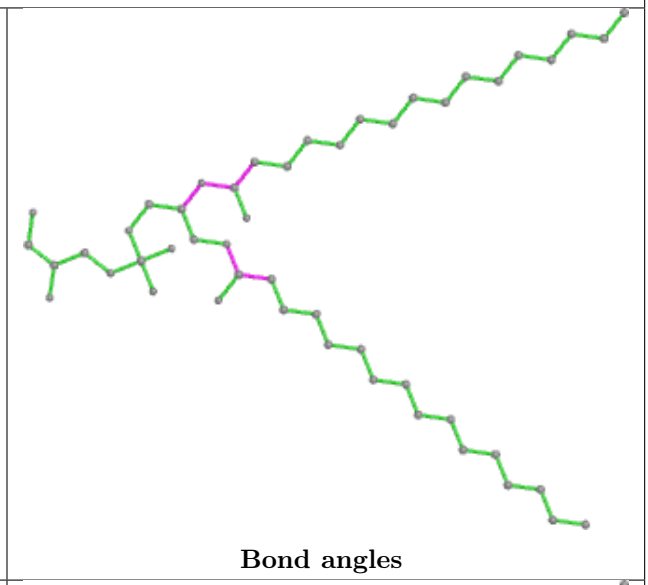


Rings

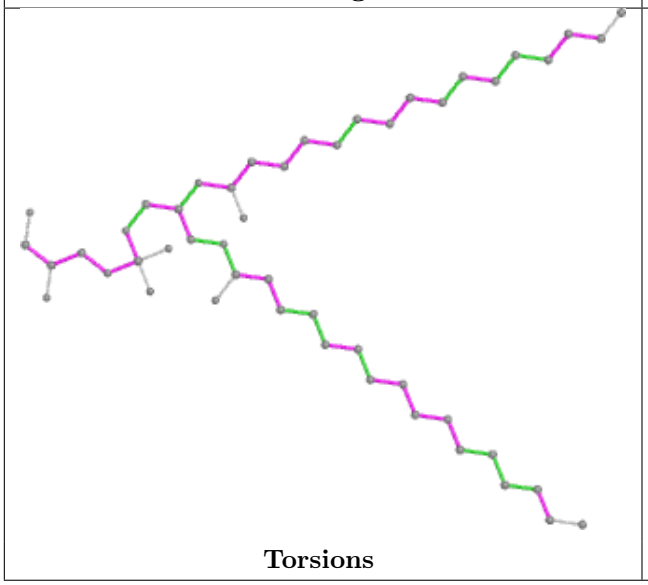
**Ligand LHG 6 801**



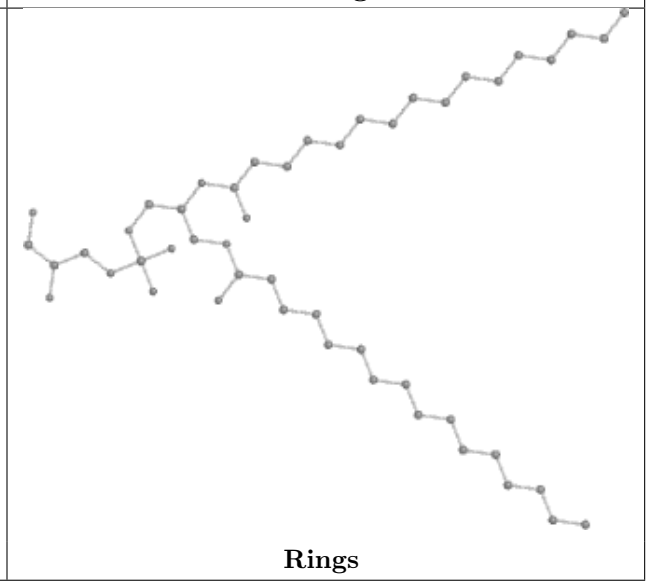
**Bond lengths**



**Bond angles**

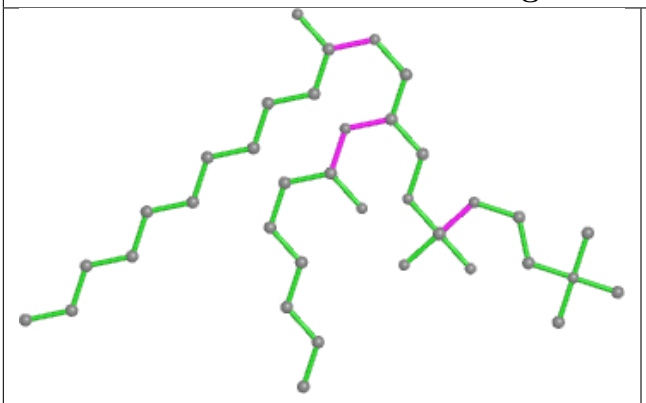


**Torsions**

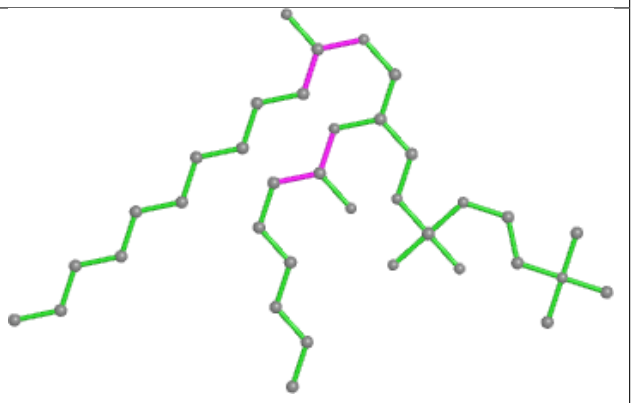


**Rings**

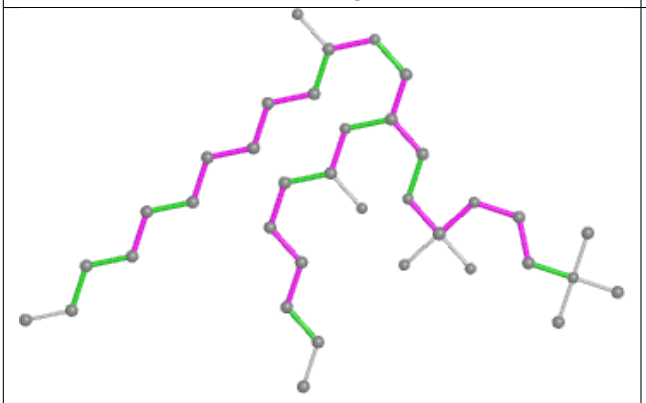
## Ligand PCW 6 803



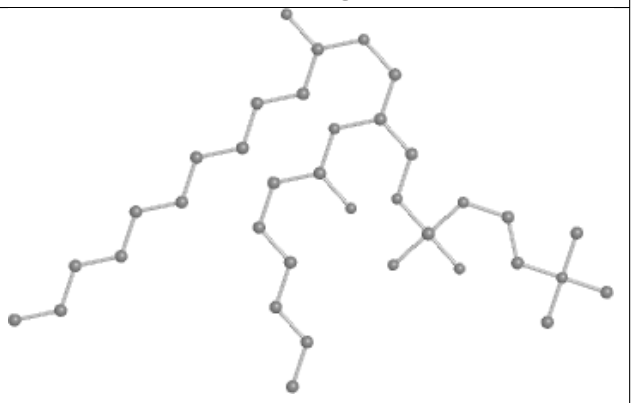
Bond lengths



Bond angles

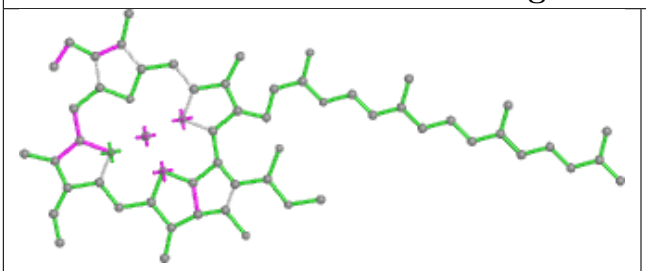


Torsions

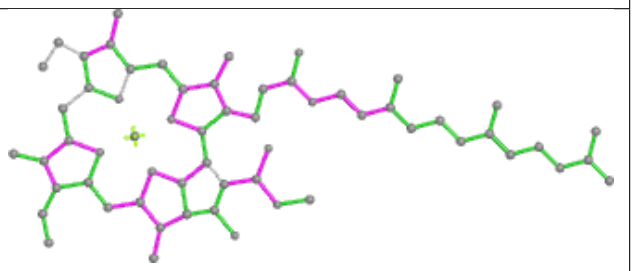


Rings

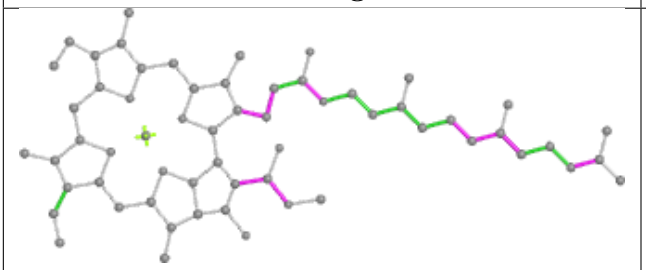
## Ligand CLA 1 601



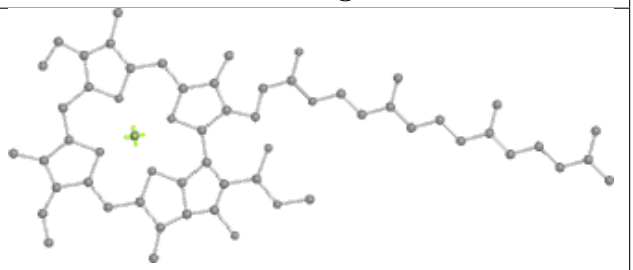
Bond lengths



Bond angles

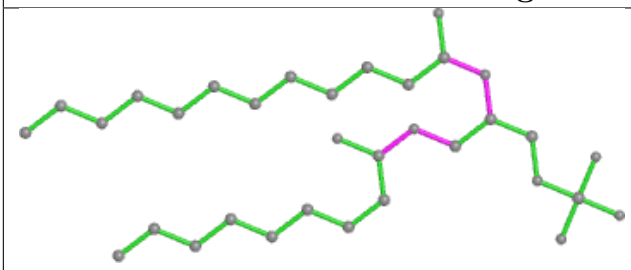


Torsions



Rings

**Ligand 3PH A 5007**



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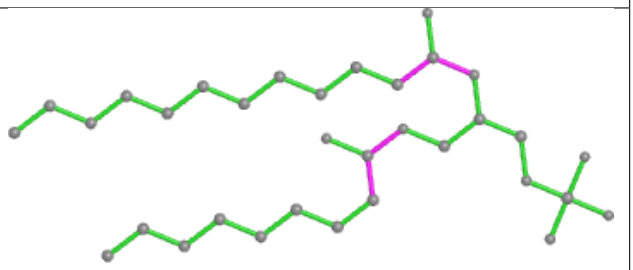
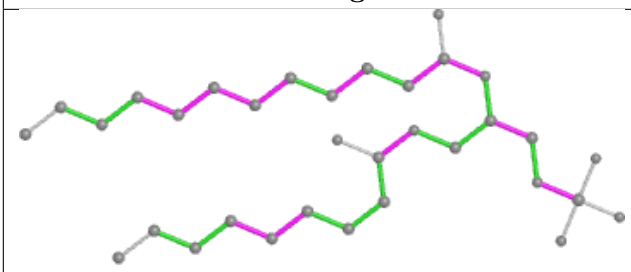
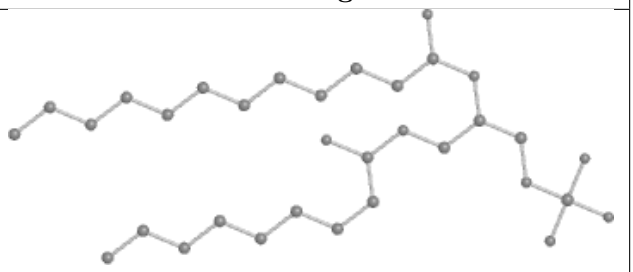


**Bond angles**

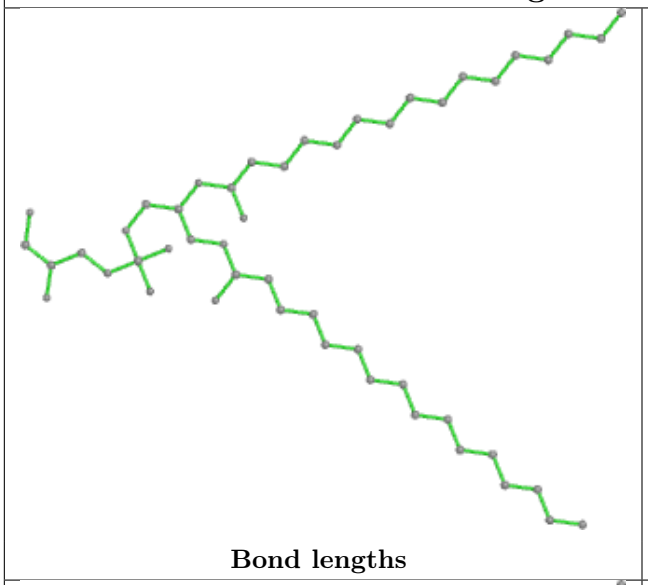


**Torsions**



**Rings**

**Ligand LHG 3 801**



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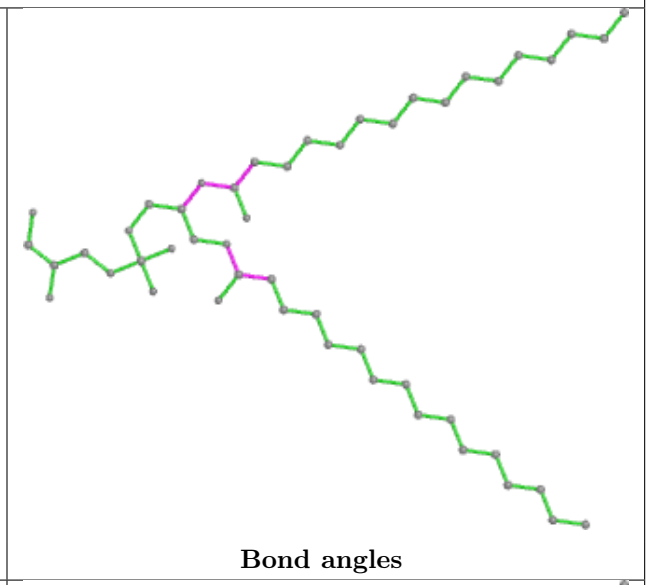

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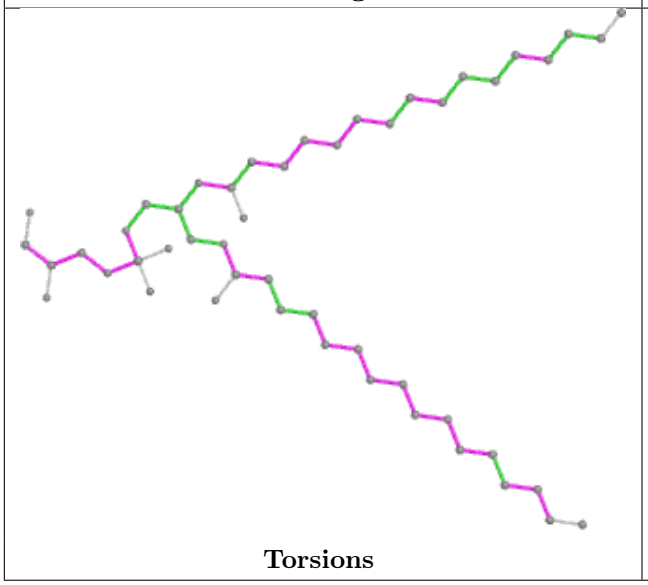

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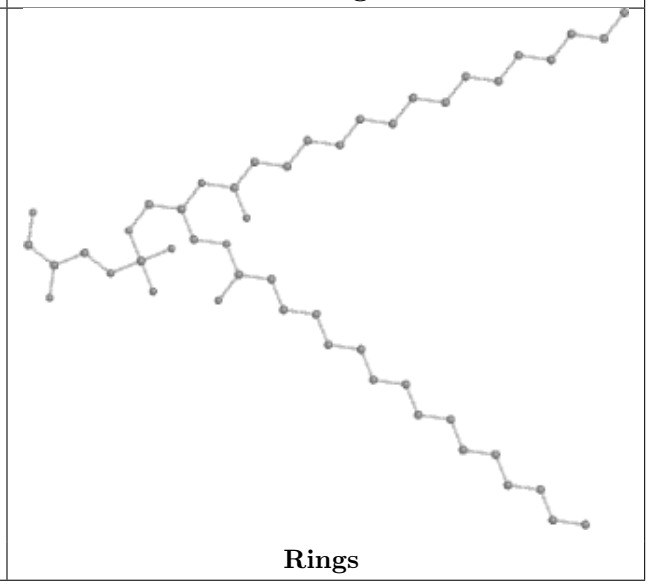
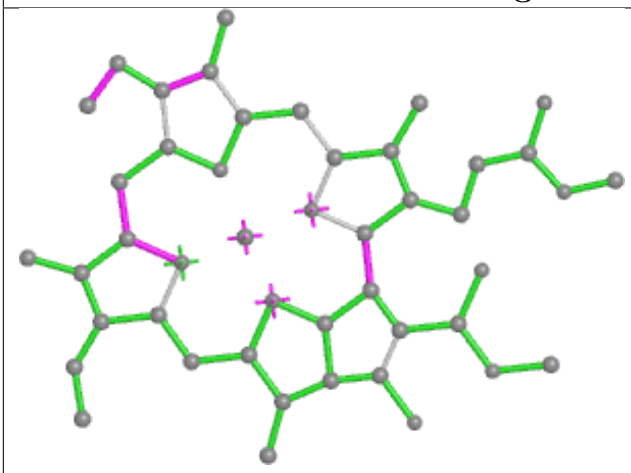


**Rings**

**Ligand CLA K 1401**



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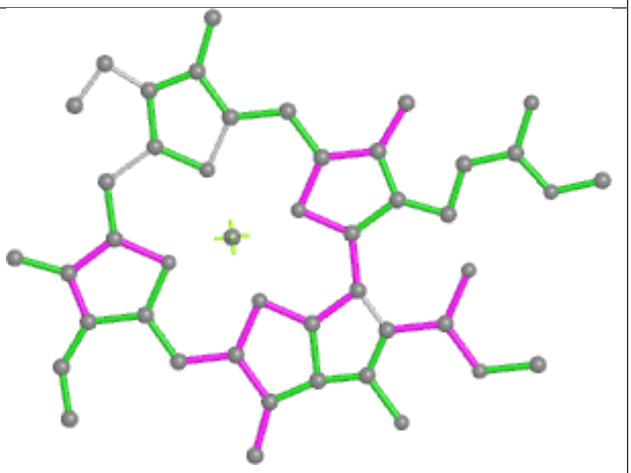
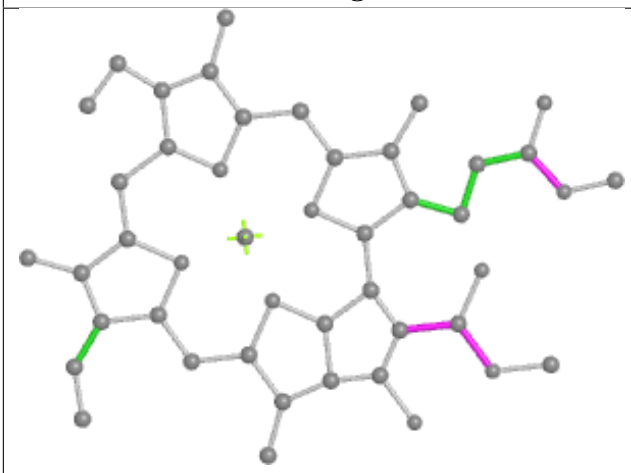


**Bond angles**



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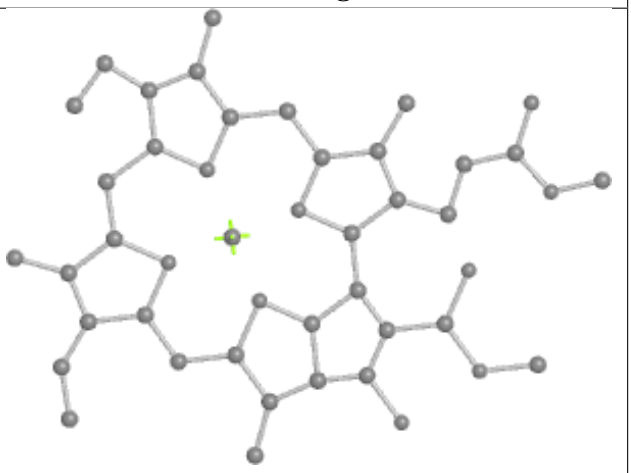
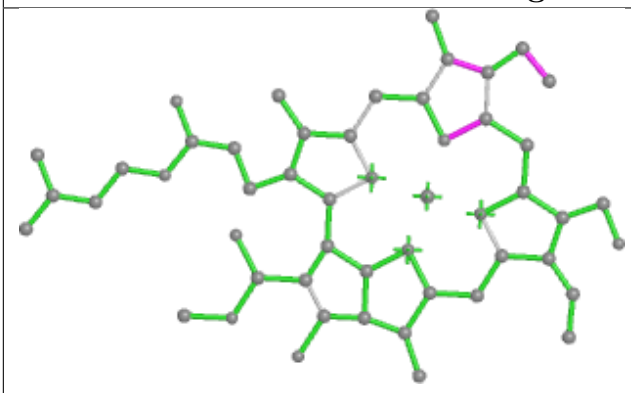


**Rings**

## Ligand CHL 7 615



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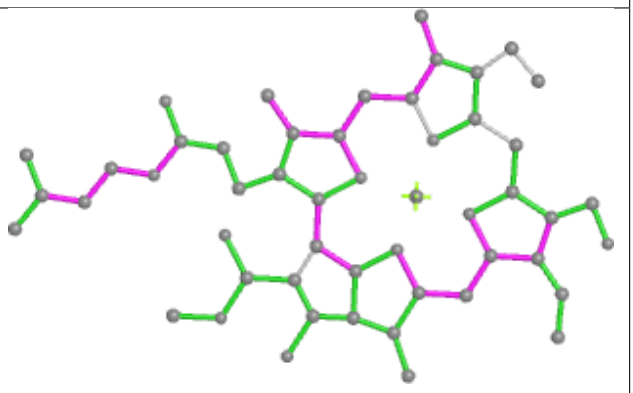
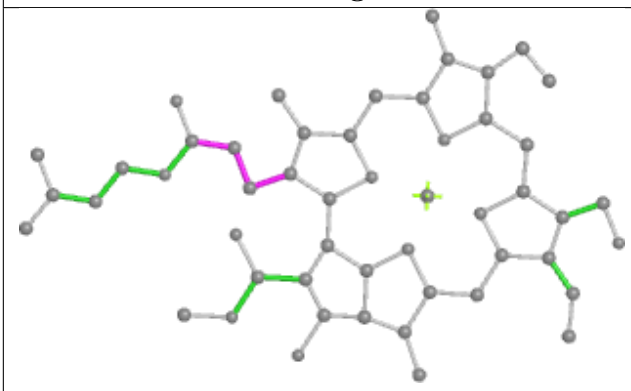


Bond angles



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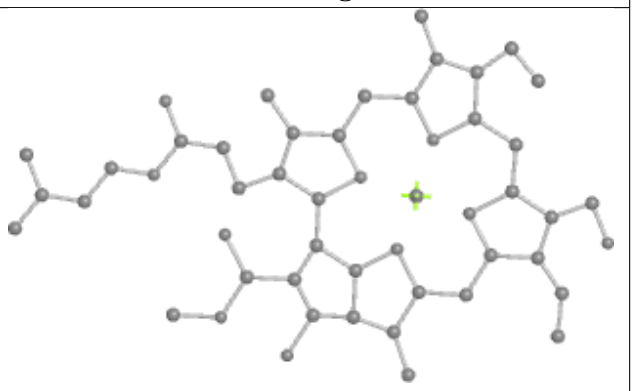
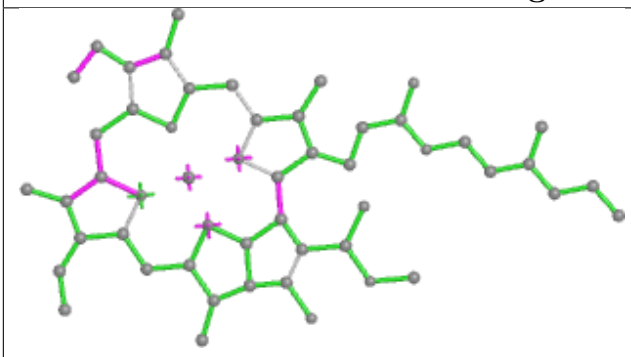


Rings

## Ligand CLA 2 602



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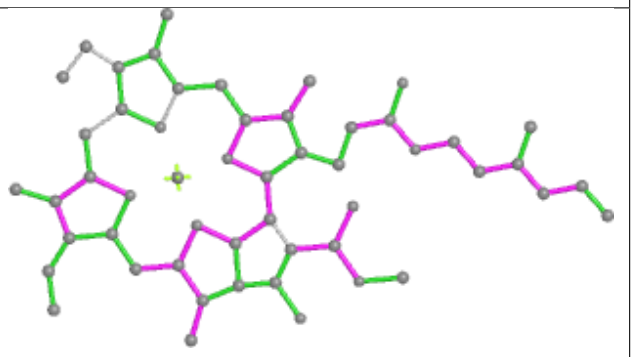
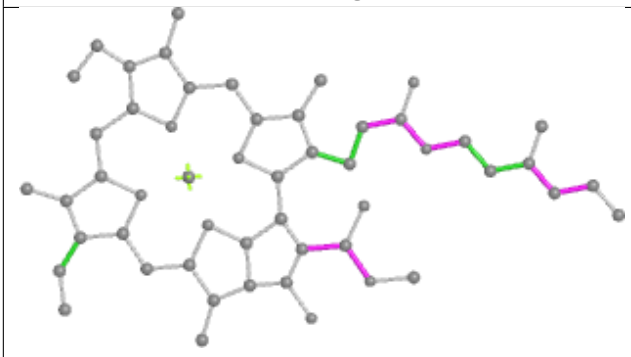


Bond angles



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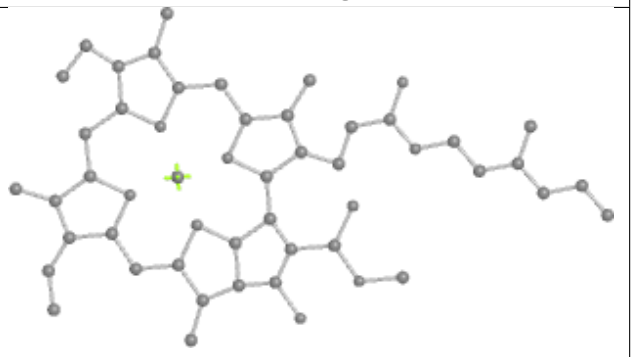
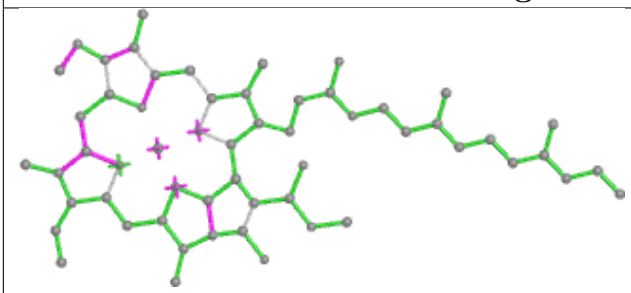


Rings

## Ligand CLA A 1105



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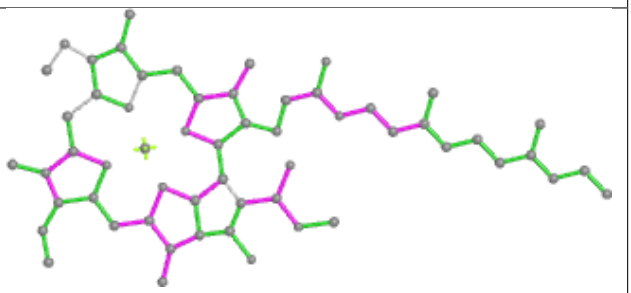

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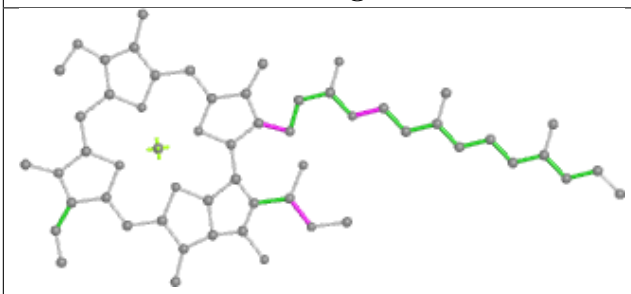

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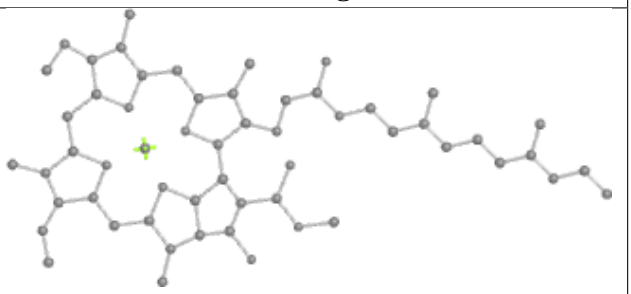
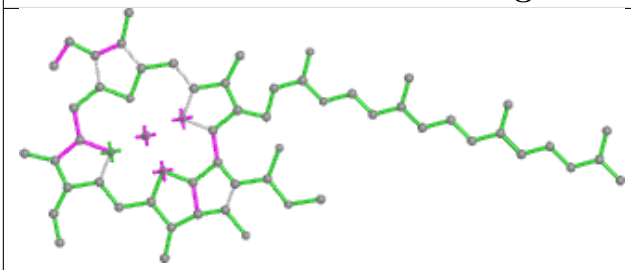


Rings

## Ligand CLA A 1122



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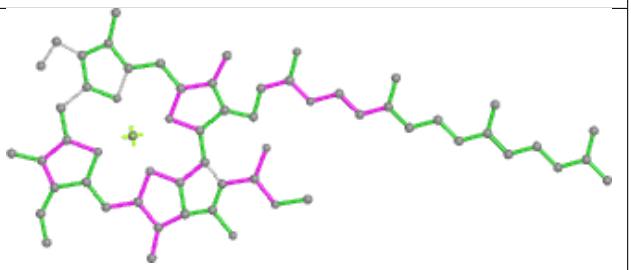
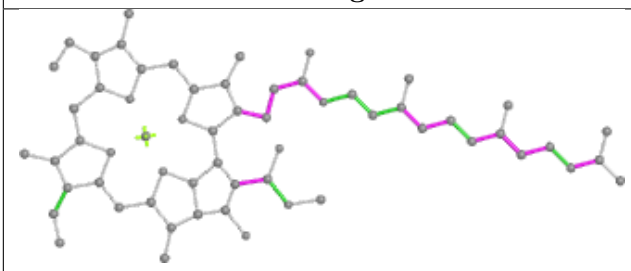
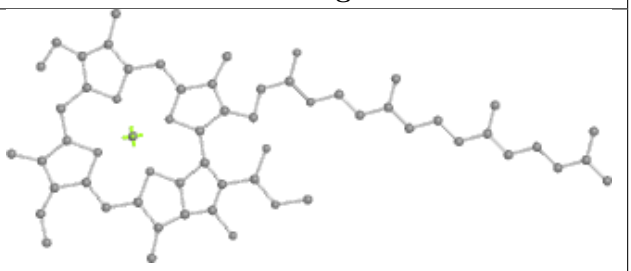


Bond angles

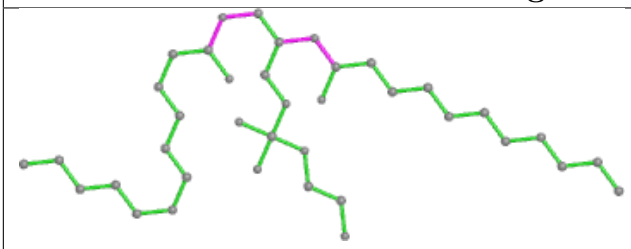


Torsions



Rings

## Ligand PTY 5 802



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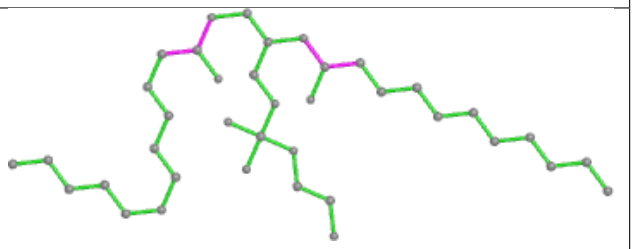
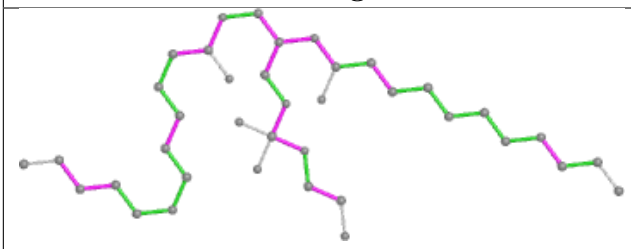


Bond angles



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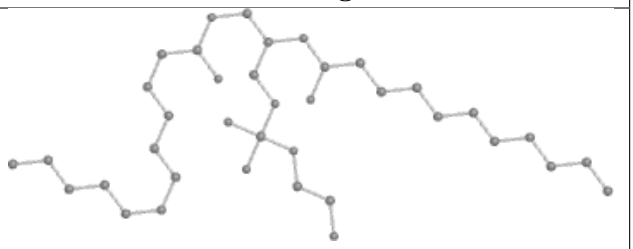
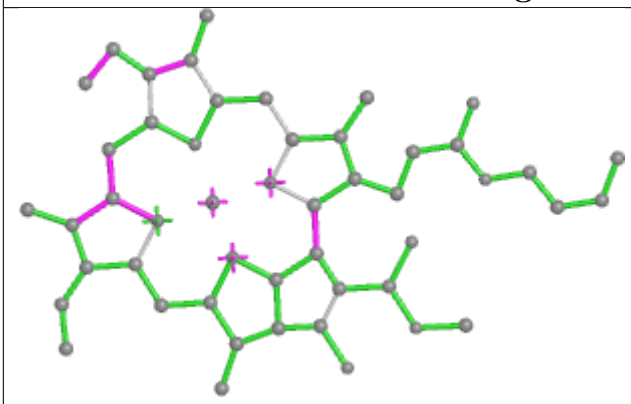


Rings

## Ligand CLA A 1120



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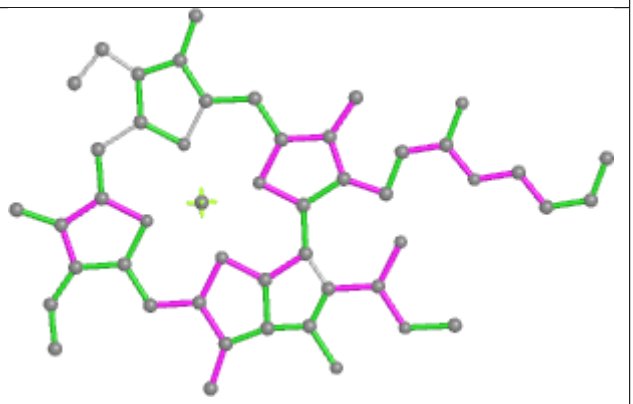
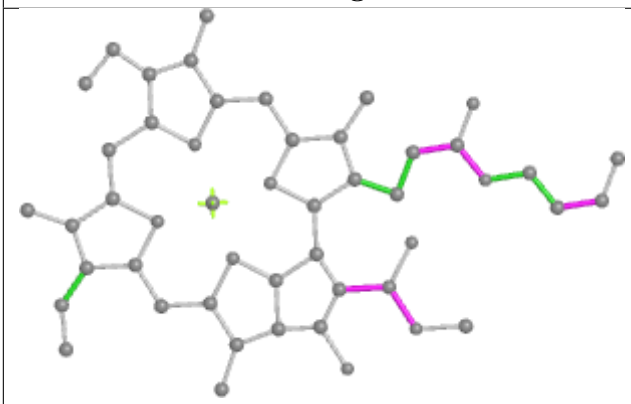


Bond angles



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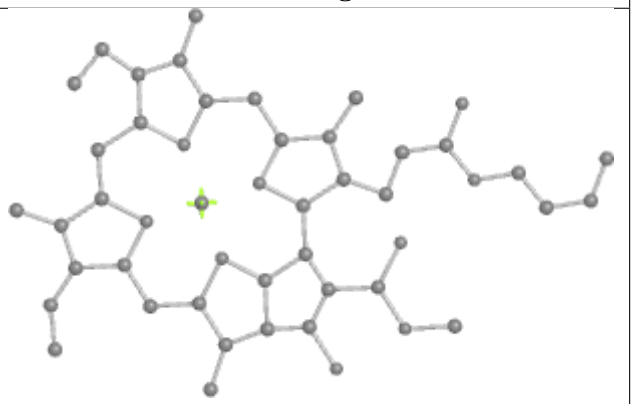
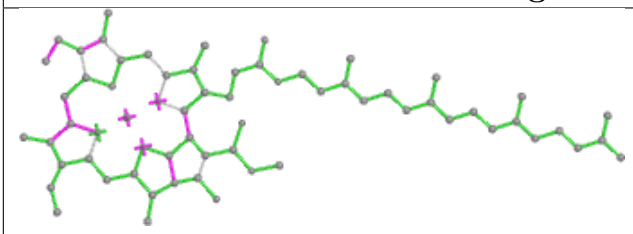


Rings

## Ligand CLA 5 612



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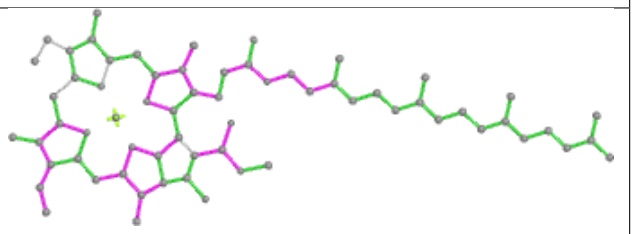
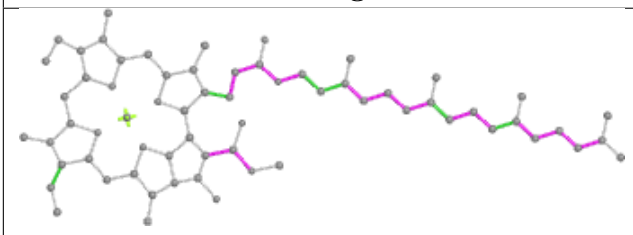


Bond angles



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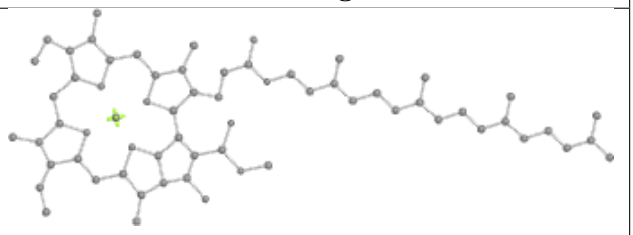
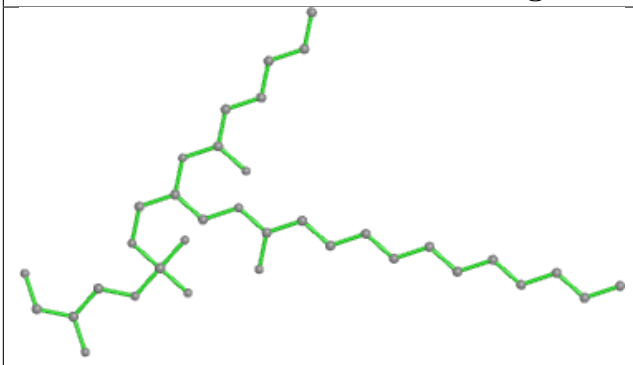


Rings

## Ligand LHG 1 801



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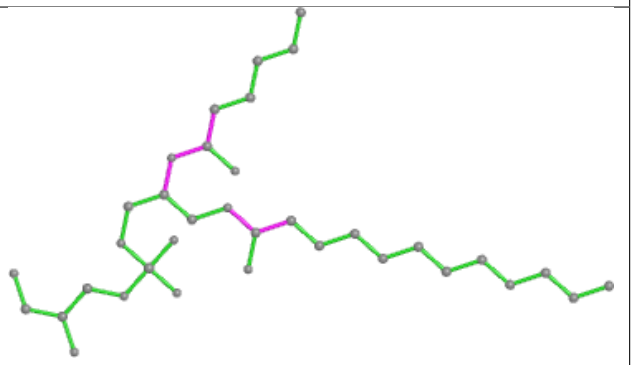
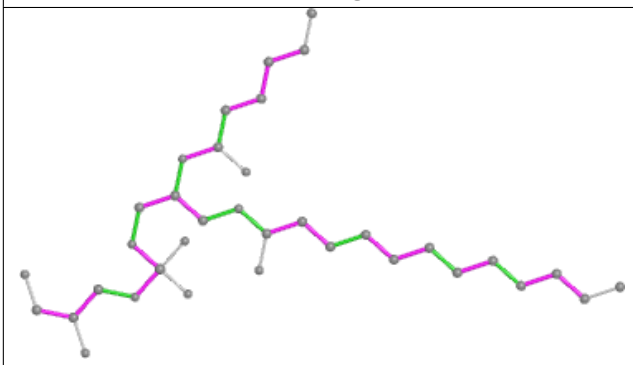


Bond angles



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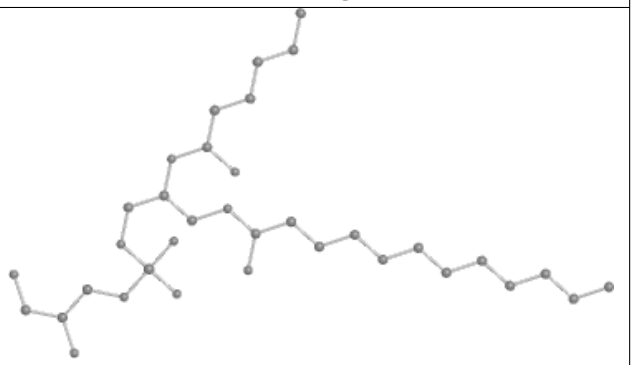
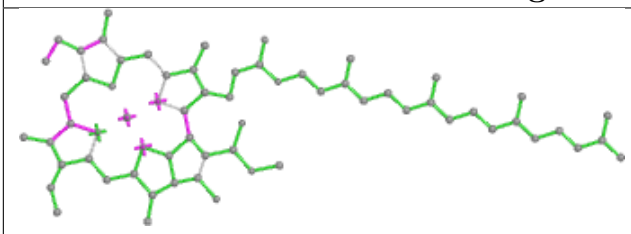
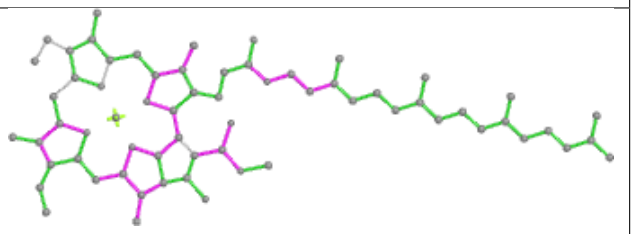


Rings

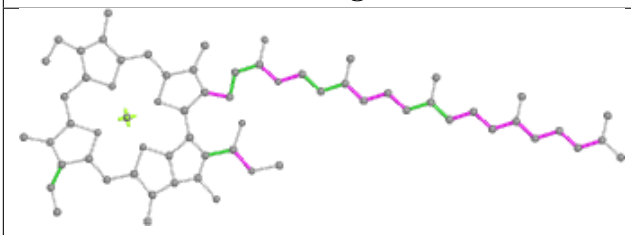
## Ligand CLA 4 610



Bond lengths



Bond angles



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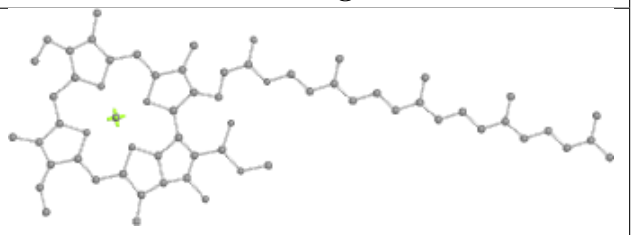

Rings

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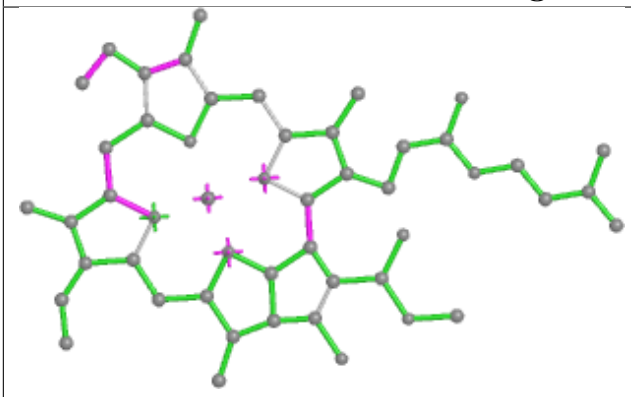
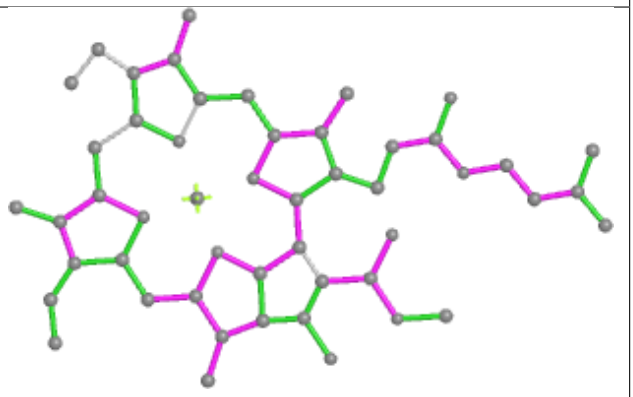
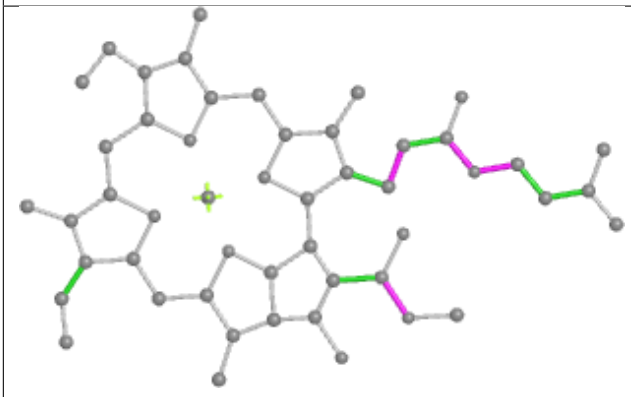


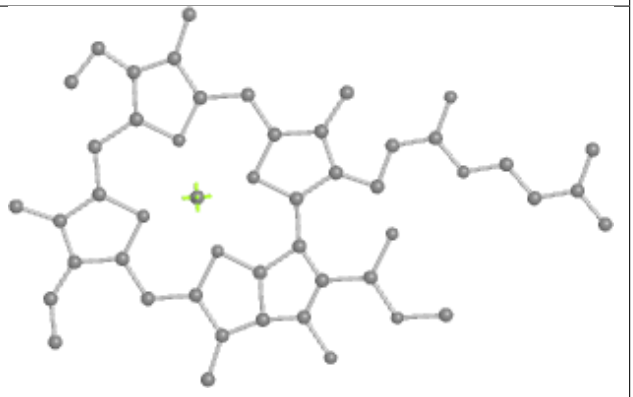
Bond lengths



Bond angles

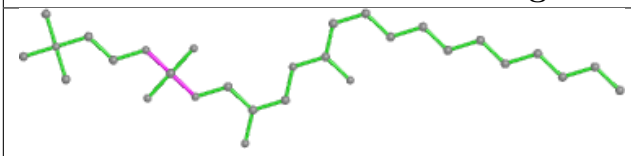


Torsions

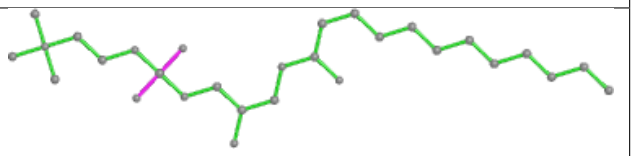


Rings

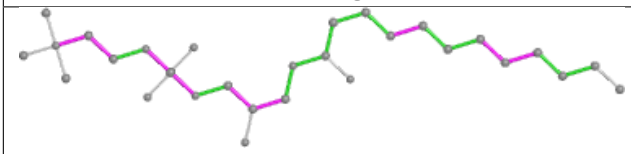
**Ligand LAP 8 810**



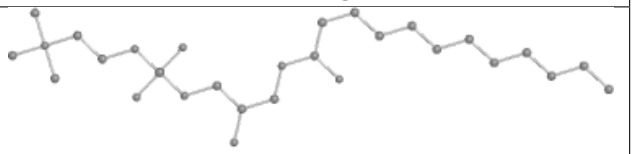
Bond lengths



Bond angles

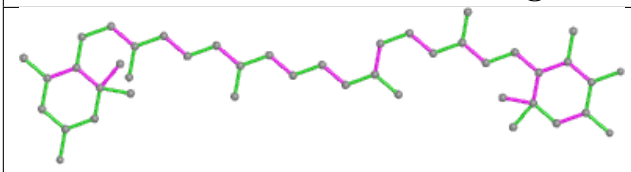


Torsions



Rings

**Ligand AXT 7 504**



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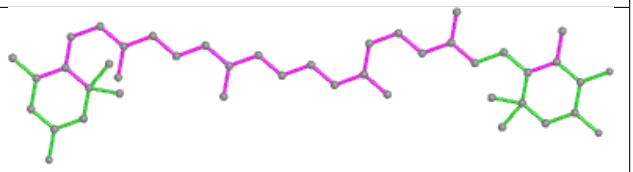
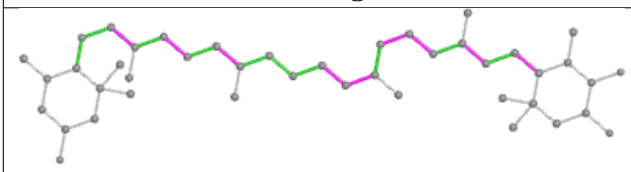
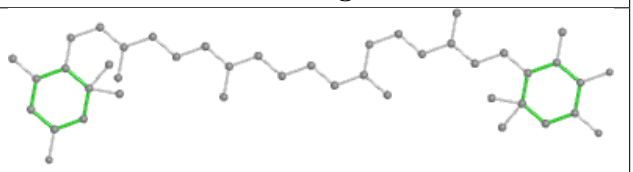


Bond angles

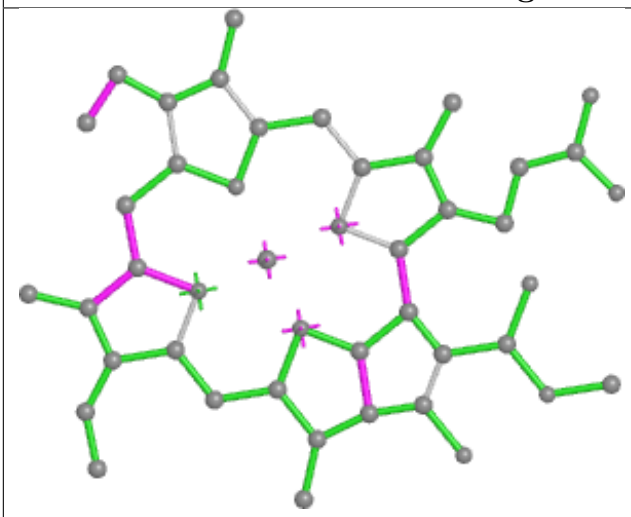


Torsions

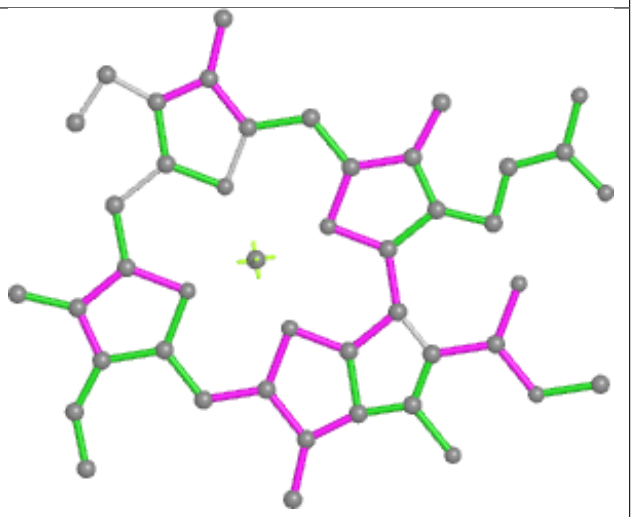


Rings

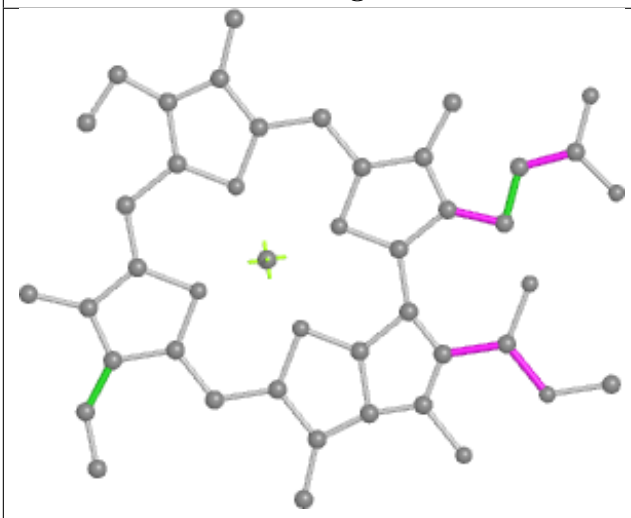
## Ligand CLA L 1503



Bond lengths



Bond angles



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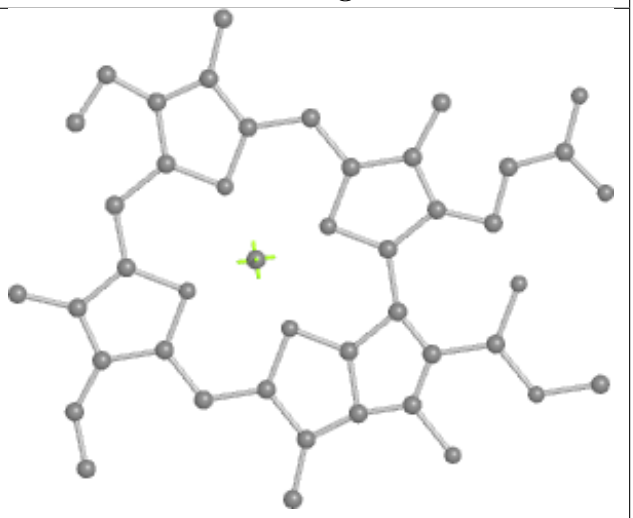
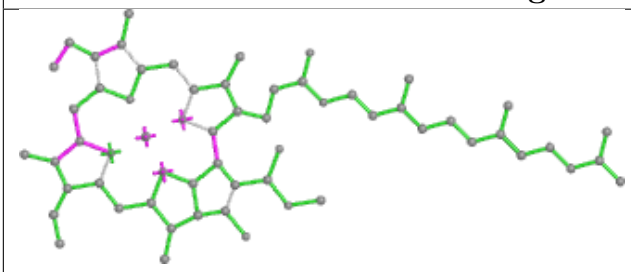
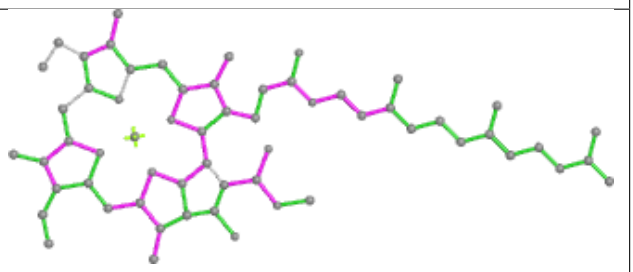


Rings

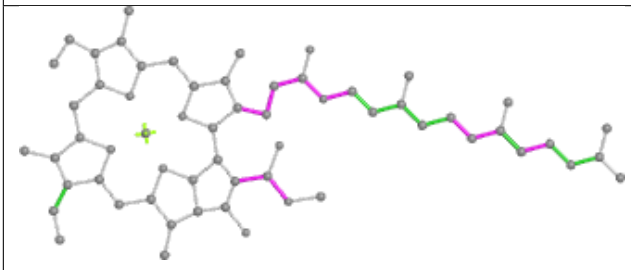
## Ligand CLA 7 612



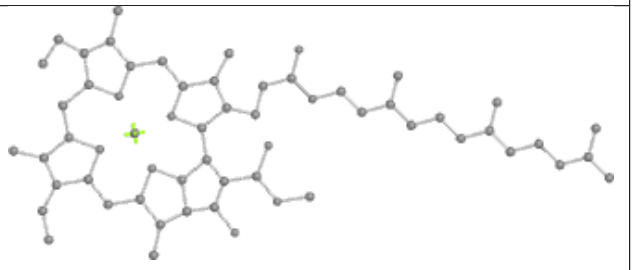
Bond lengths



Bond angles

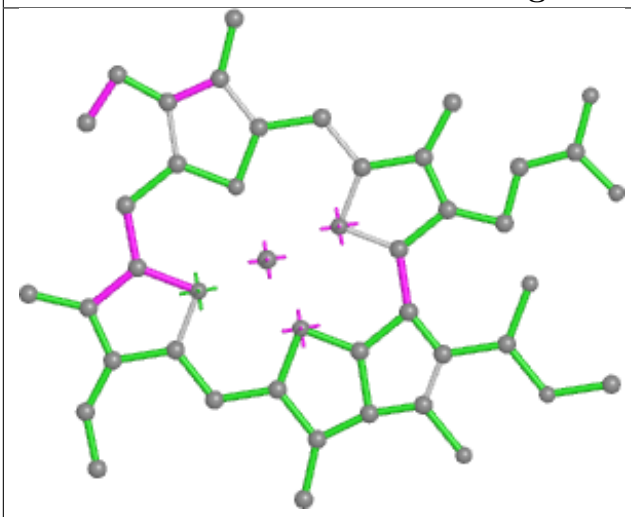


Torsions

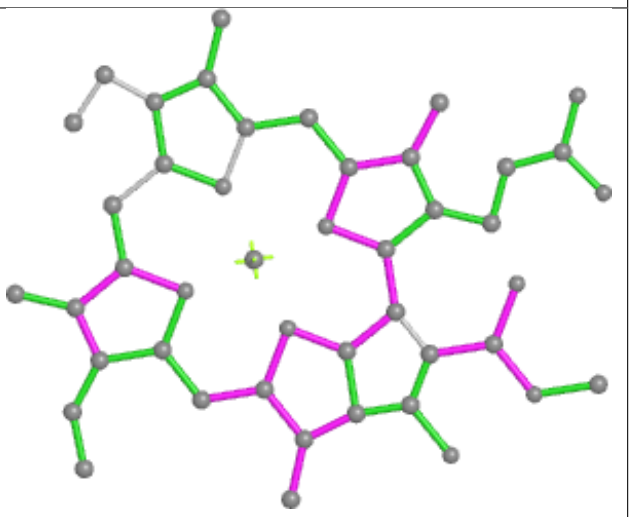


Rings

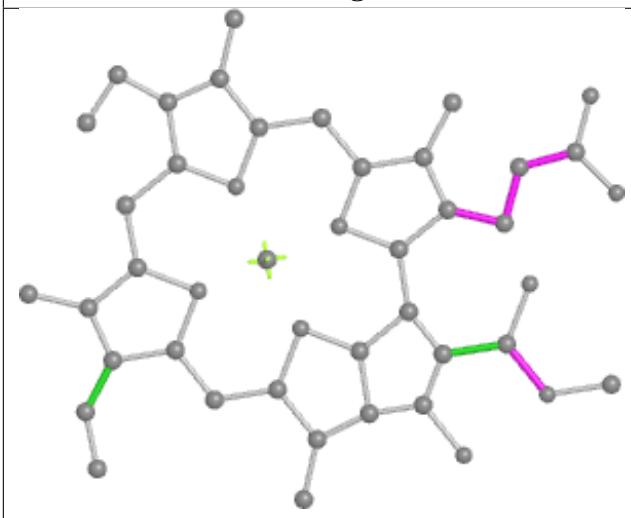
## Ligand CLA 4 617



Bond lengths



Bond angles



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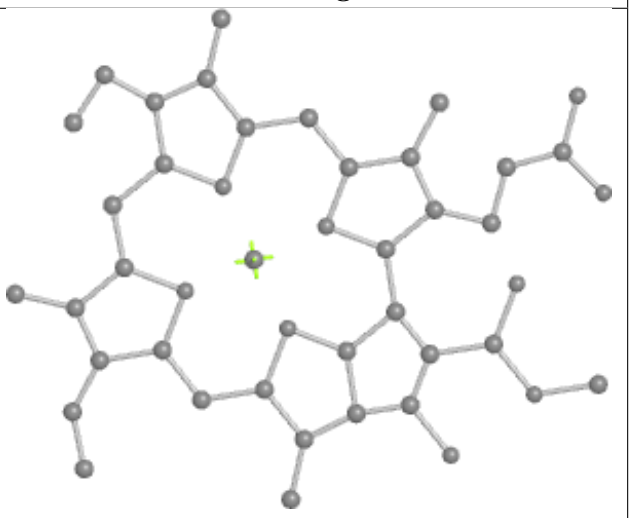
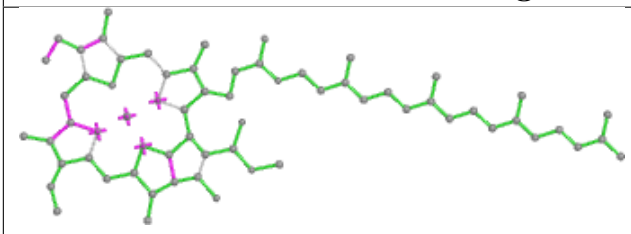
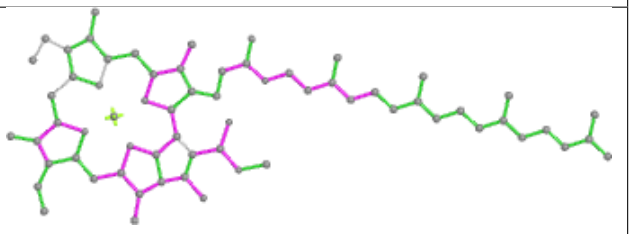


Rings

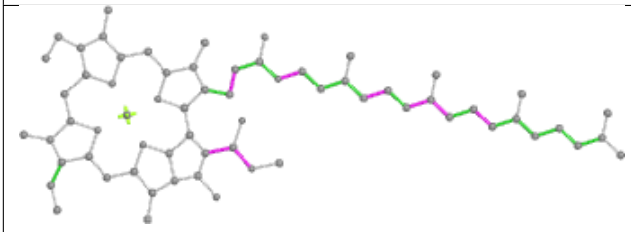
## Ligand CLA B 1022



Bond lengths



Bond angles



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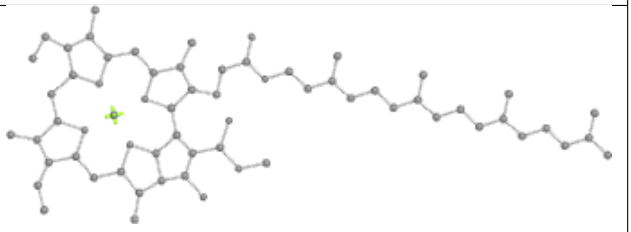
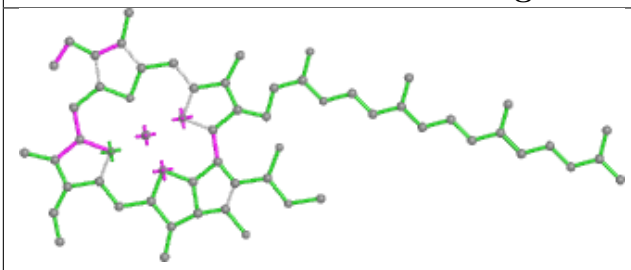
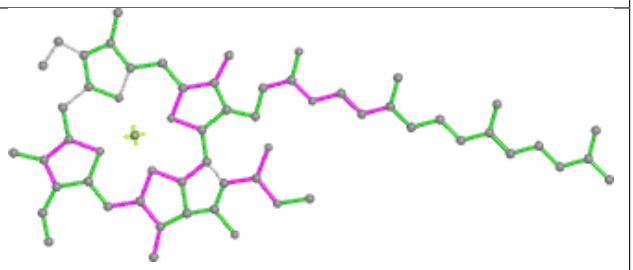


Rings

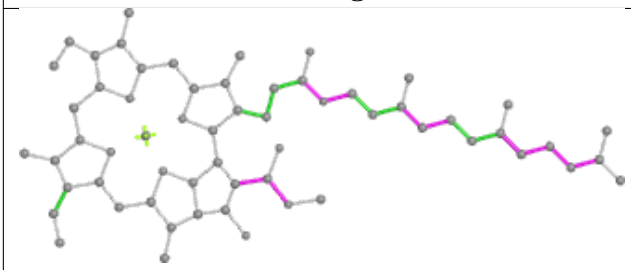
## Ligand CLA A 1115



Bond lengths



Bond angles



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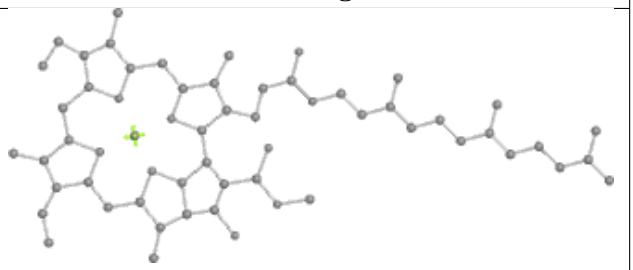
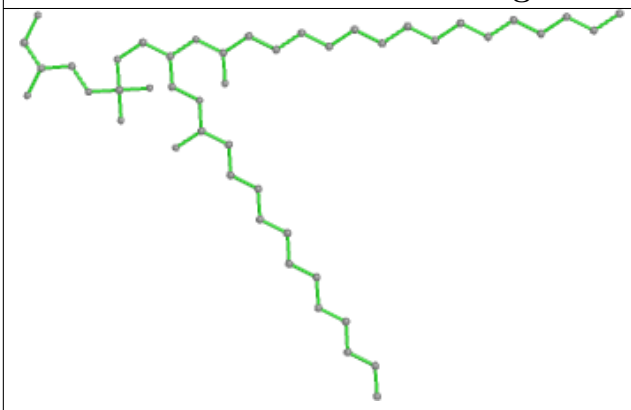
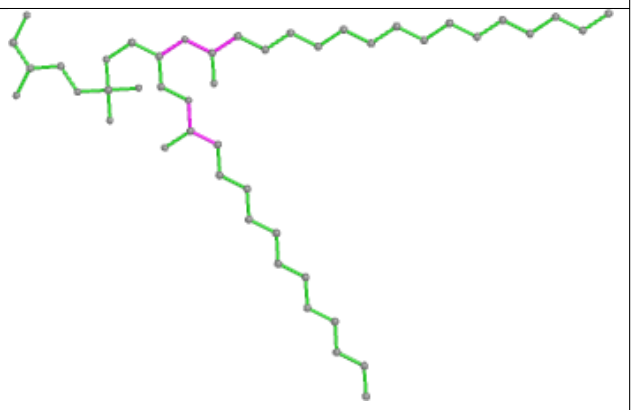


Rings

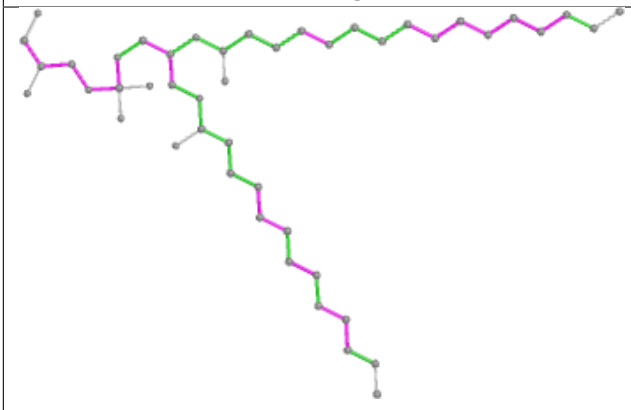
## Ligand LHG A 5003



Bond lengths



Bond angles



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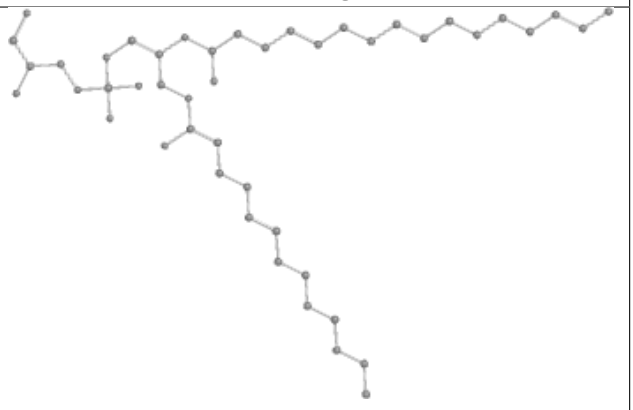
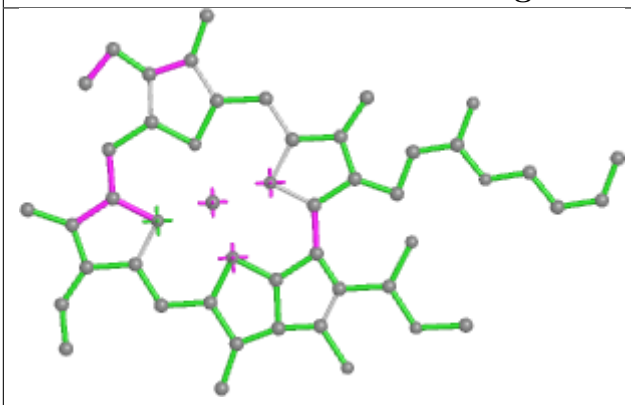


Rings

## Ligand CLA K 1403



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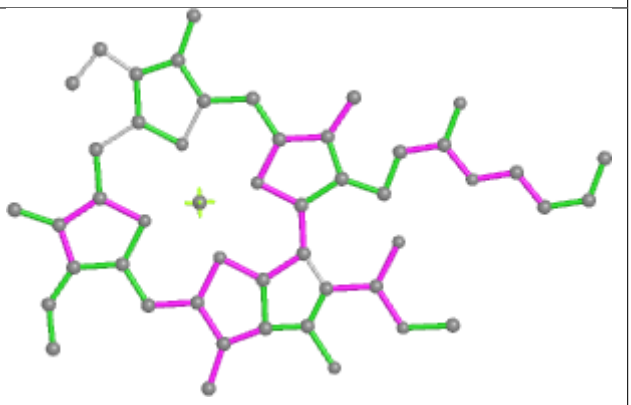
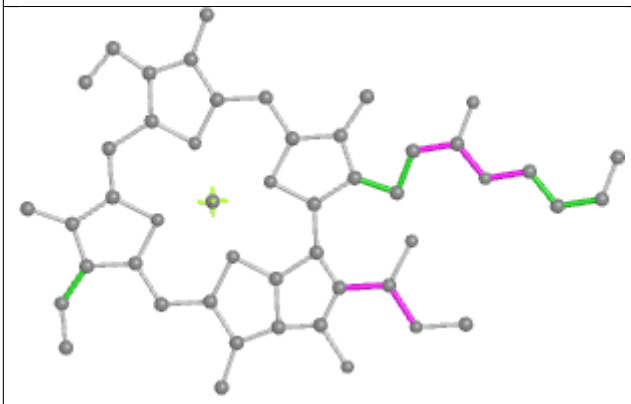


Bond angles



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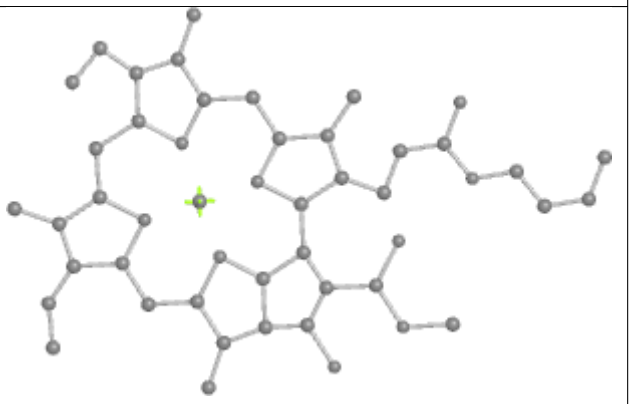
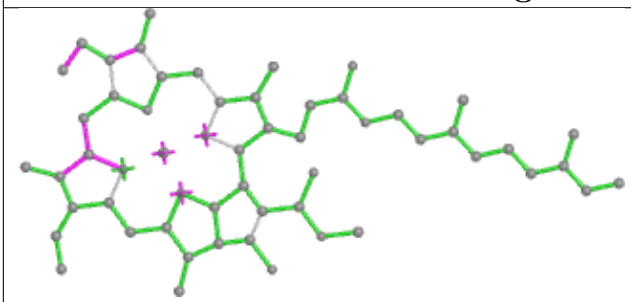


Rings

## Ligand CLA A 1130



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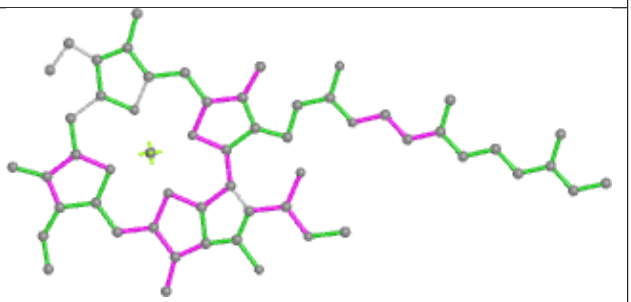
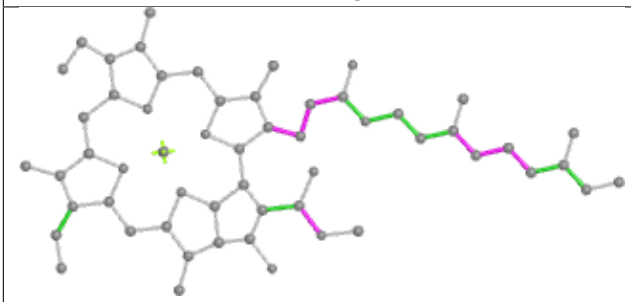


Bond angles



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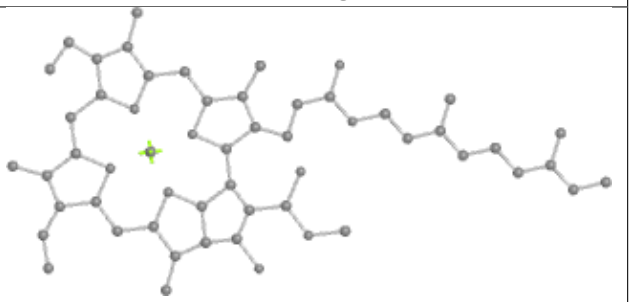
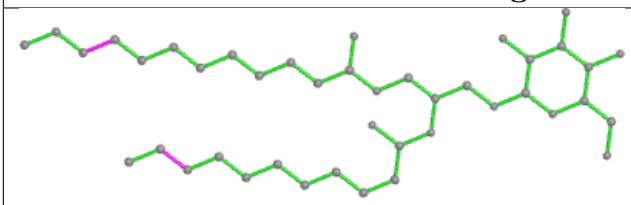
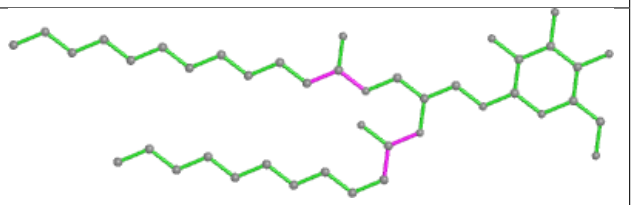
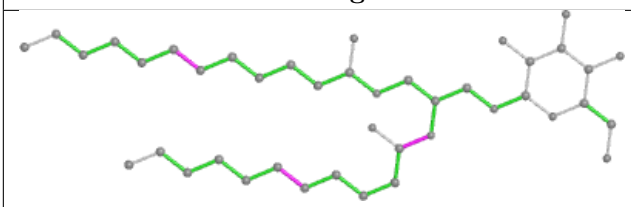


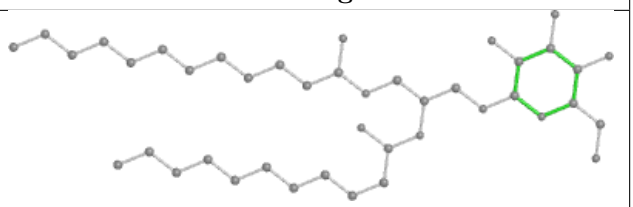
Rings

## Ligand LMG A 5004

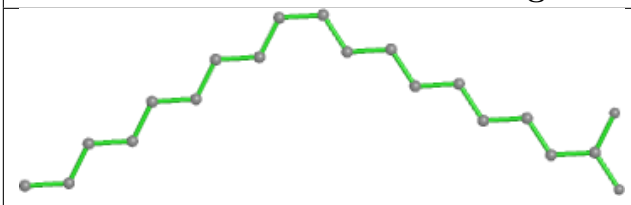

Bond lengths

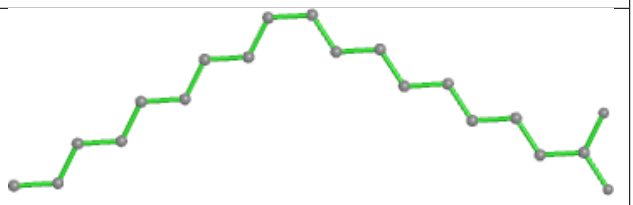

Bond angles

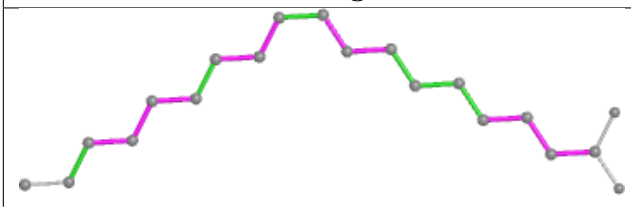

Torsions


Rings

## Ligand OLA 8 809


Bond lengths


Bond angles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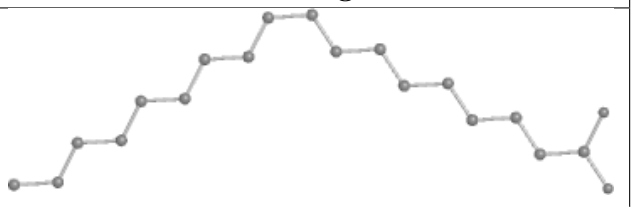
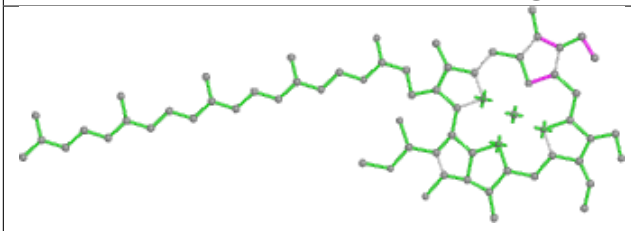

Rings

## Ligand CHL 5 610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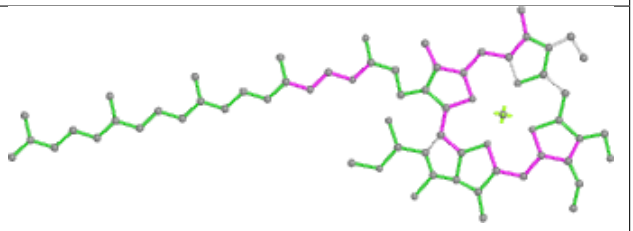
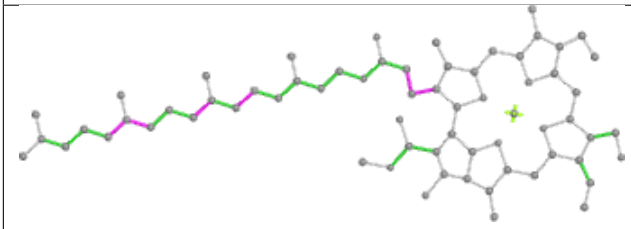
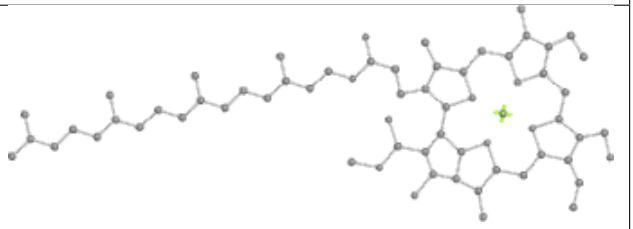
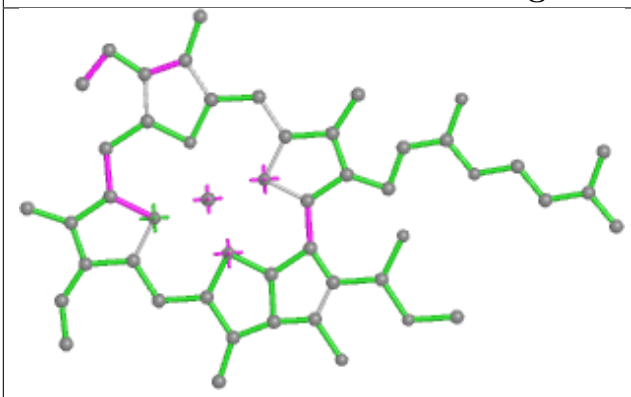

Bond angles

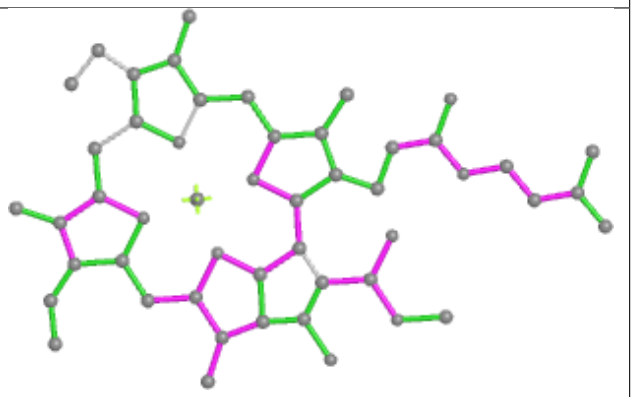

Torsions


Rings

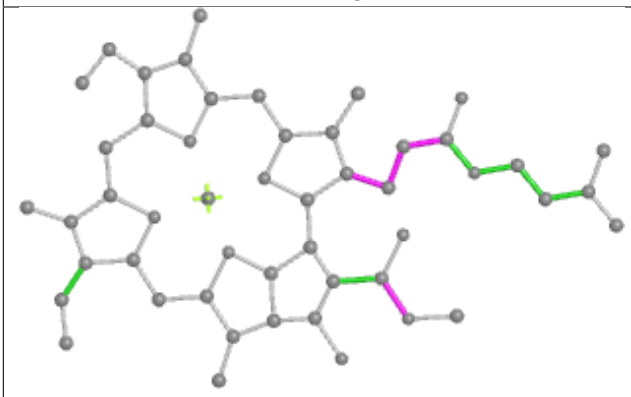
**Ligand CLA 3 612**



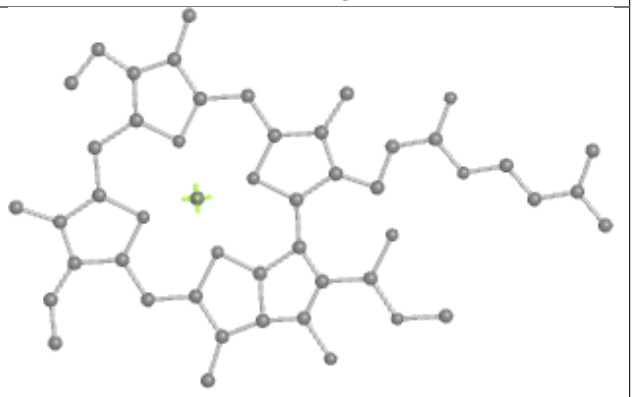
**Bond lengths**



**Bond angles**

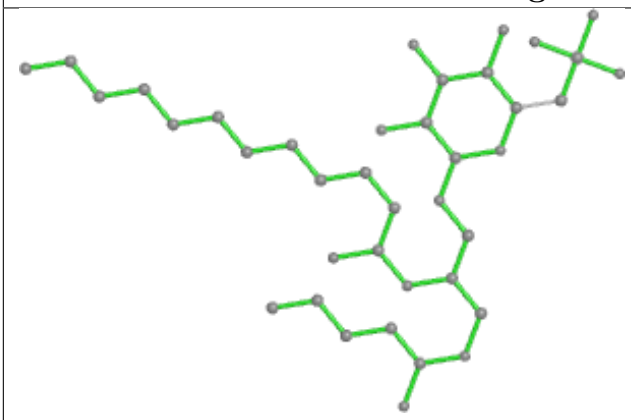


**Torsions**

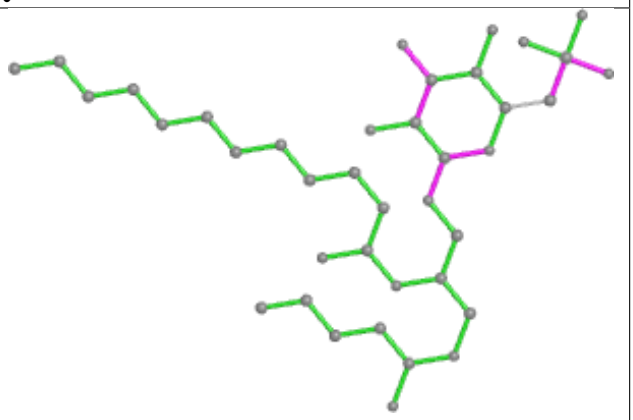


**Rings**

**Ligand SQD 7 805**



Bond lengths



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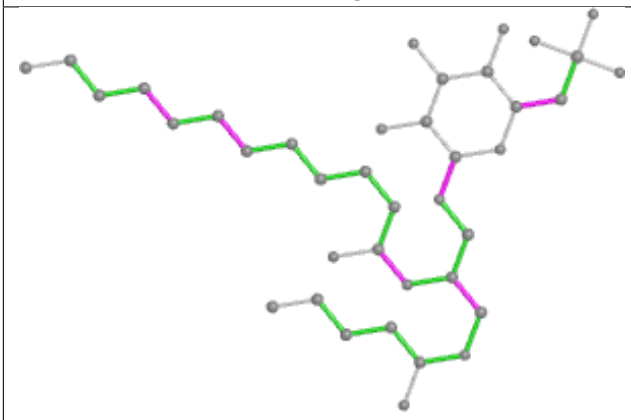

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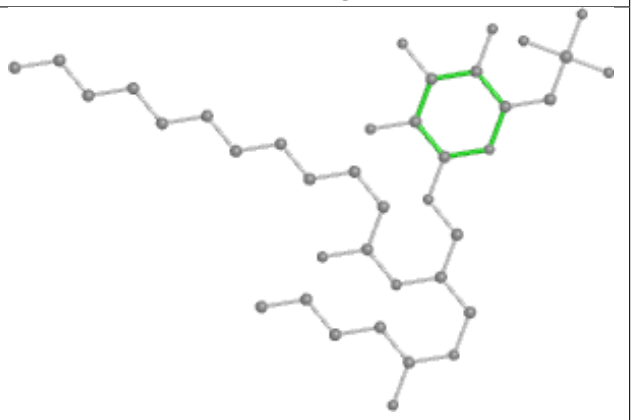
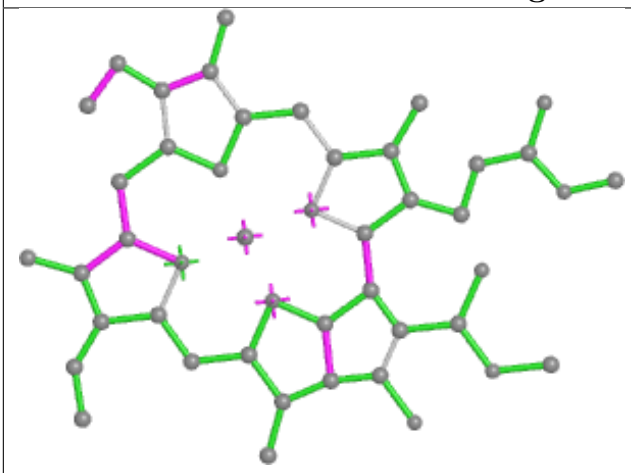


Rings

**Ligand CLA 5 605**



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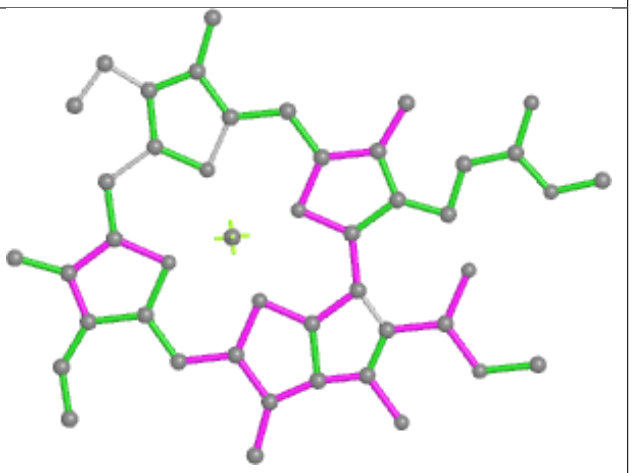
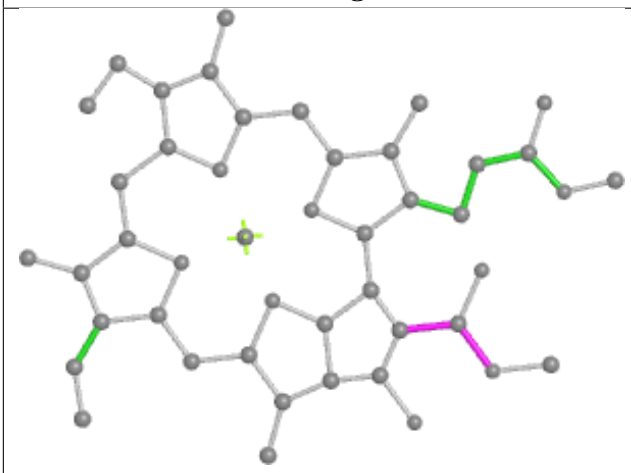
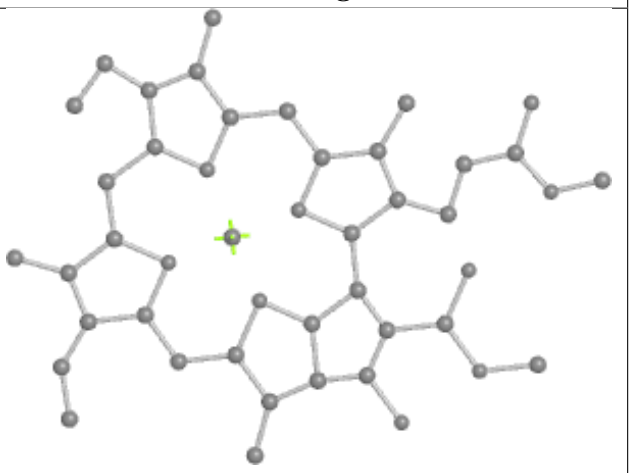


**Bond angles**



**Torsions**



**Rings**

| Ligand CLA 5 606 | |
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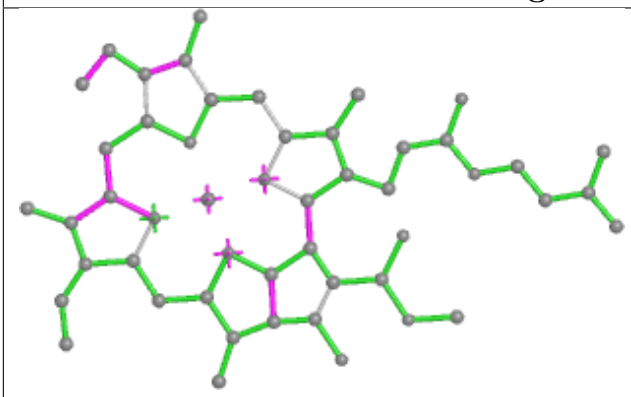
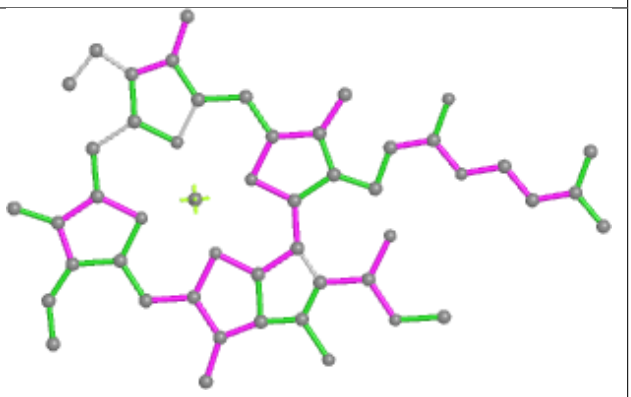
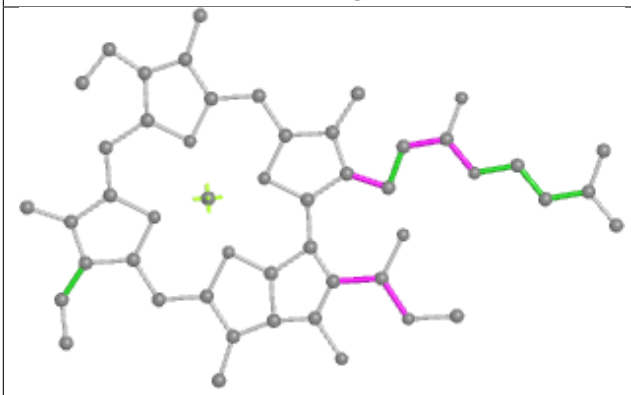
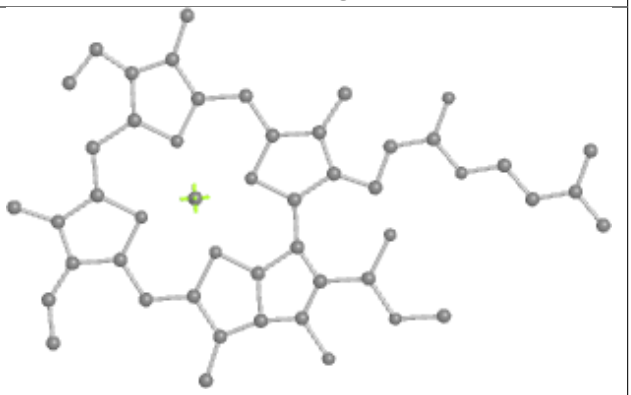
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand DGA 8 804 | |
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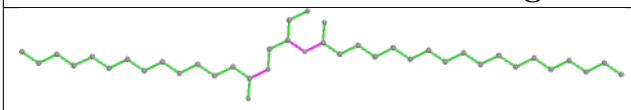
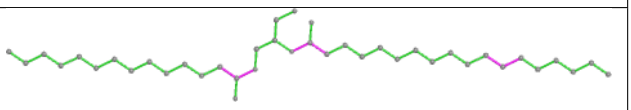
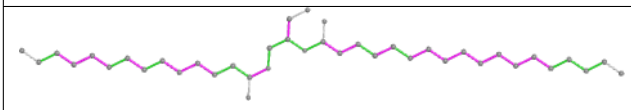
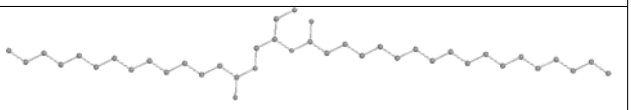
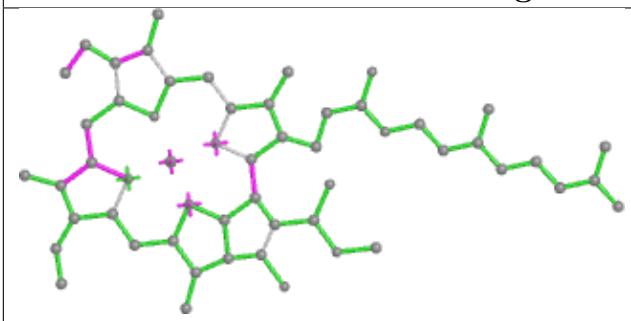
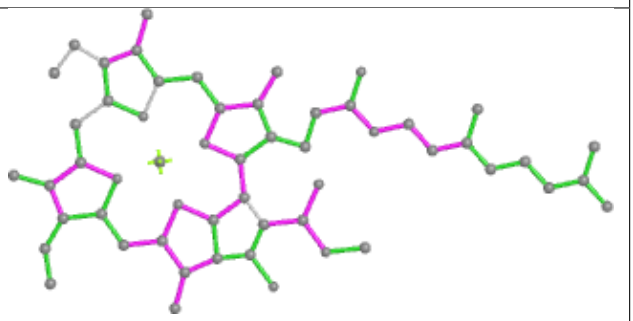
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

**Ligand CLA O 1802**



**Bond lengths**



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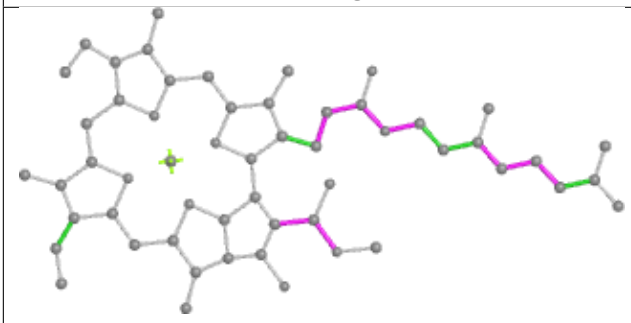
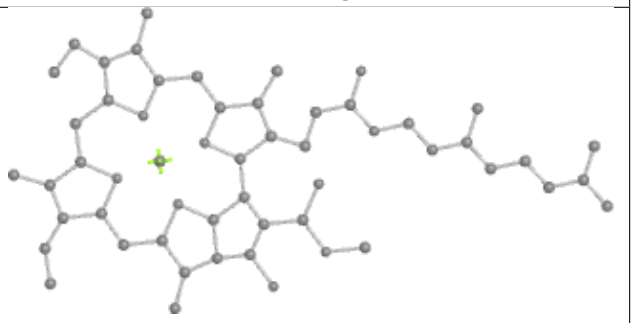
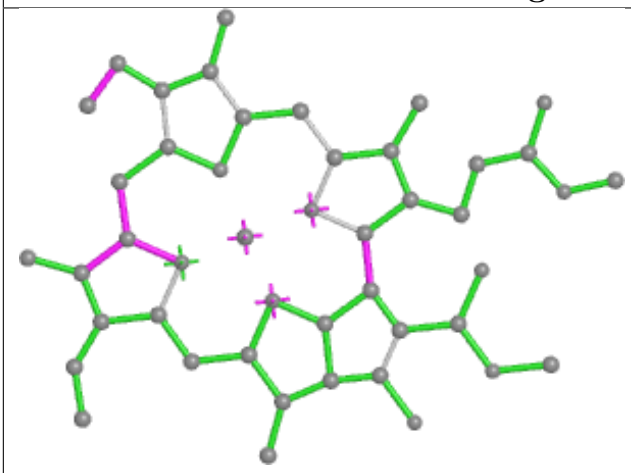


**Torsions**

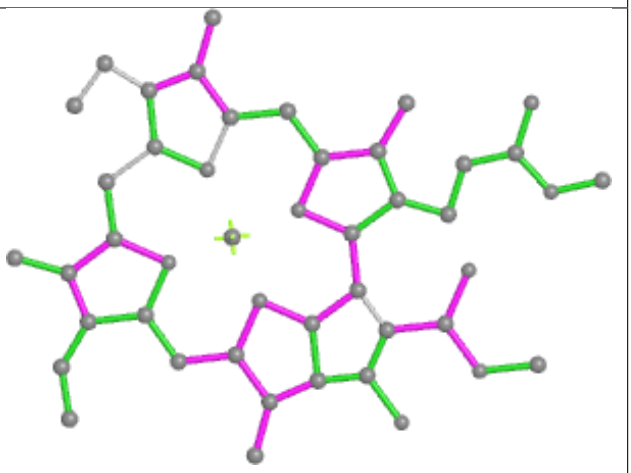


**Rings**

**Ligand CLA 2 606**



**Bond lengths**



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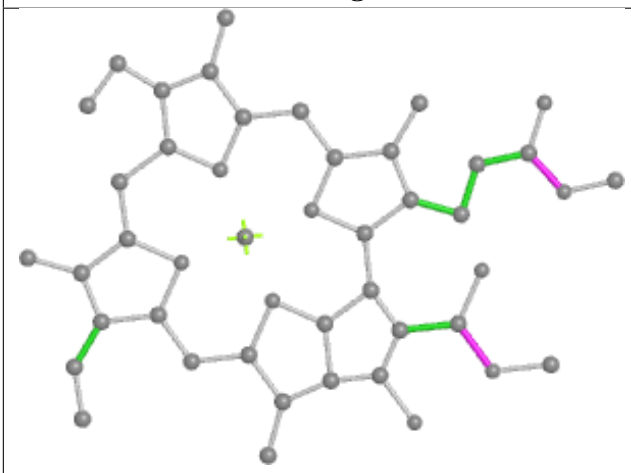
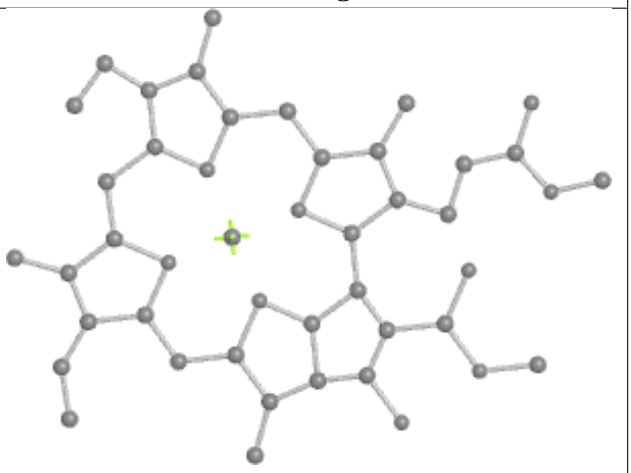
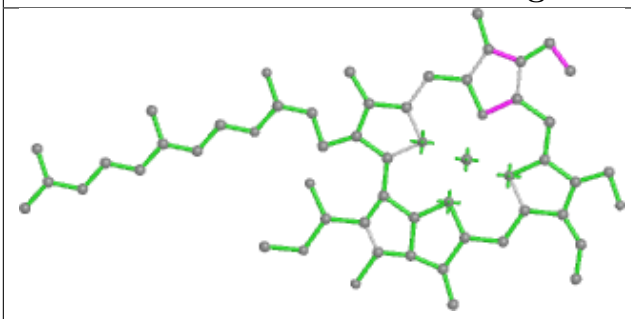


**Torsions**



**Rings**

## Ligand CHL 6 610



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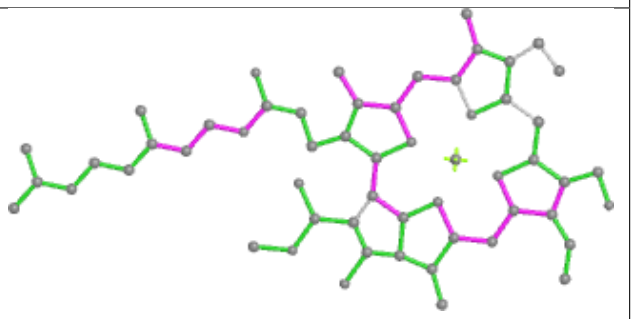
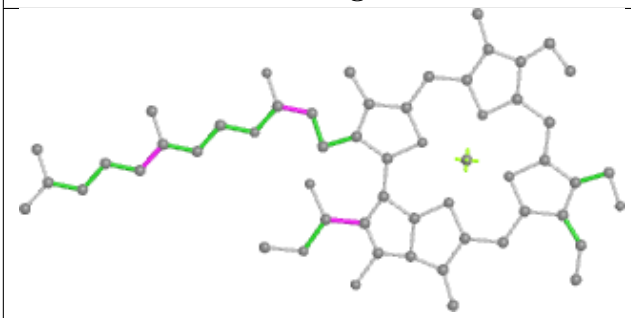
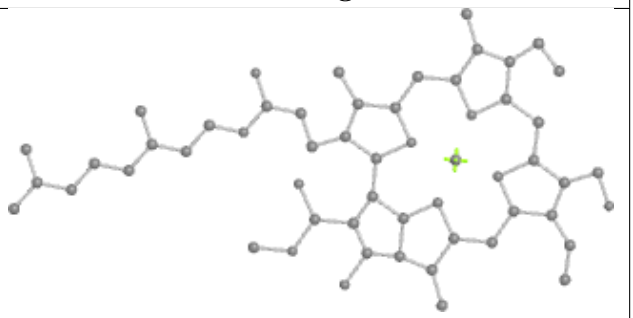


Bond angles

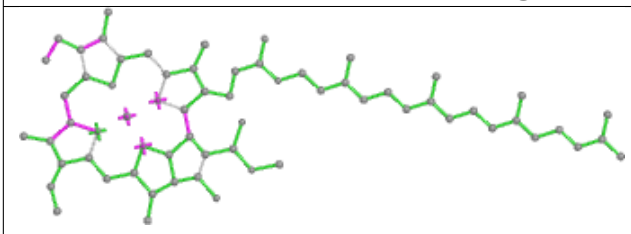


Torsions



Rings

## Ligand CLA A 1106



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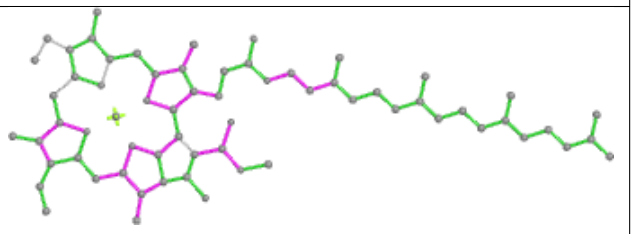
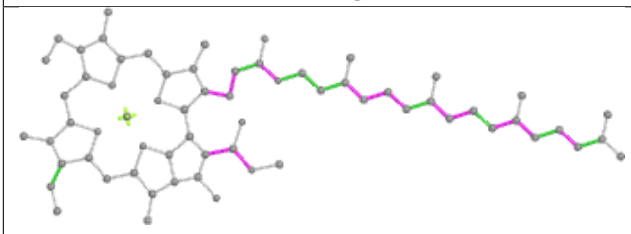
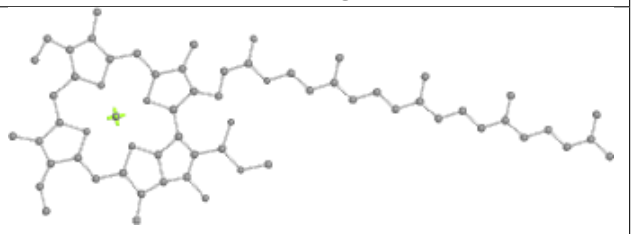


Bond angles

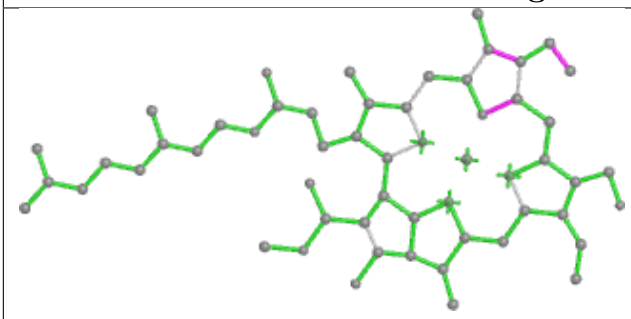


Torsions



Rings

## Ligand CHL a 606



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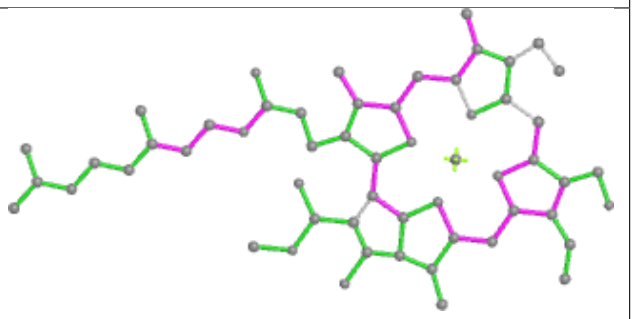
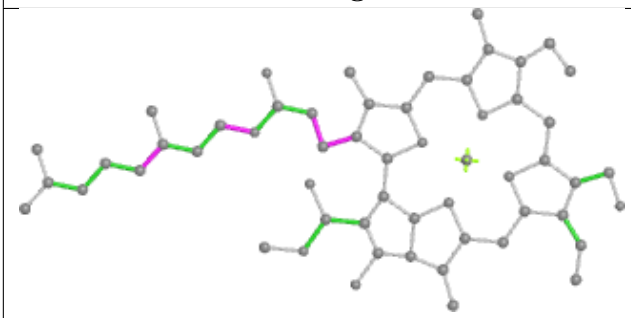


Bond angles



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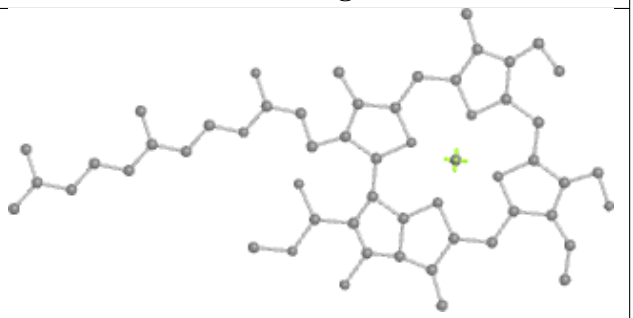
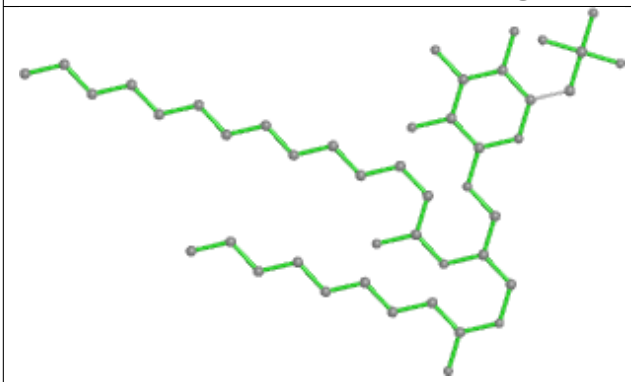


Rings

## Ligand SQD H 5001



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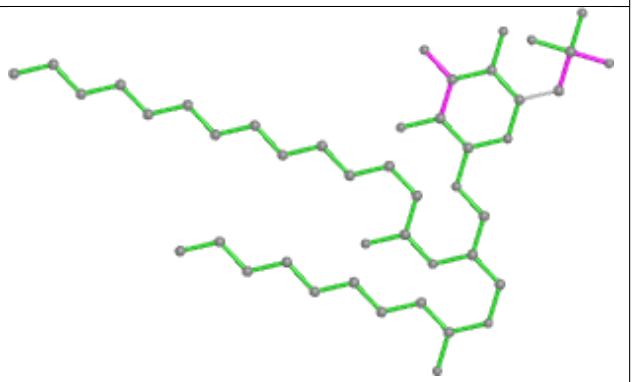
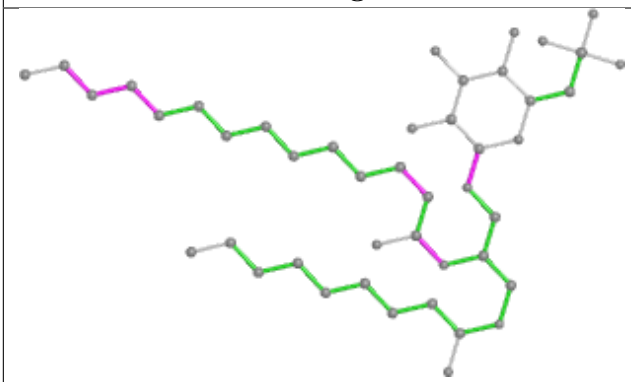


Bond angles



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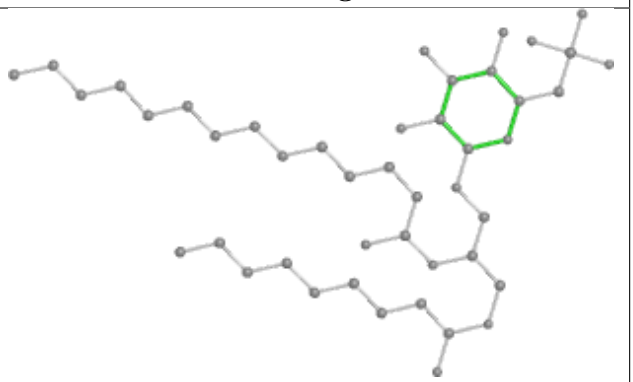
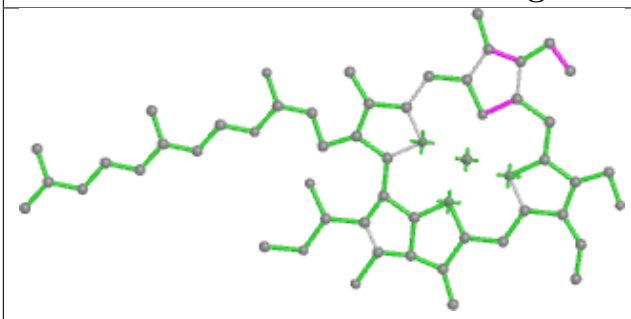


Rings

## Ligand CHL 4 618



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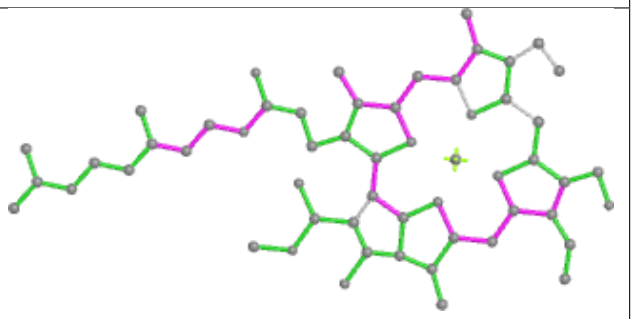
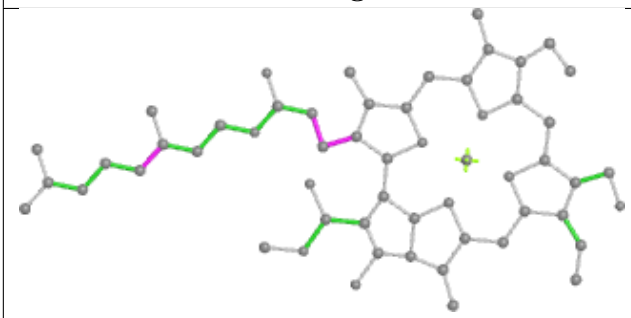


Bond angles



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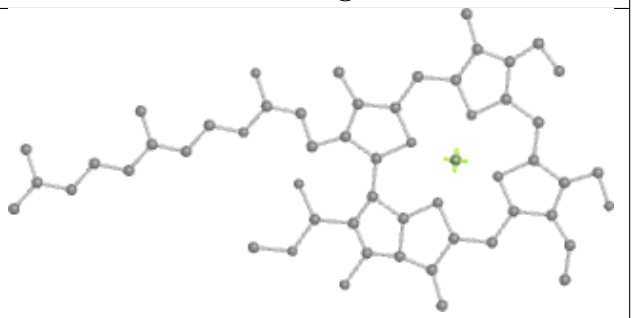
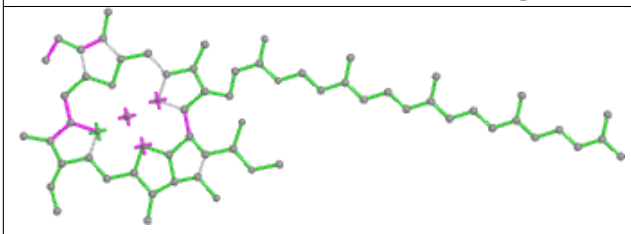
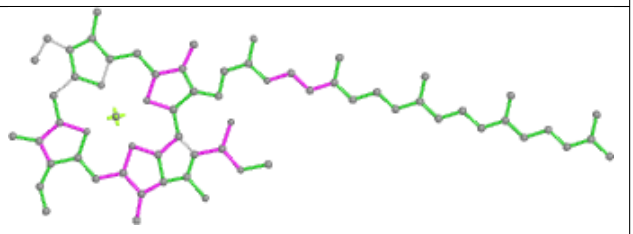


Rings

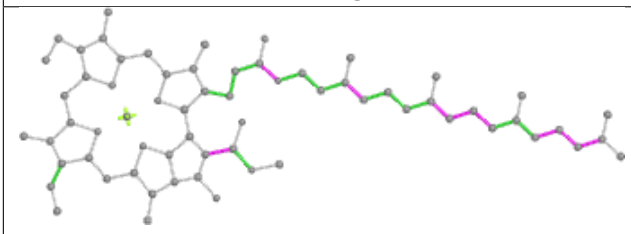
## Ligand CLA A 1136



Bond lengths



Bond angles



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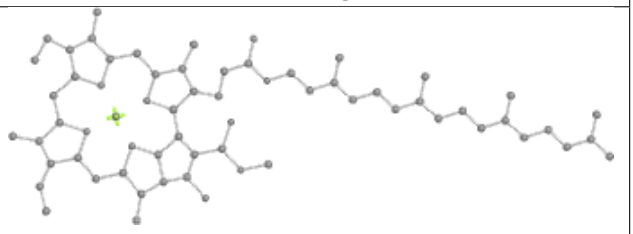
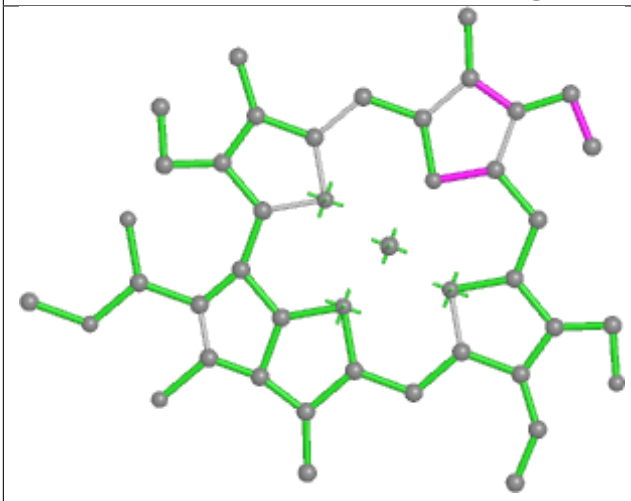
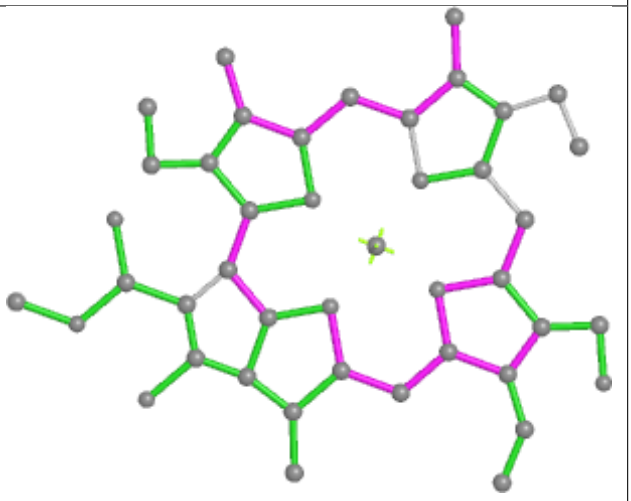


Rings

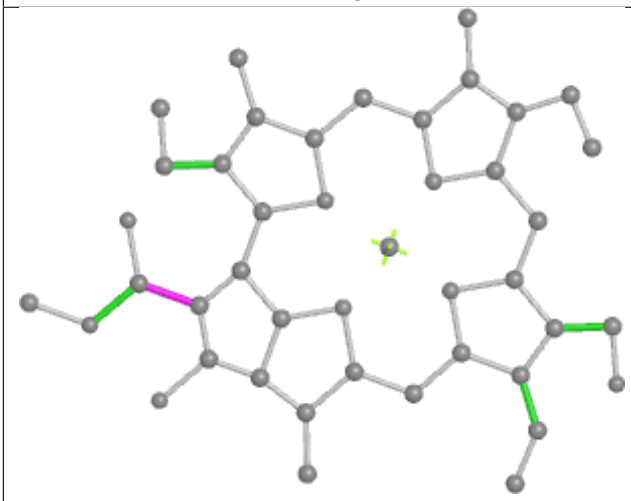
## Ligand CHL 3 608



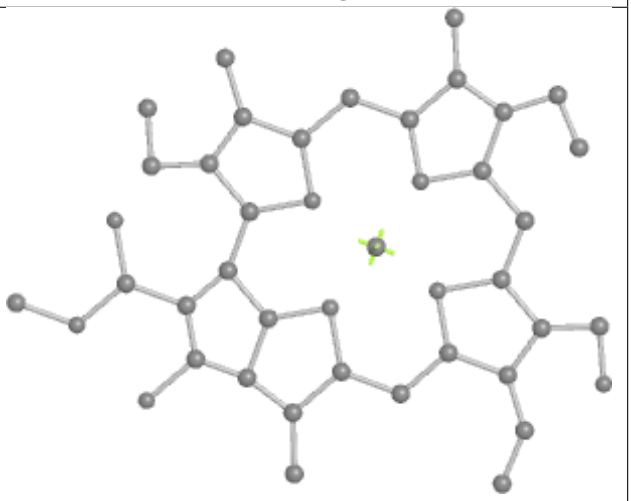
Bond lengths



Bond angles

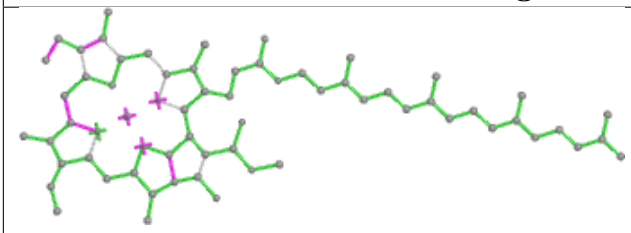


Torsions

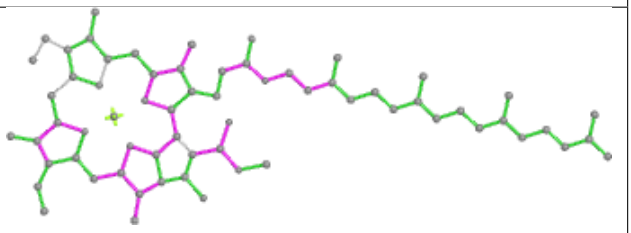


Rings

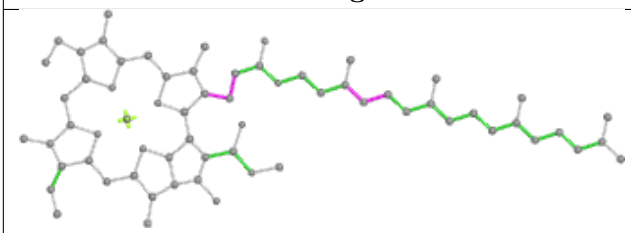
## Ligand CLA B 1225



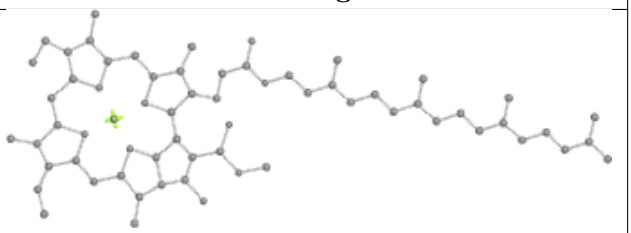
Bond lengths



Bond angles

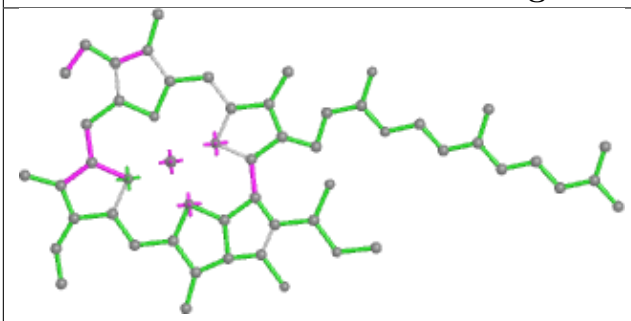


Torsions

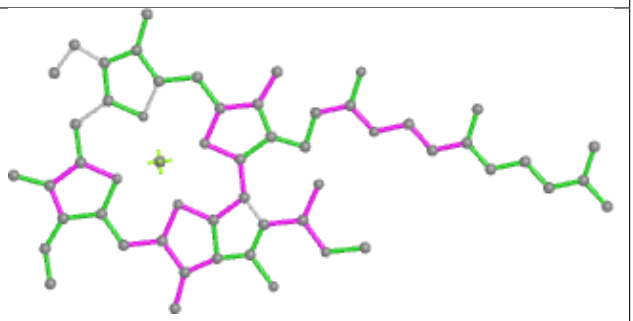


Rings

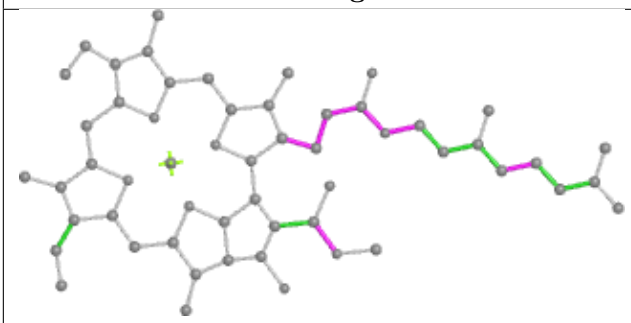
## Ligand CLA 7 608



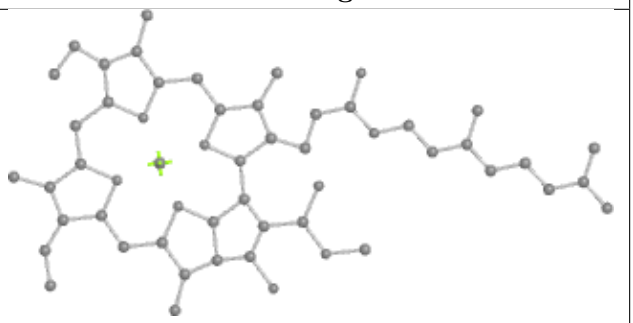
Bond lengths



Bond angles

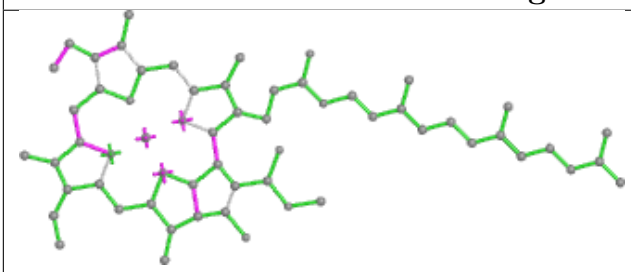


Torsions



Rings

## Ligand CLA 9 605



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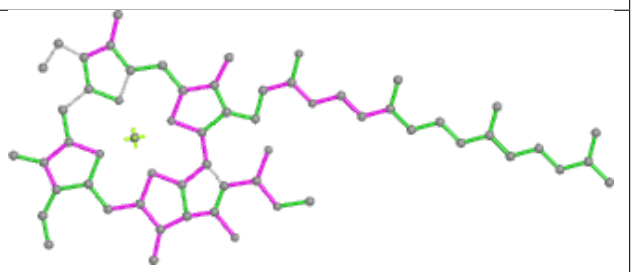
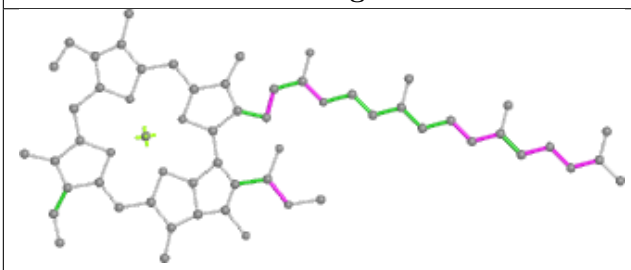


Bond angles



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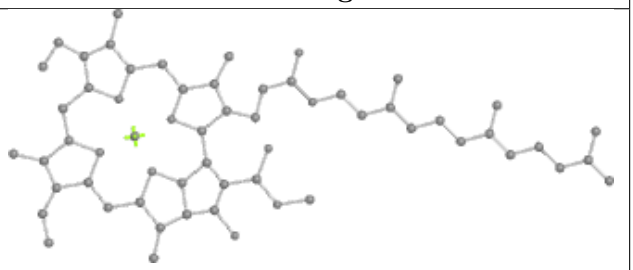
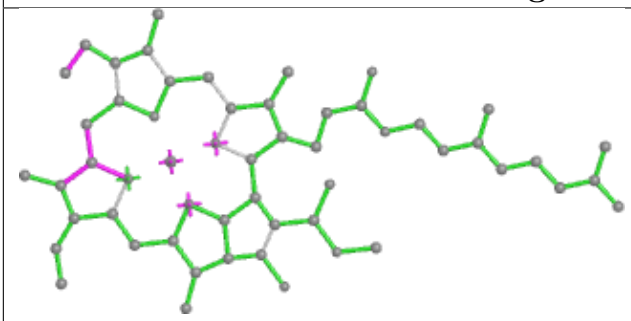


Rings

## Ligand CLA 9 606



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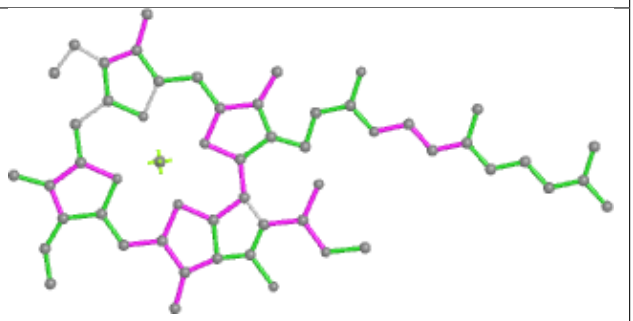
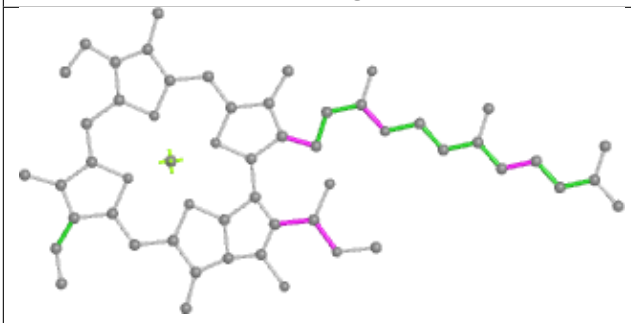


Bond angles



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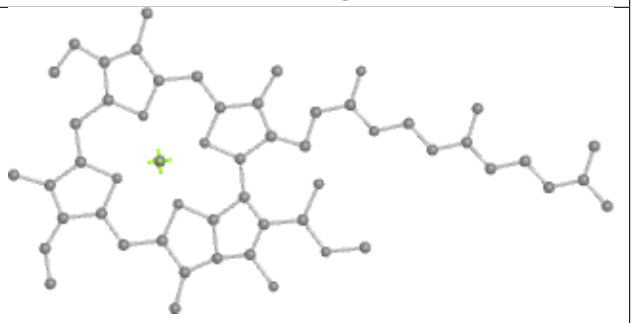
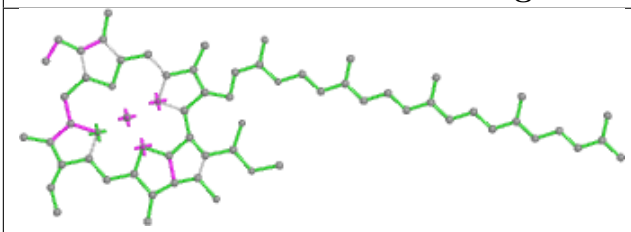


Rings

## Ligand CLA A 1104



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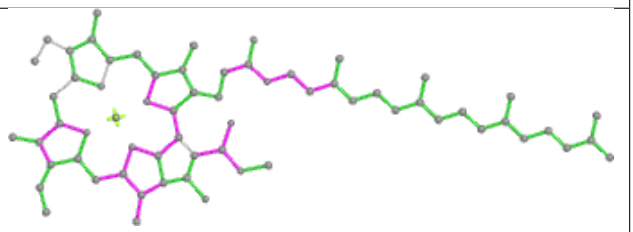
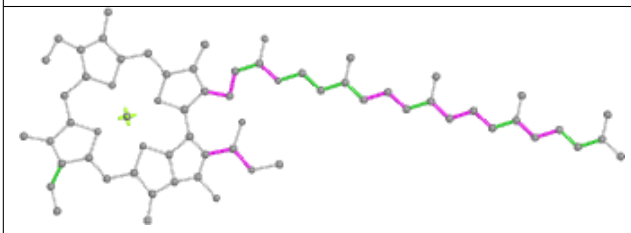


Bond angles



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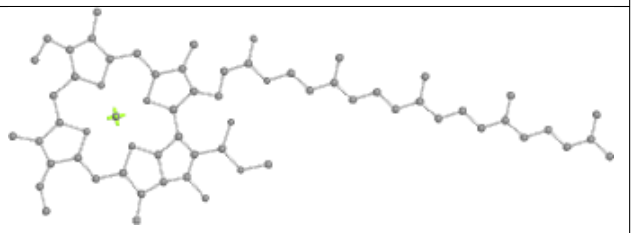
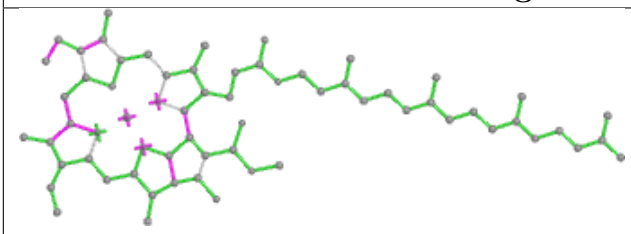


Rings

## Ligand CLA A 1131



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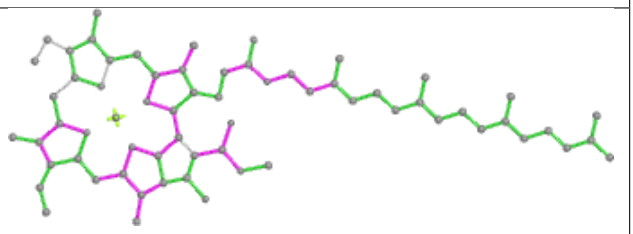

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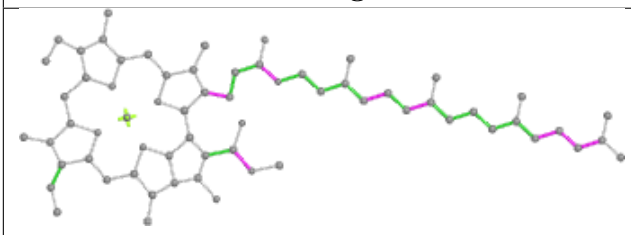

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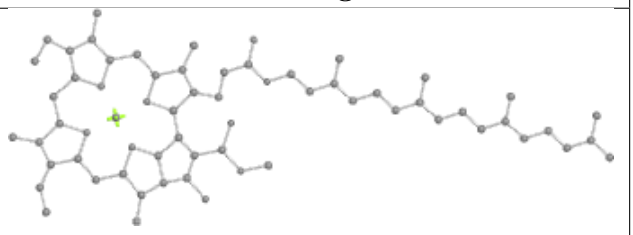
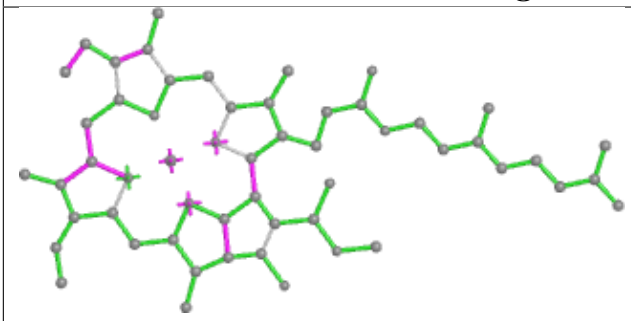


Rings

## Ligand CLA A 1118



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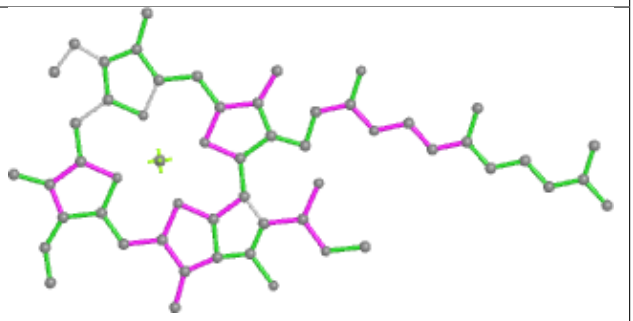
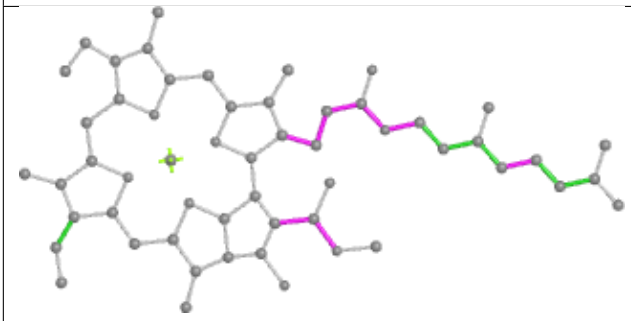


Bond angles



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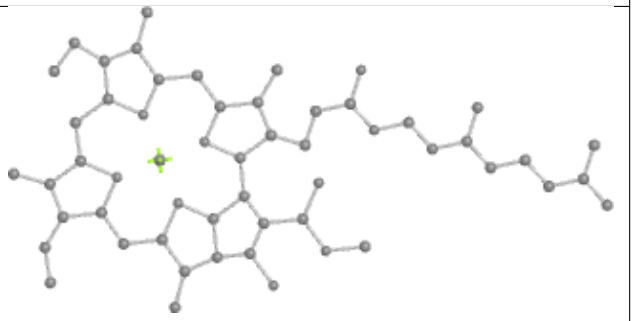
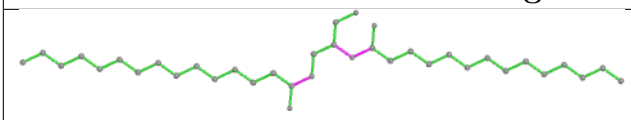


Rings

## Ligand DGA 2 803



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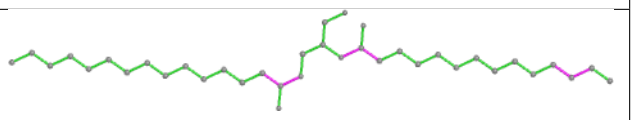
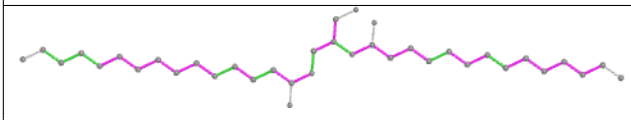


Bond angles



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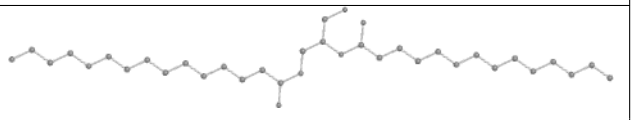
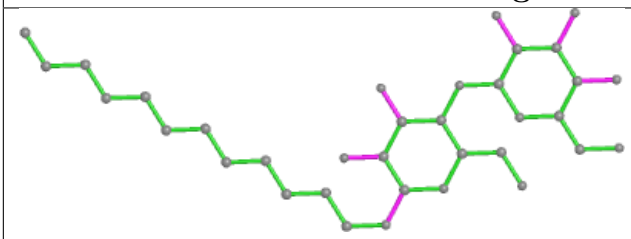


Rings

## Ligand LMT B 5006



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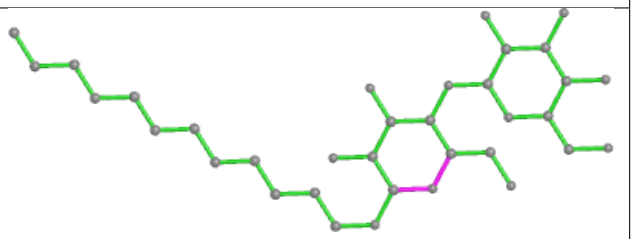
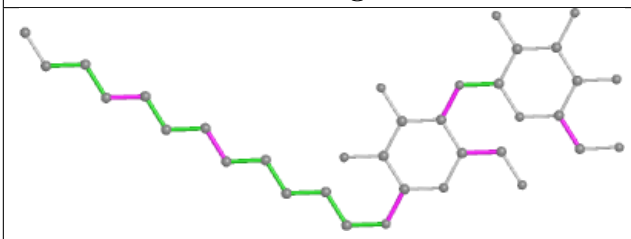


Bond angles



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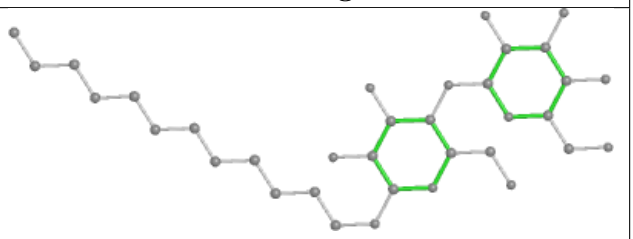
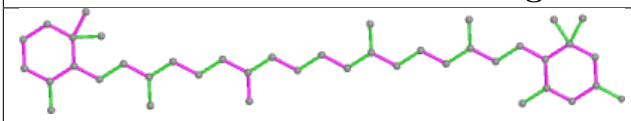


Rings

## Ligand RRX 3 506



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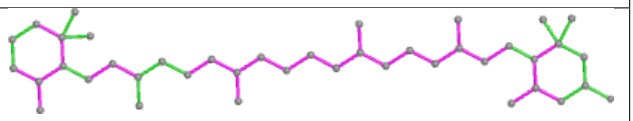
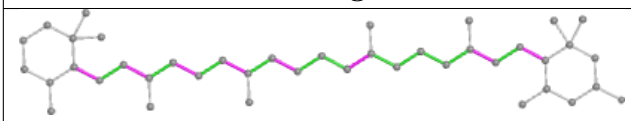


Bond angles



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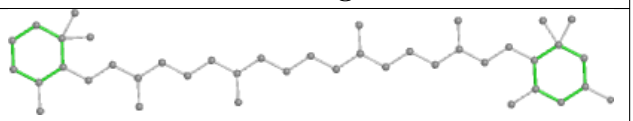
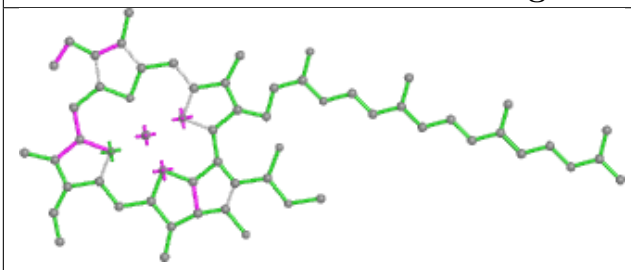


Rings

## Ligand CLA 7 601



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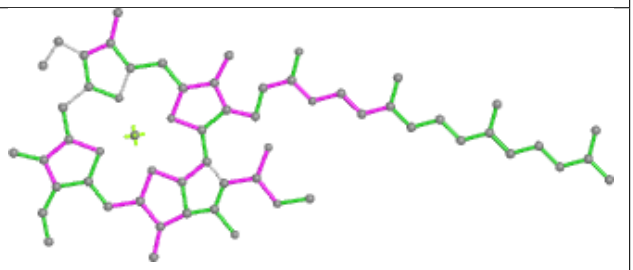
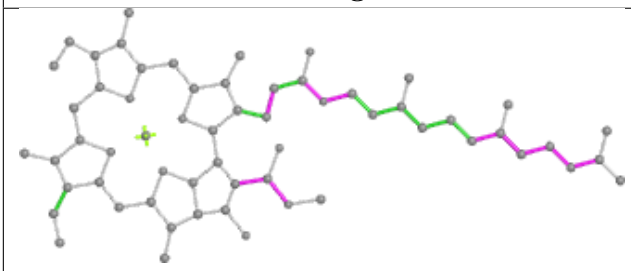


Bond angles



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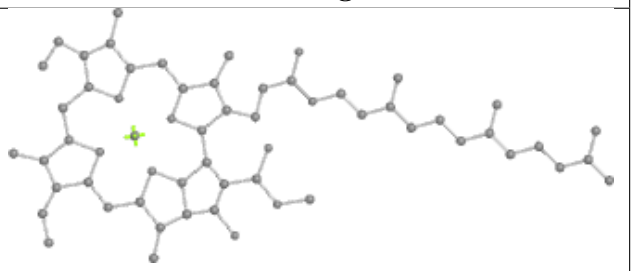
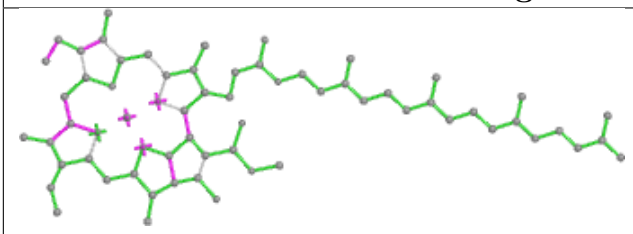


Rings

## Ligand CLA B 1223



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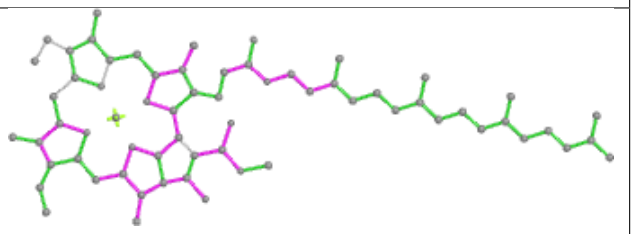
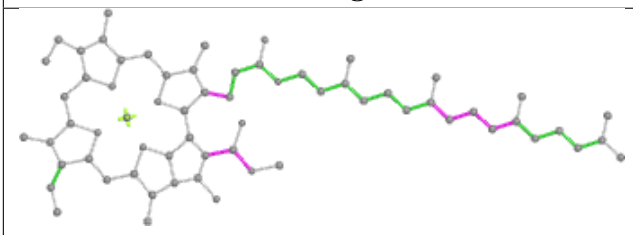


Bond angles



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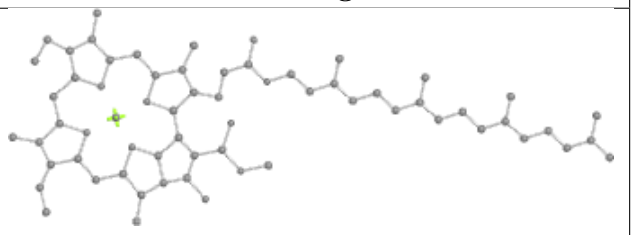
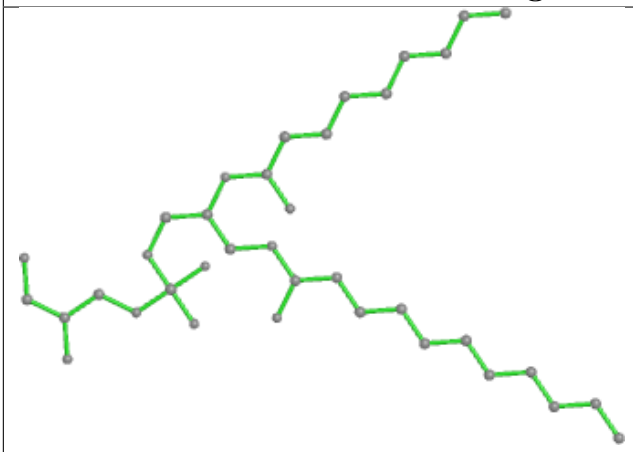


Rings

## Ligand LHG 7 801



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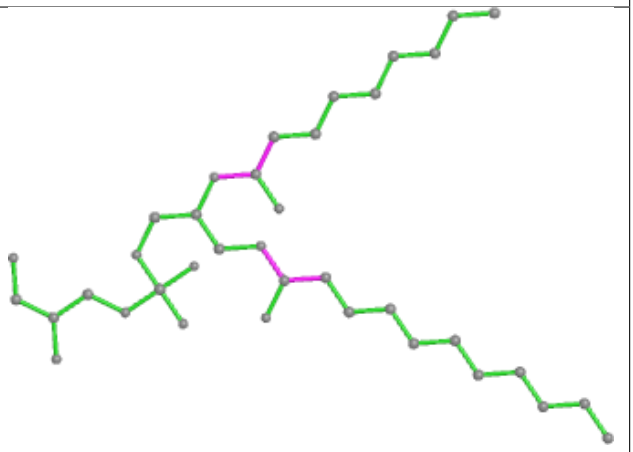
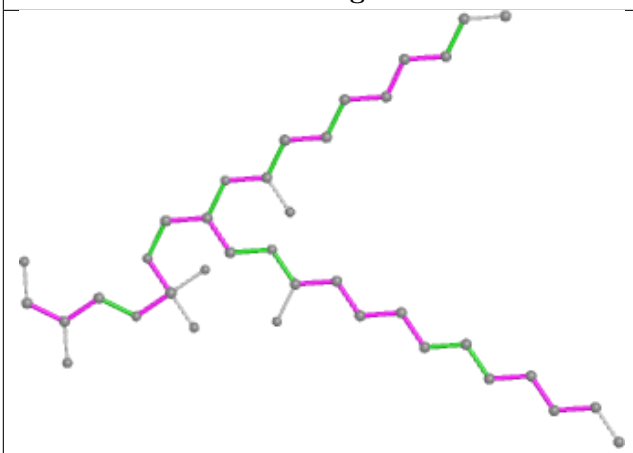


Bond angles



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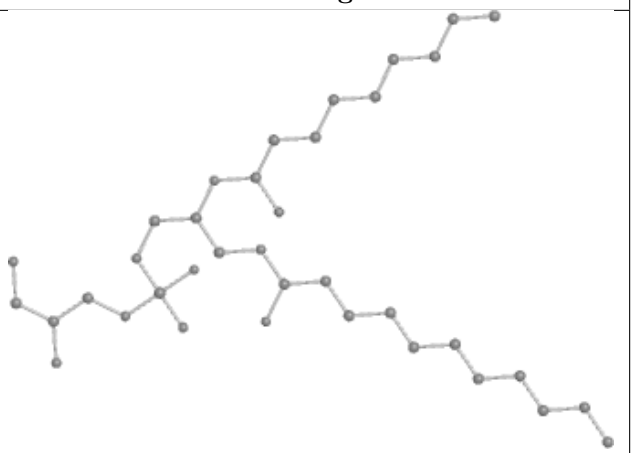
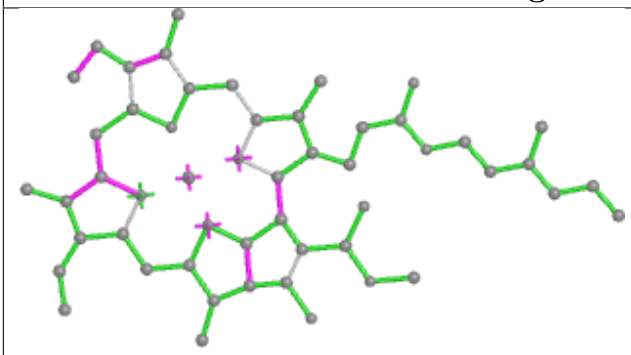
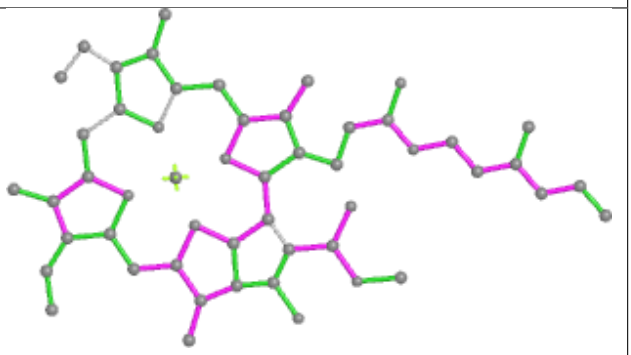
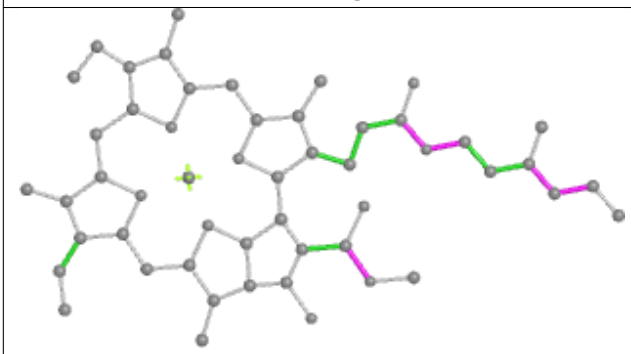
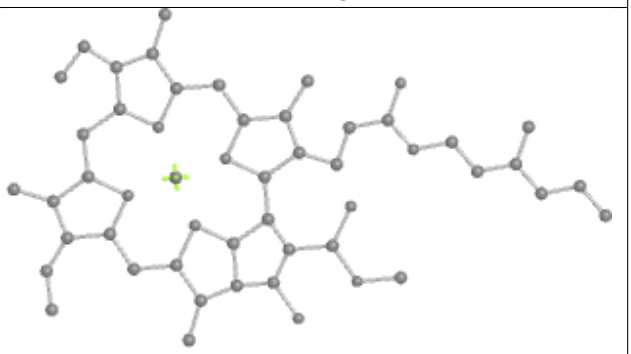


Rings

| Ligand CLA 6 602 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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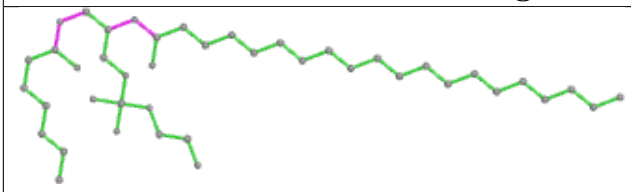
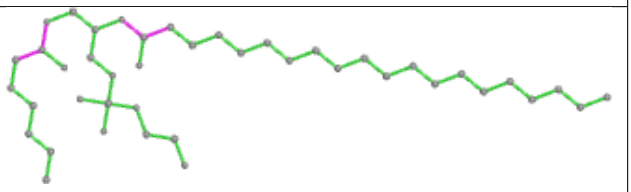
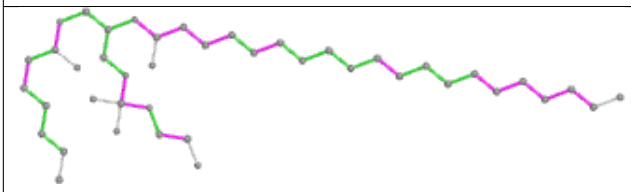
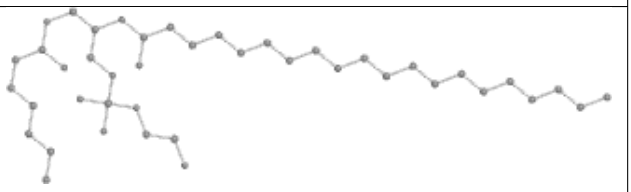
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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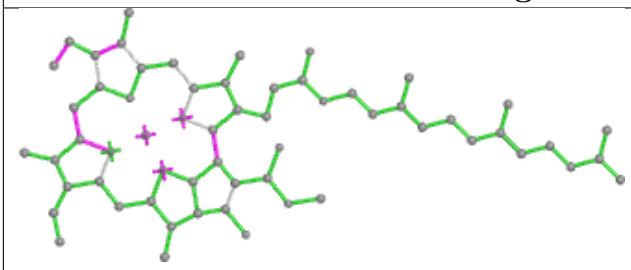

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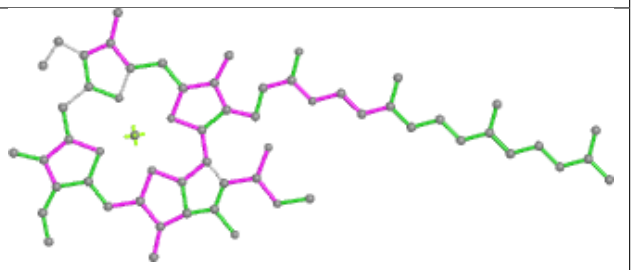

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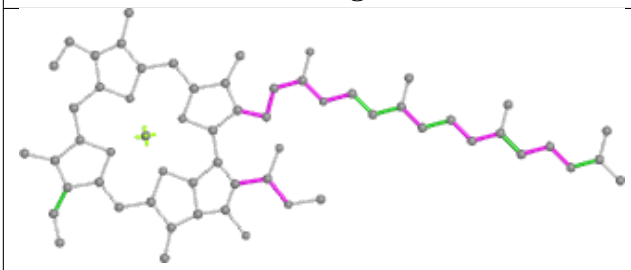

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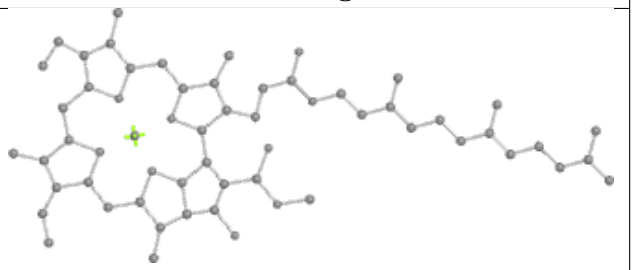

Rings

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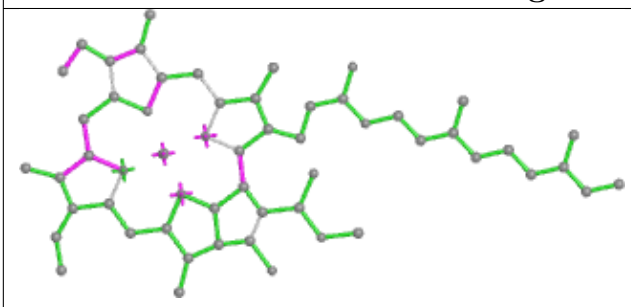

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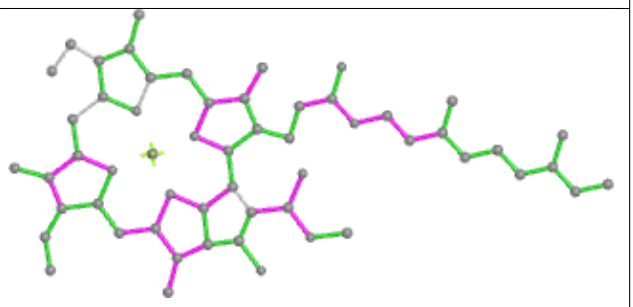

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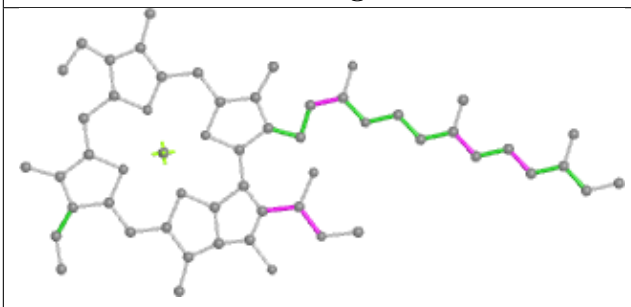

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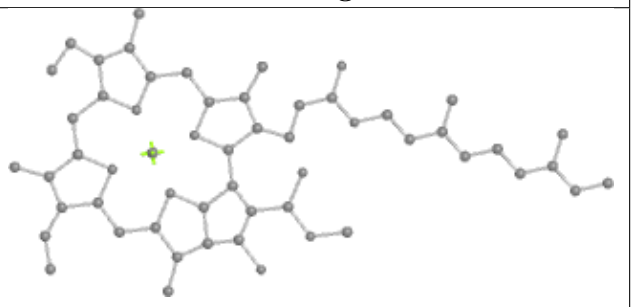
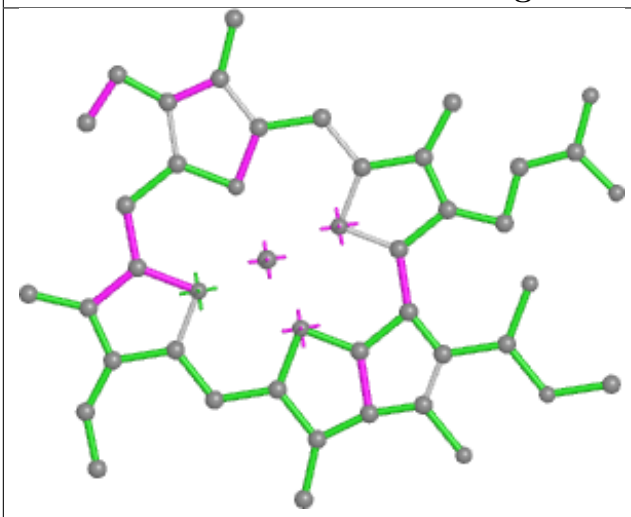


Rings

## Ligand CLA K 1404



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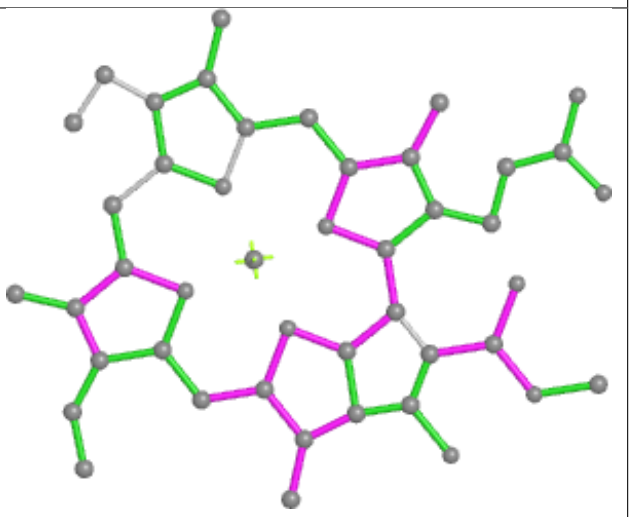

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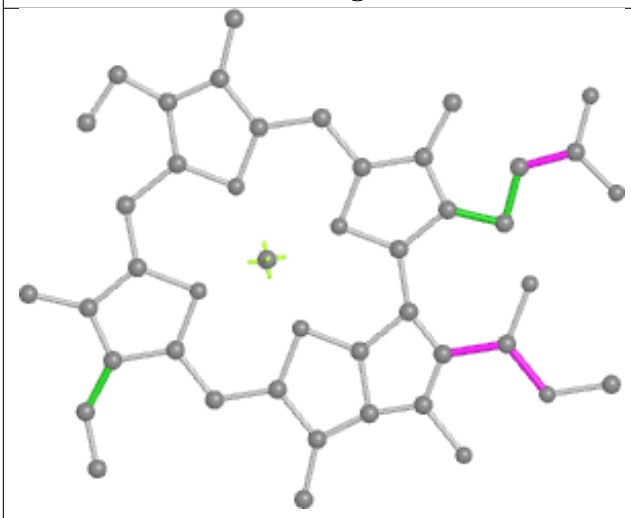

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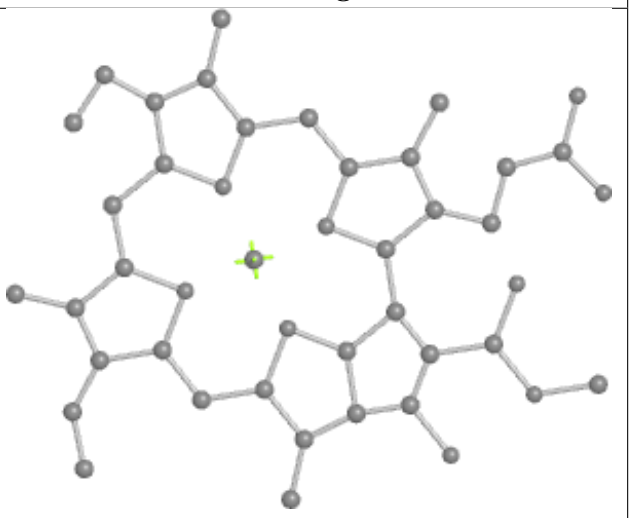

Rings

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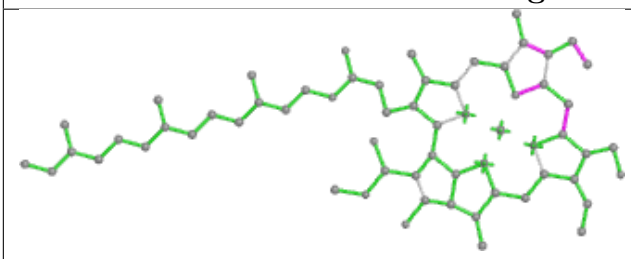

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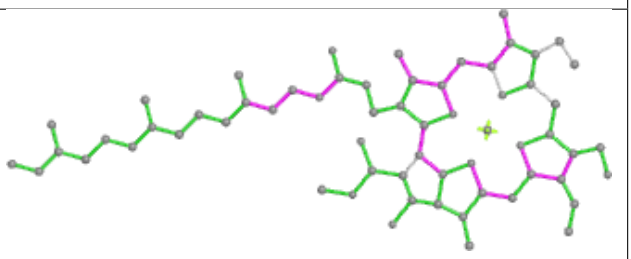

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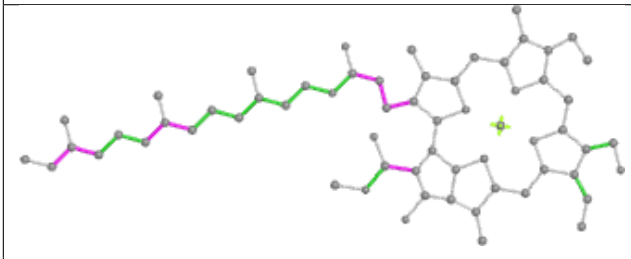

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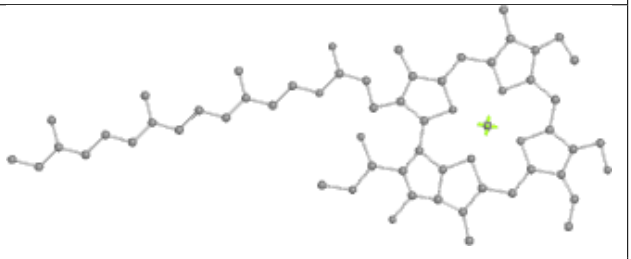

Rings

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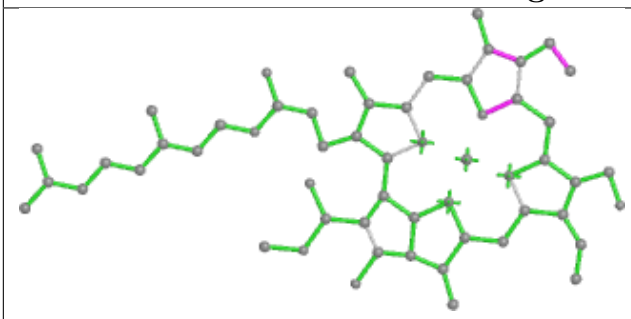

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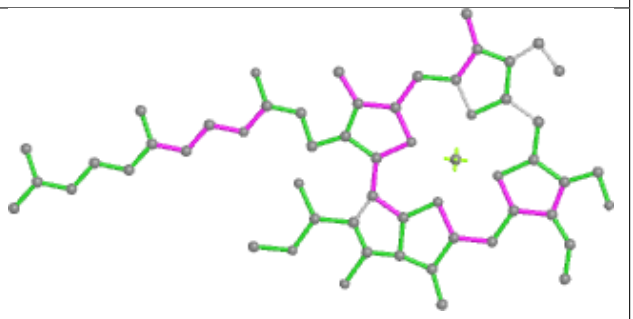
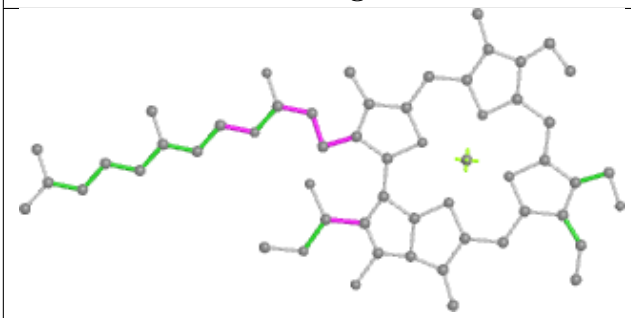


Bond angles



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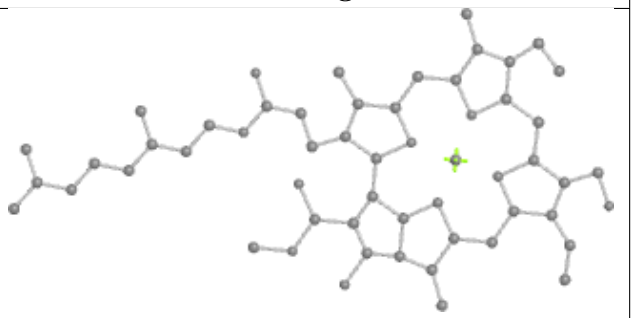

Rings

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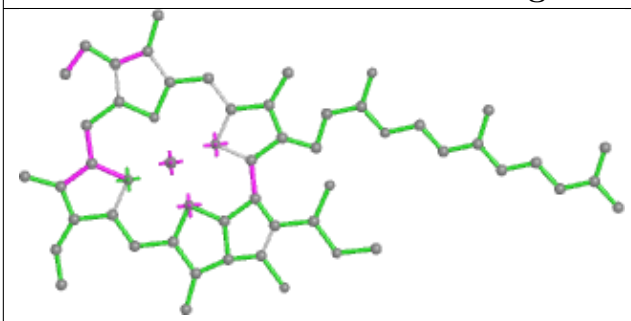

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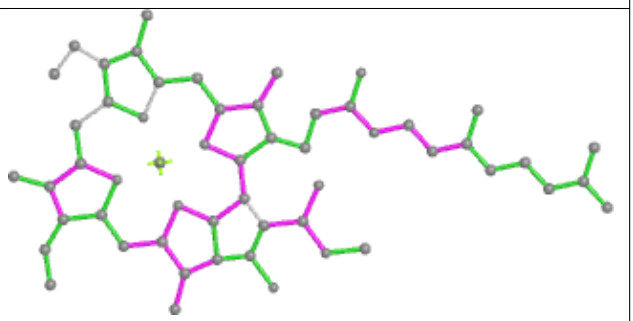

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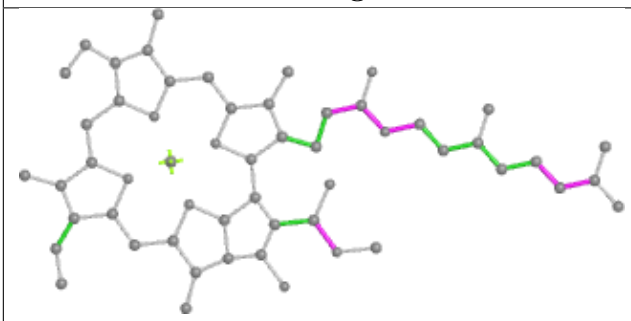

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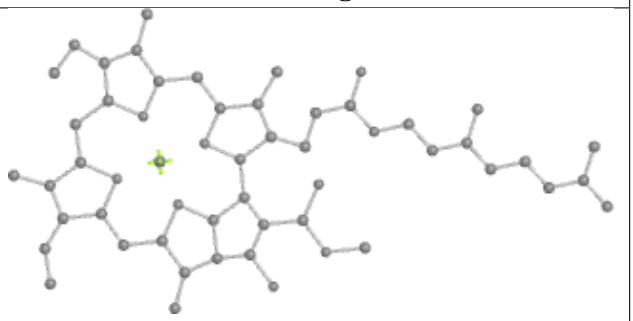

Rings

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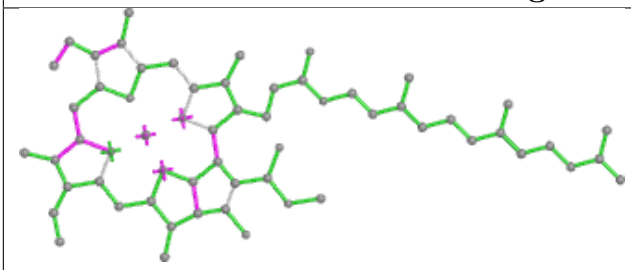

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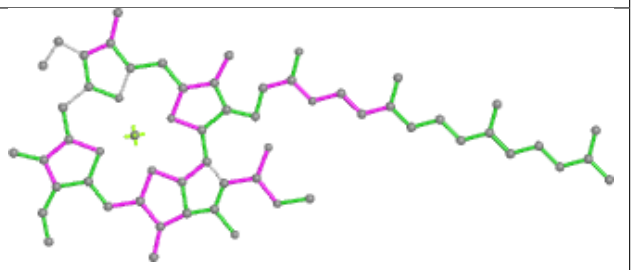

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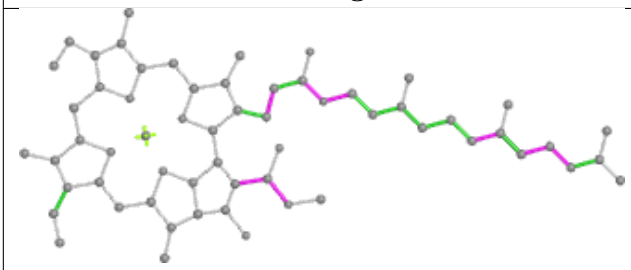

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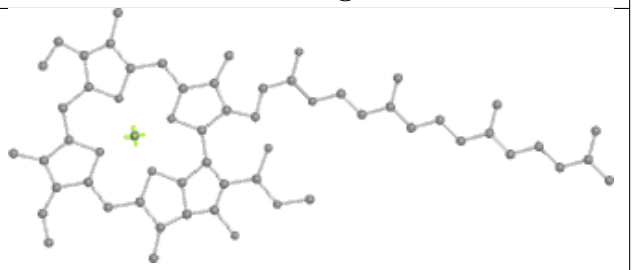

Rings

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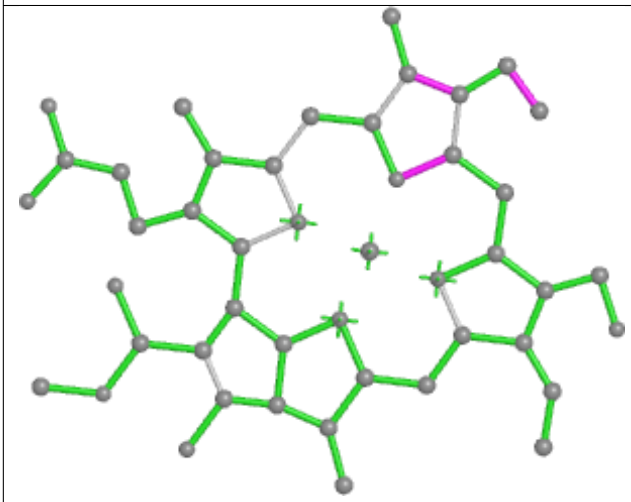

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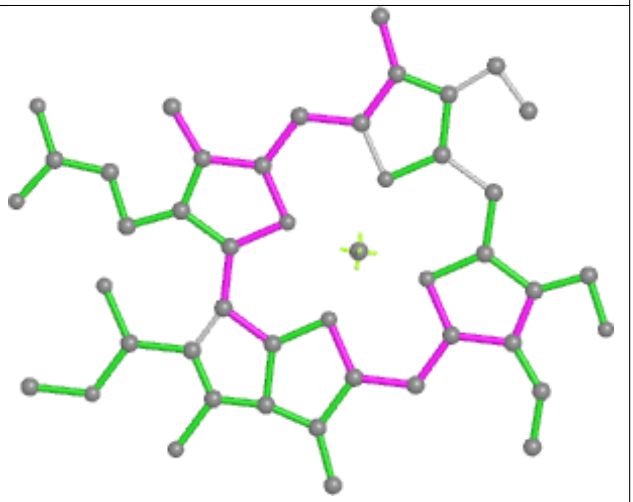
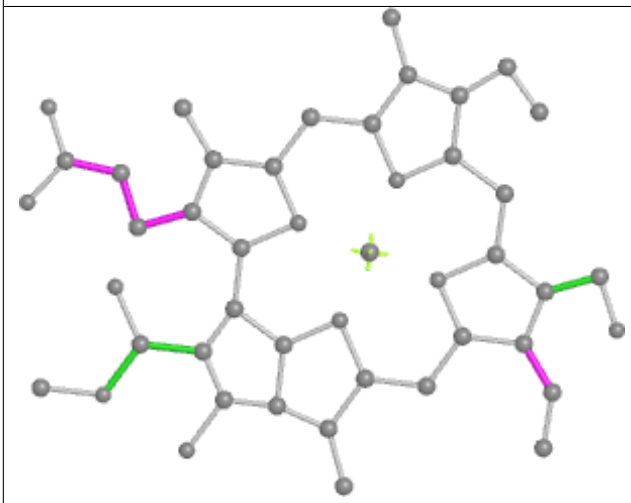


Bond angles



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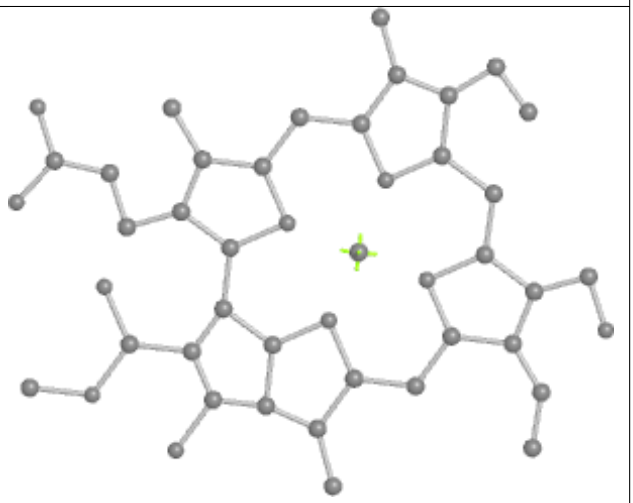

Rings

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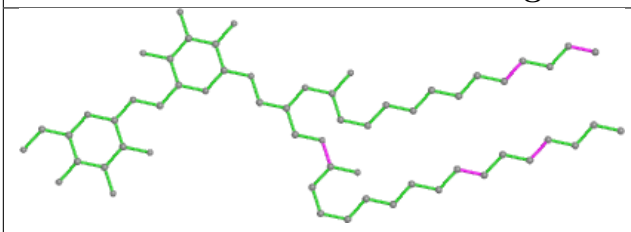

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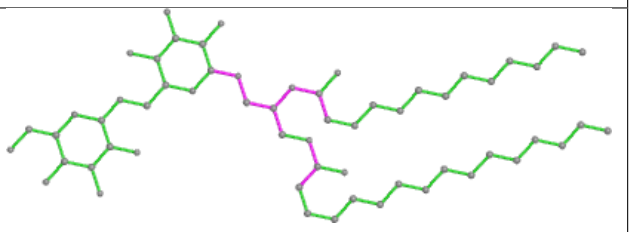
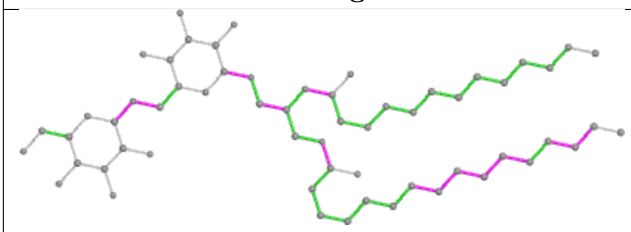


Bond angles



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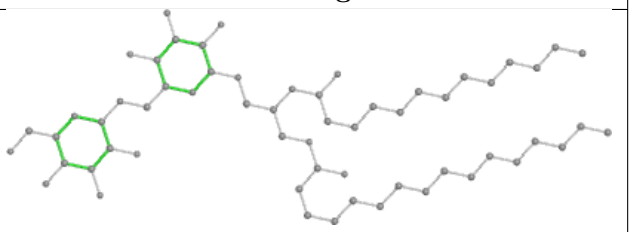
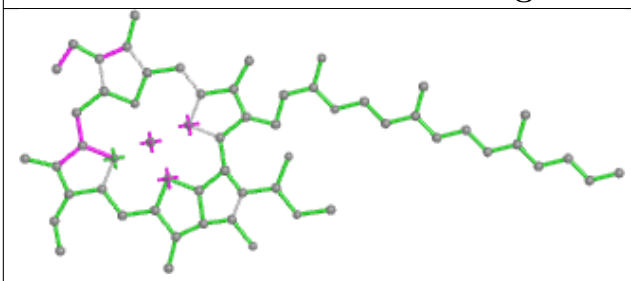


Rings

## Ligand CLA B 1222



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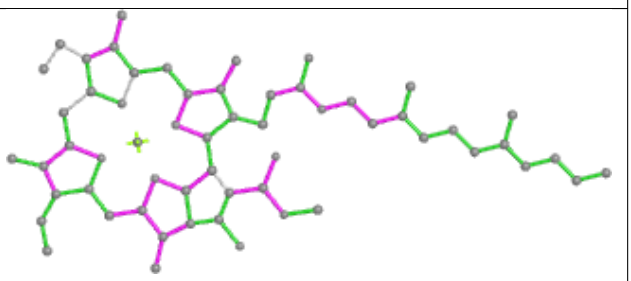
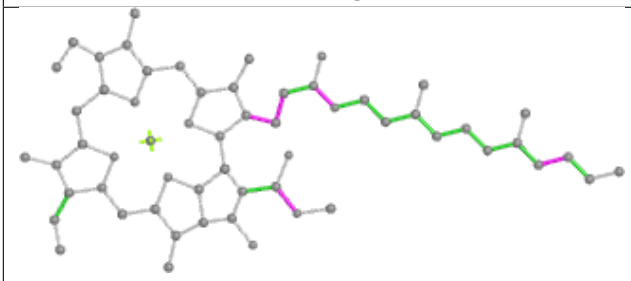


Bond angles



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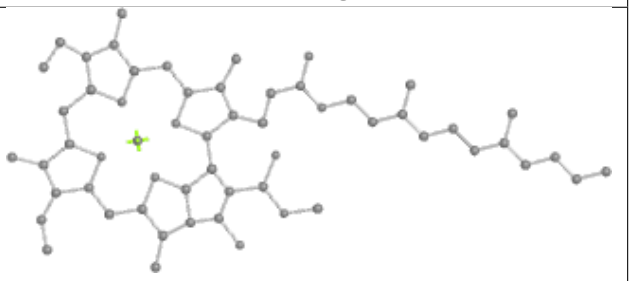
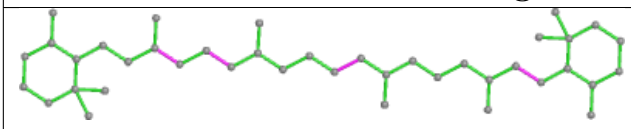
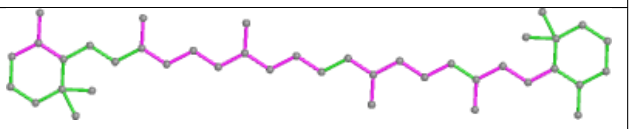


Rings

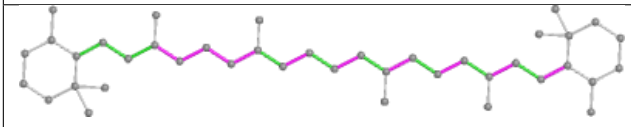
## Ligand BCR B 4006



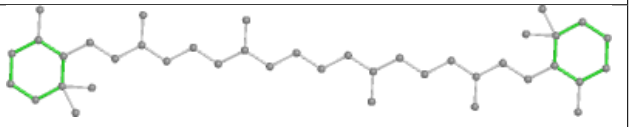
Bond lengths



Bond angles

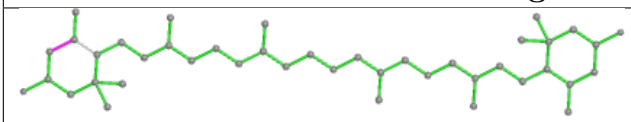


Torsions

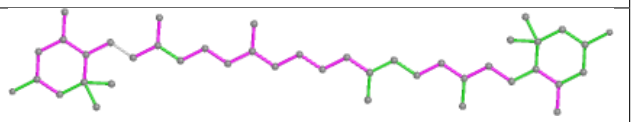


Rings

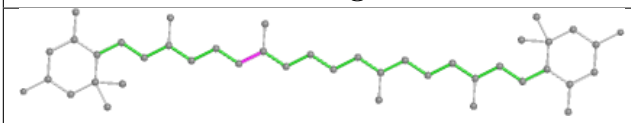
## Ligand LUT 2 502



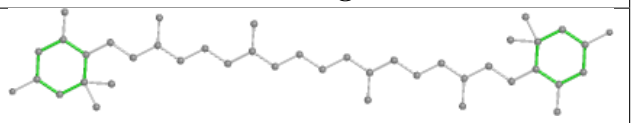
Bond lengths



Bond angles

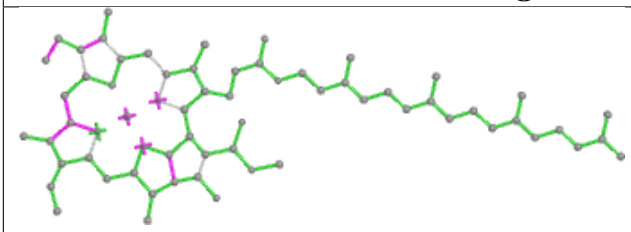


Torsions

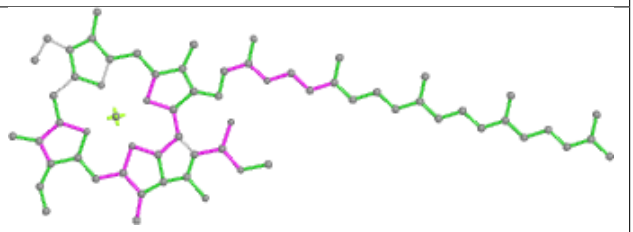


Rings

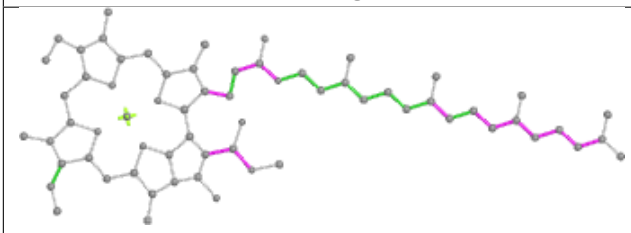
## Ligand CLA B 1021



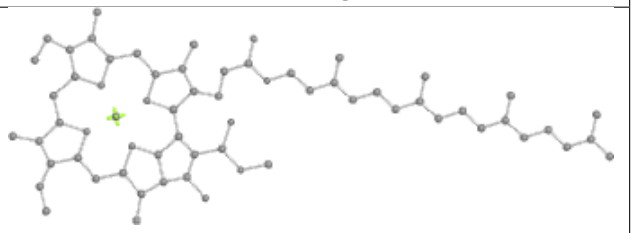
Bond lengths



Bond angles

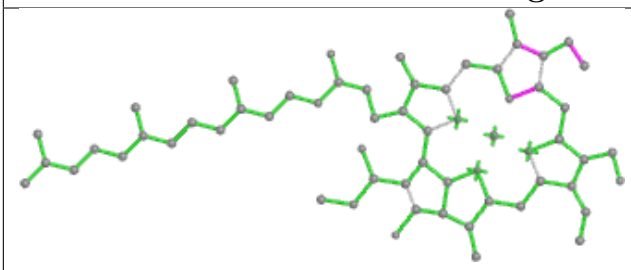


Torsions



Rings

## Ligand CHL 3 611



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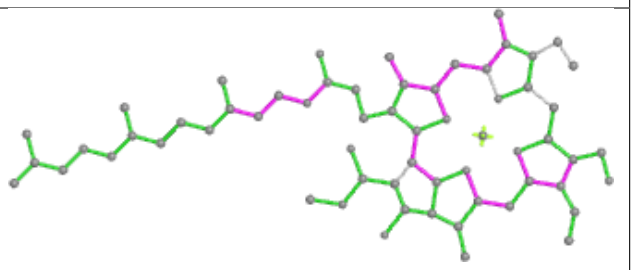
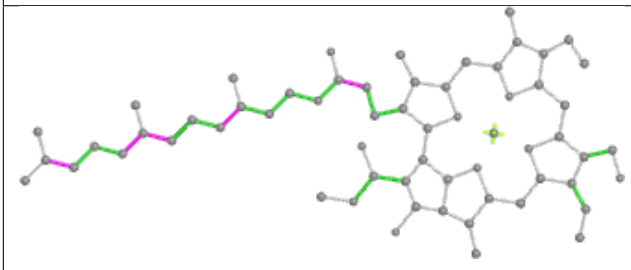
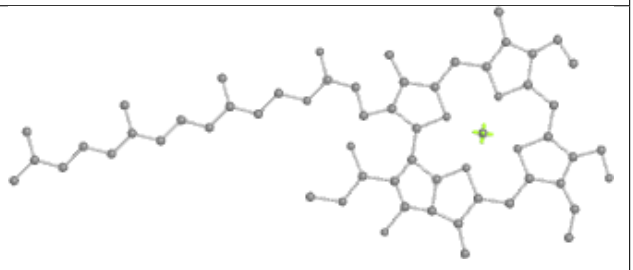


Bond angles

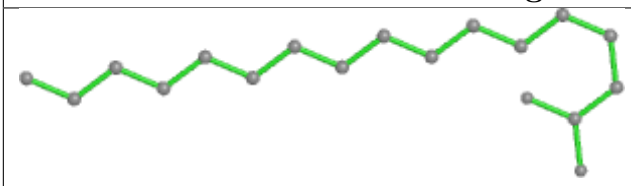


Torsions

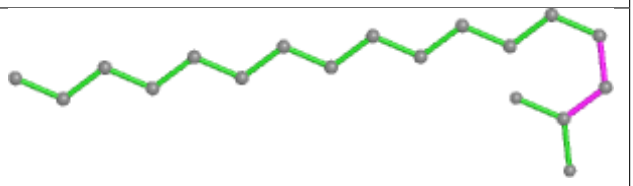


Rings

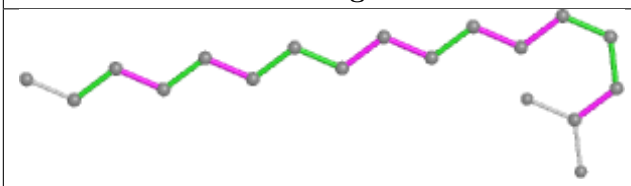
## Ligand PLM 6 804



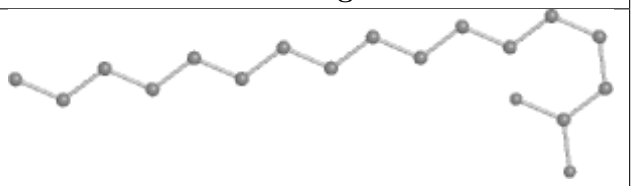
Bond lengths



Bond angles

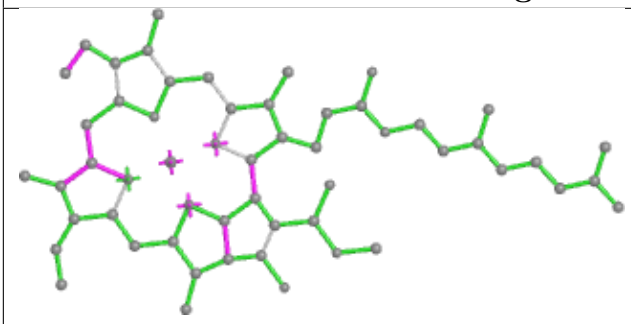


Torsions

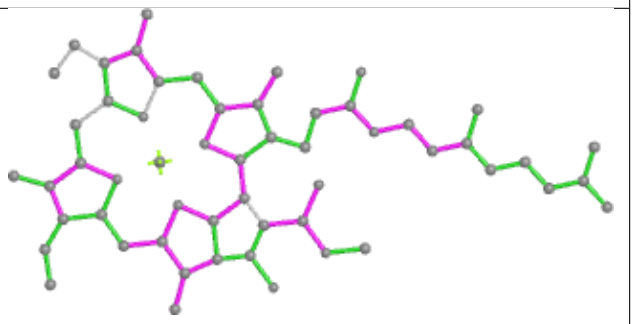


Rings

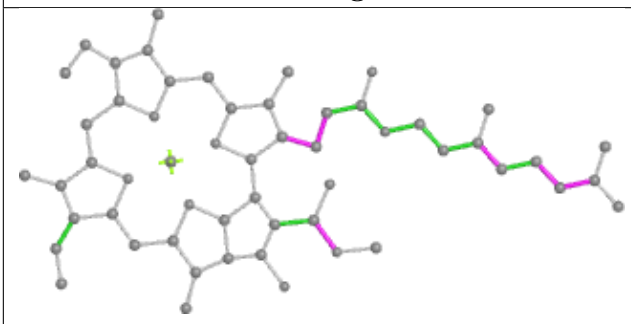
## Ligand CLA A 1107



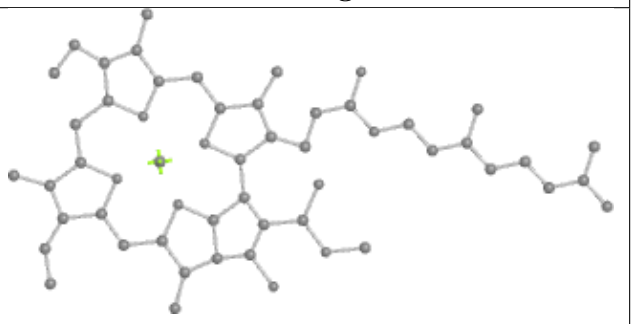
Bond lengths



Bond angles

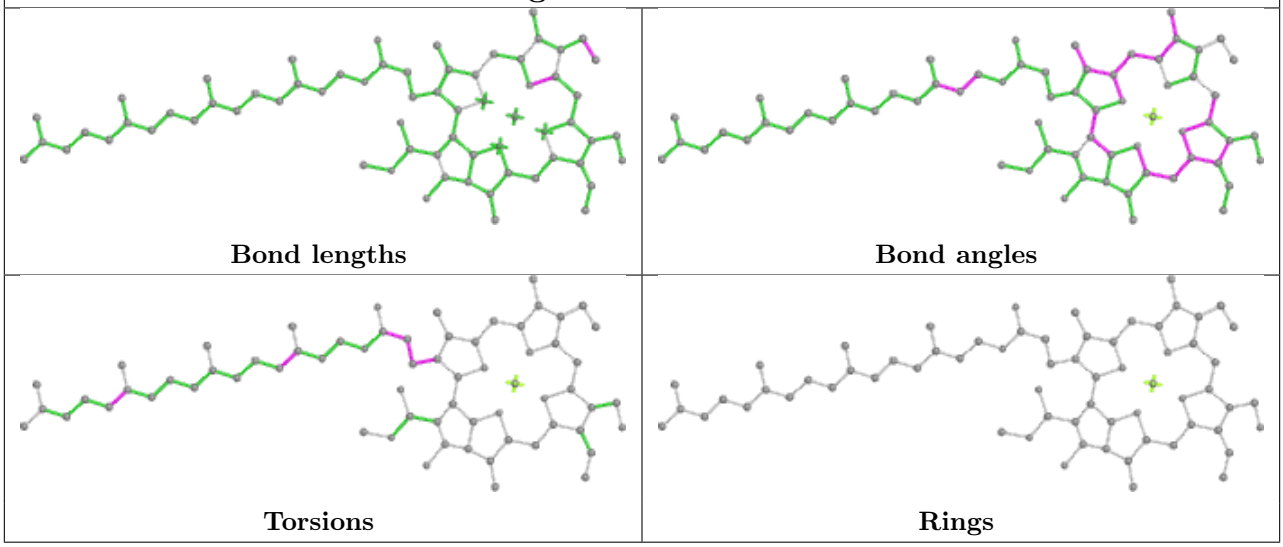


Torsions

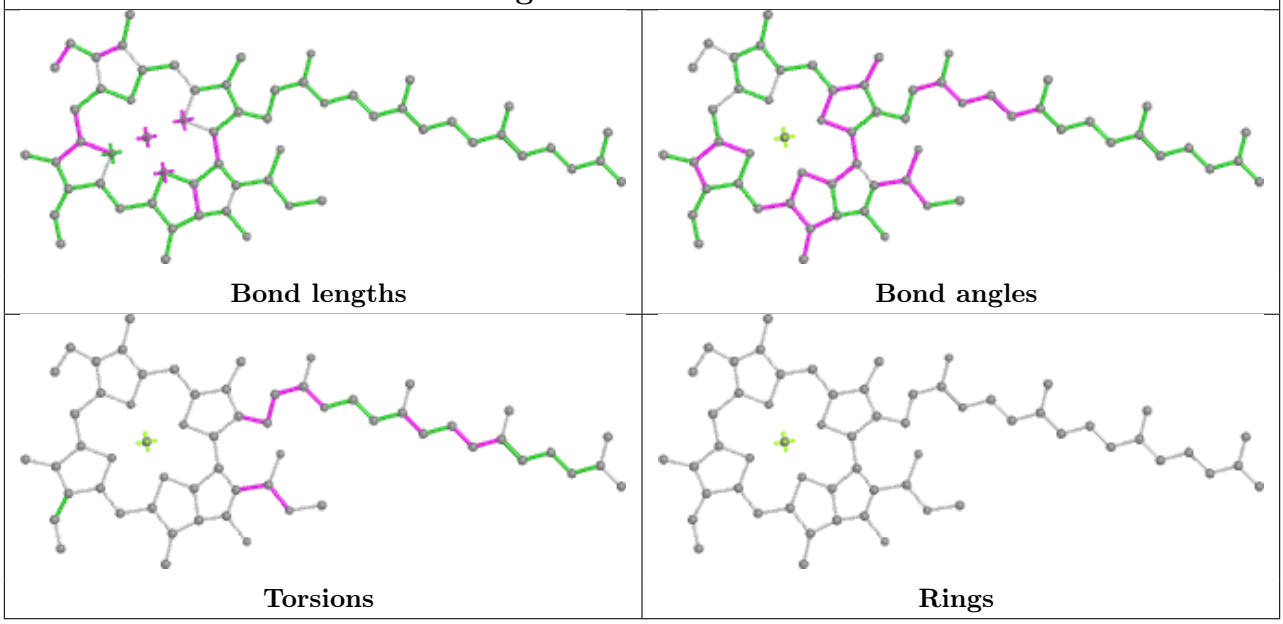


Rings

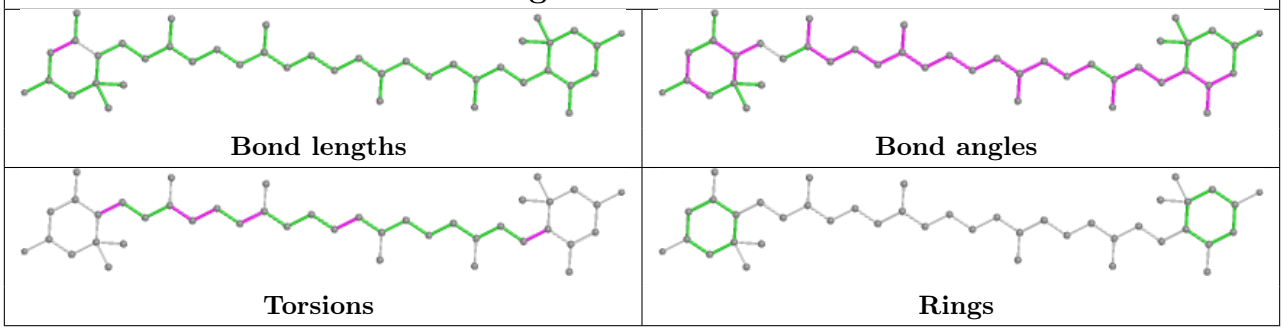
## Ligand CHL 9 601



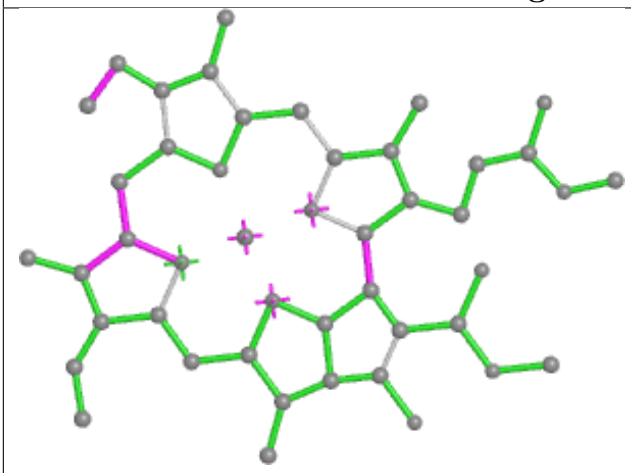

## Ligand CLA A 1134



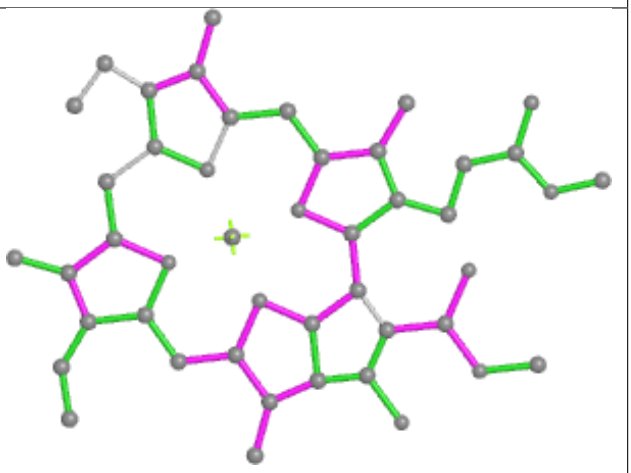

## Ligand LUT 1 503



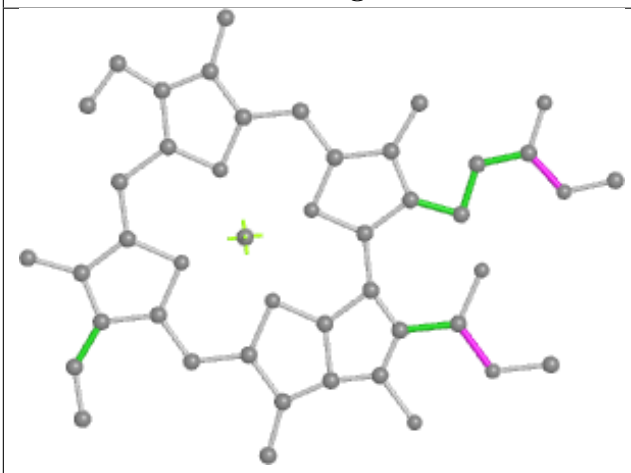
**Ligand CLA 9 602**



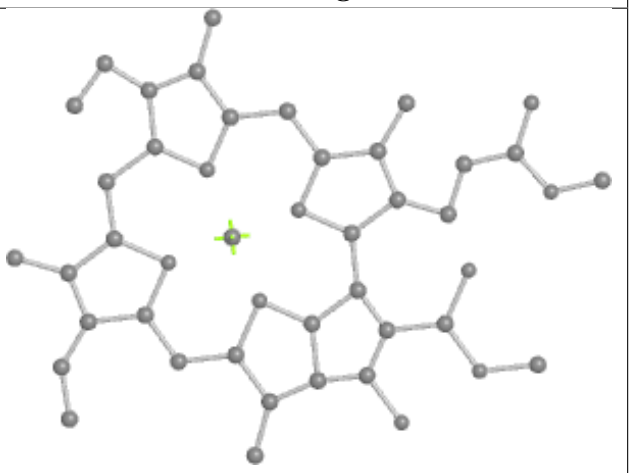
**Bond lengths**



**Bond angles**

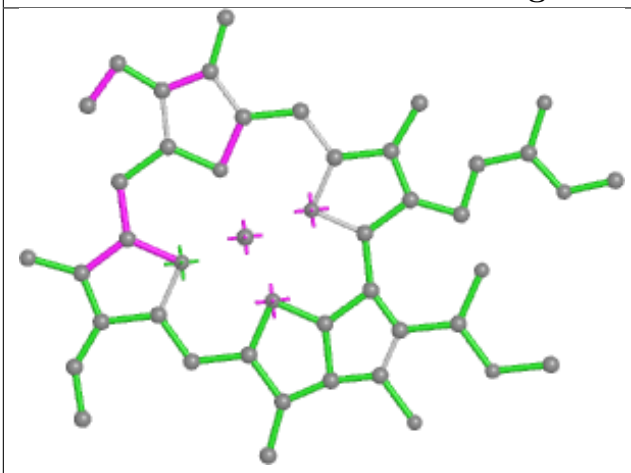


**Torsions**

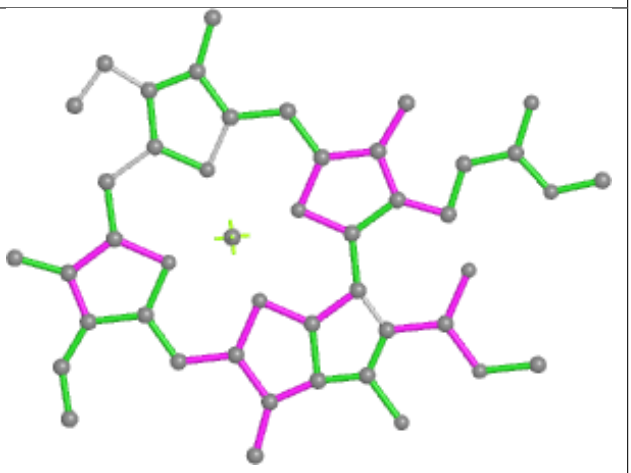


**Rings**

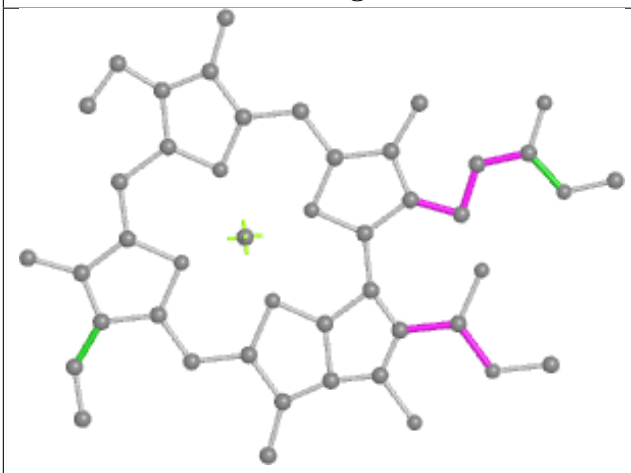
**Ligand CLA 6 618**



**Bond lengths**



**Bond angles**



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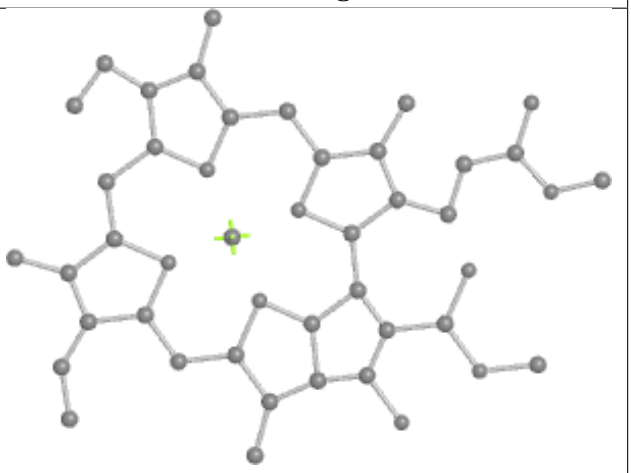

**Rings**

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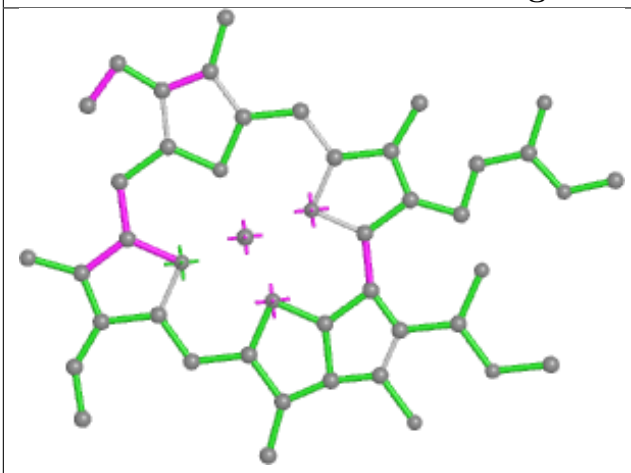

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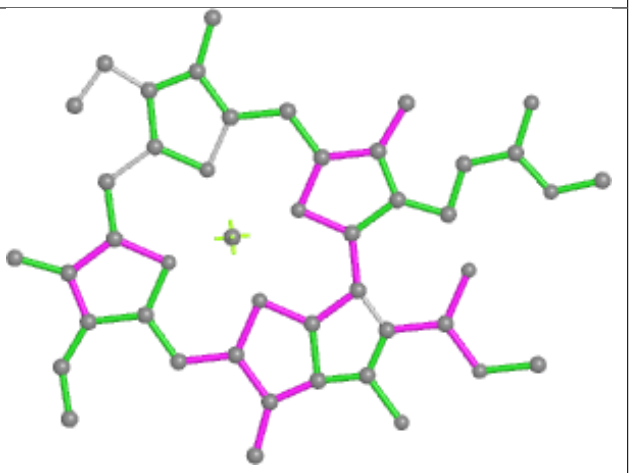
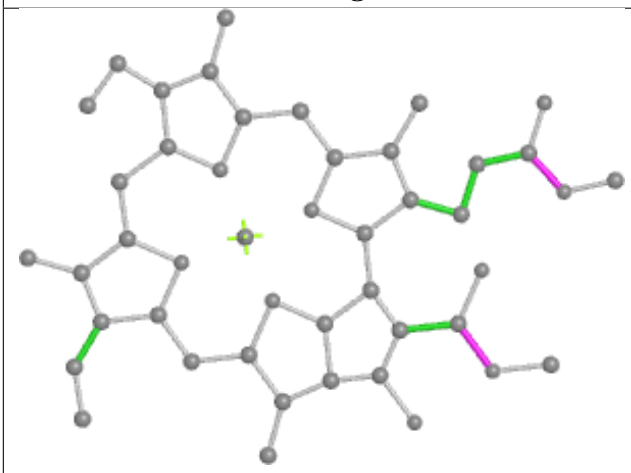
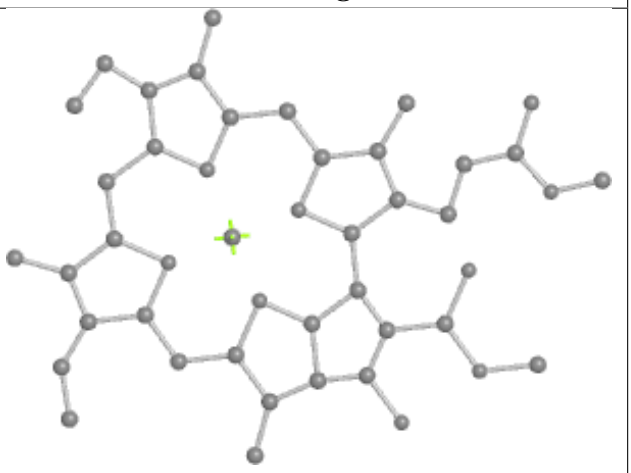


**Bond angles**

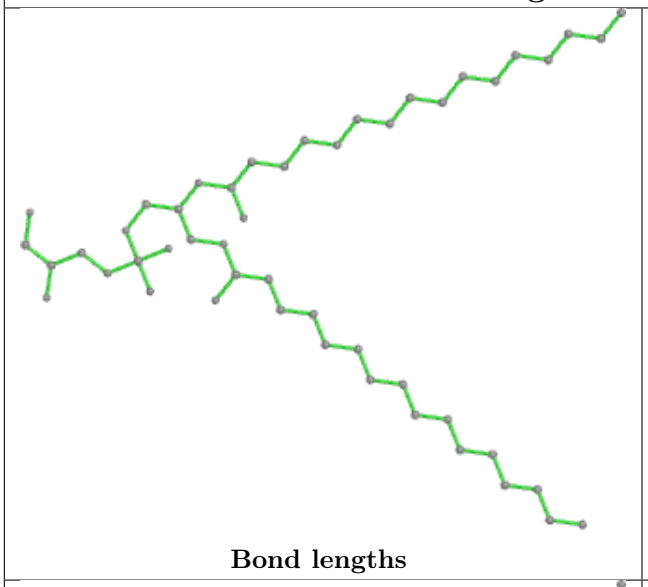


**Torsions**

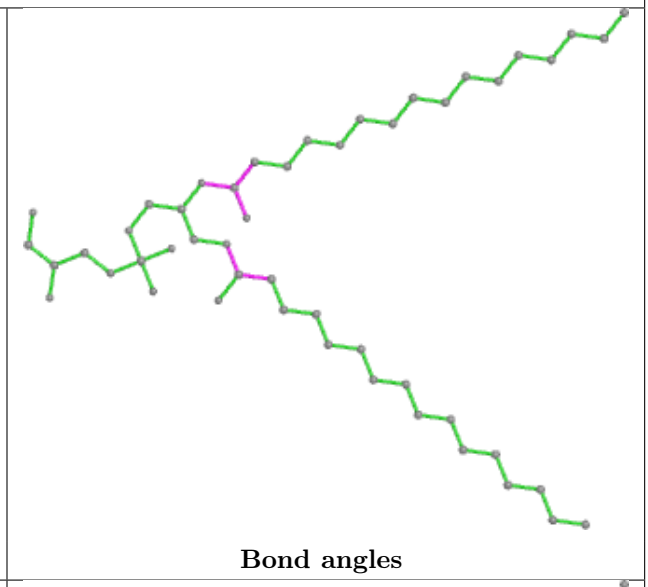


**Rings**

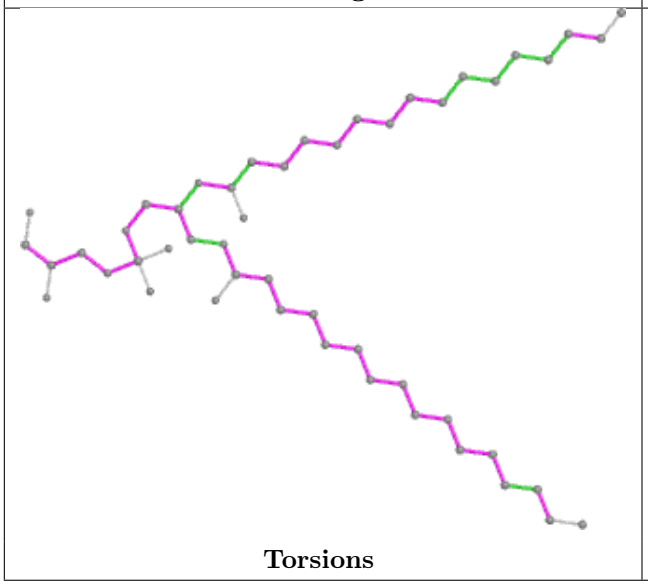
## Ligand LHG 2 802



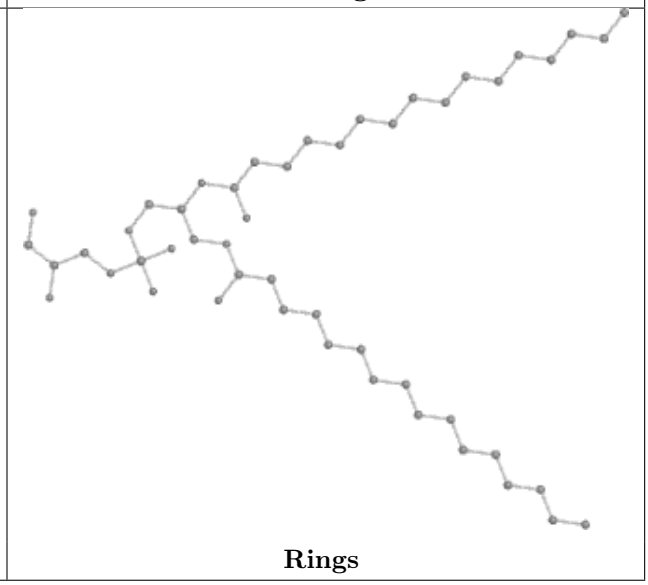
Bond lengths



Bond angles

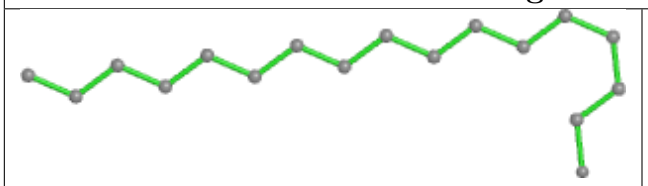


Torsions



Rings

## Ligand PLM 4 803



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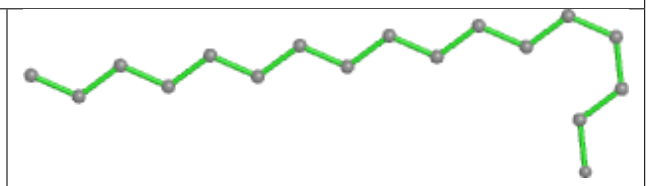
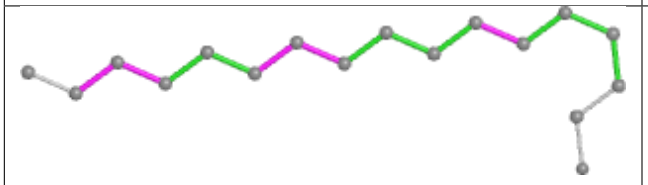
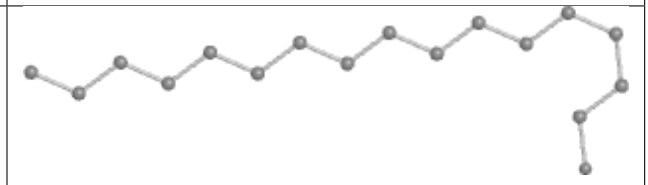


Bond angles

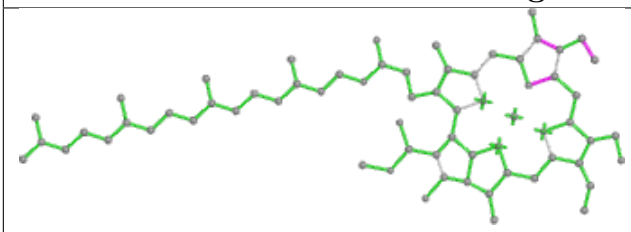


Torsions



Rings

## Ligand CHL 7 617



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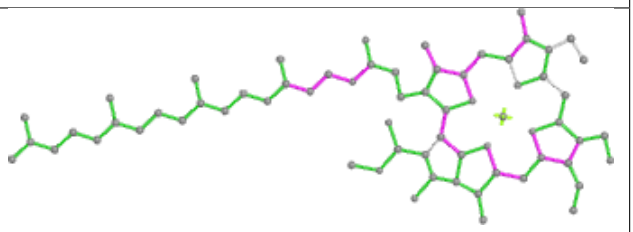
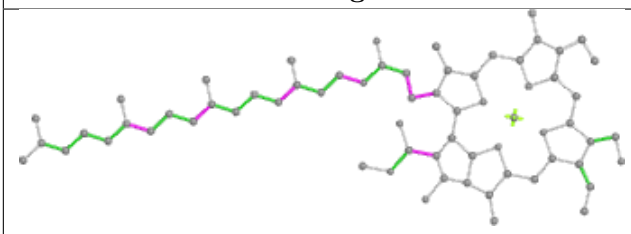
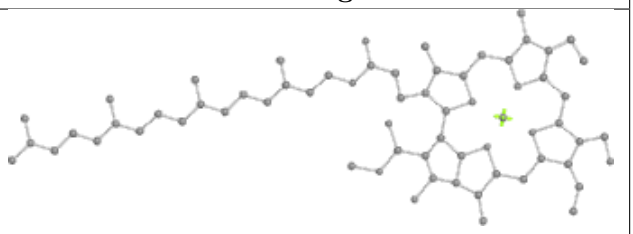


Bond angles

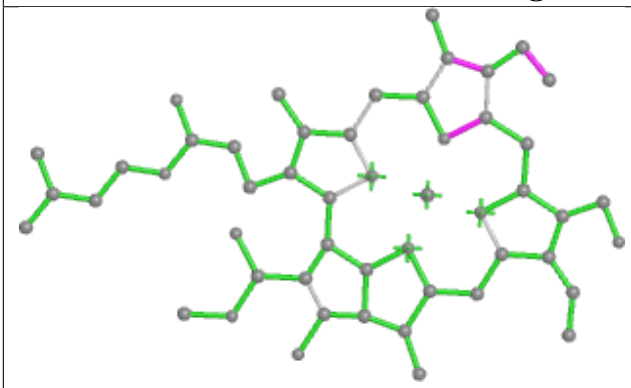


Torsions

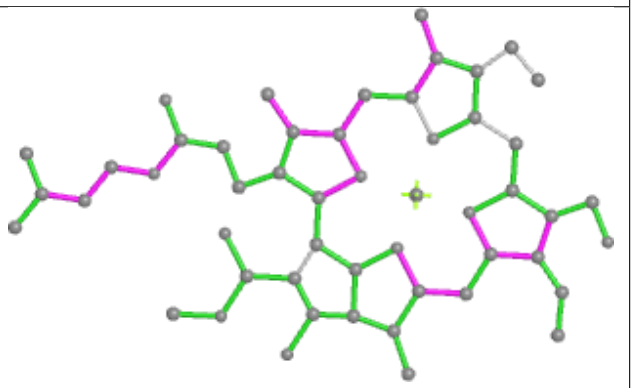


Rings

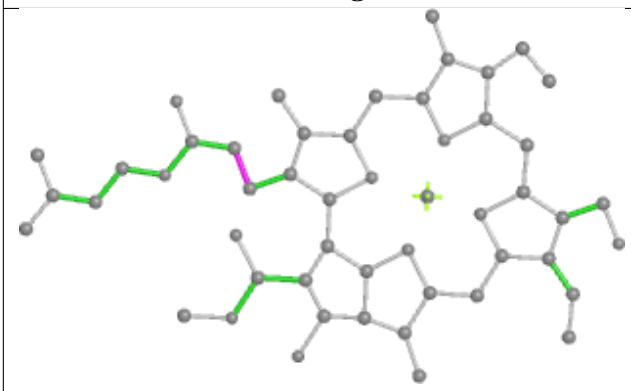
## Ligand CHL 2 613



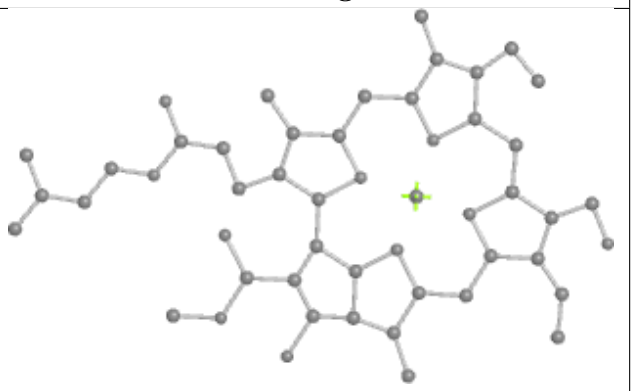
Bond lengths



Bond angles

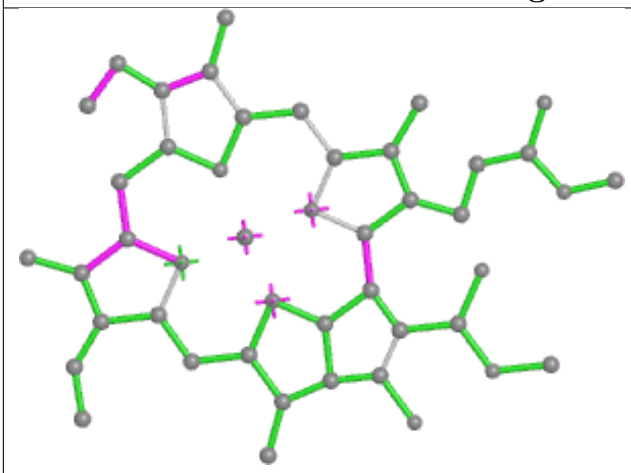


Torsions

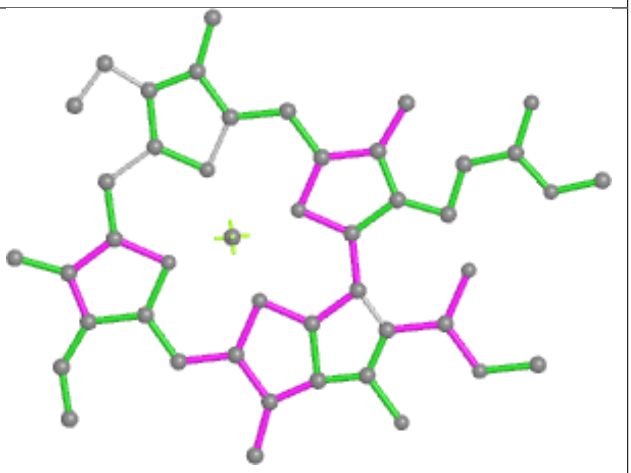


Rings

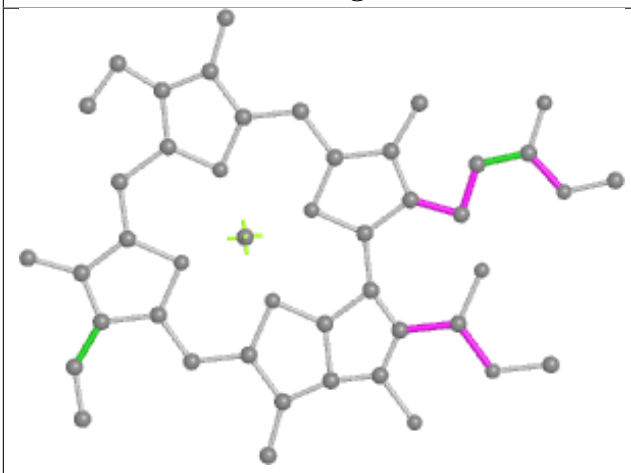
## Ligand CLA 5 615



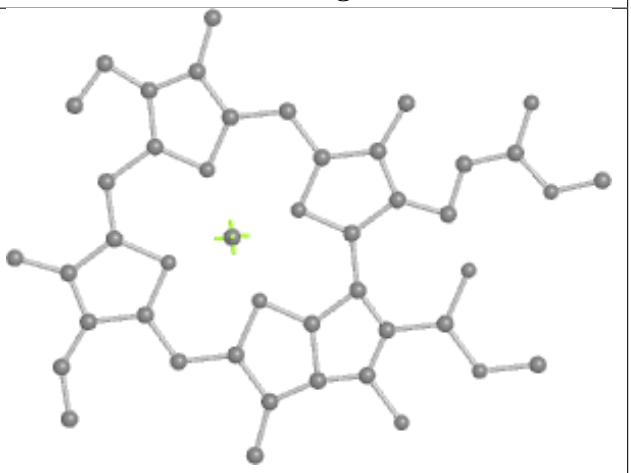
Bond lengths



Bond angles

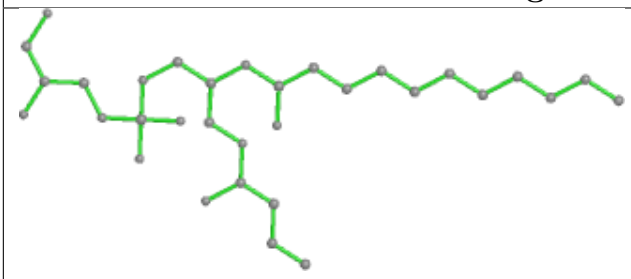


Torsions



Rings

## Ligand LHG 4 802



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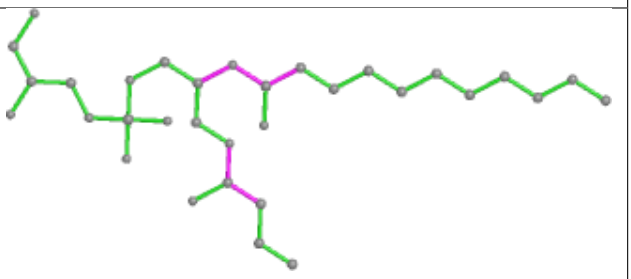
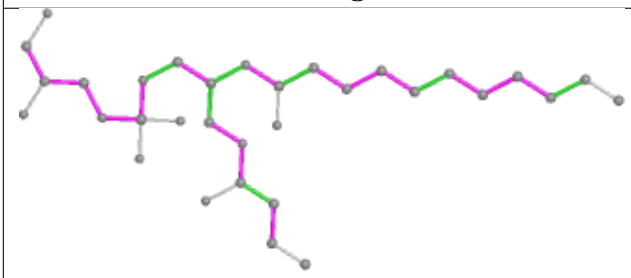
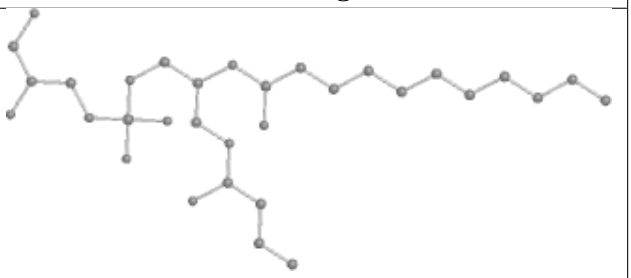


Bond angles

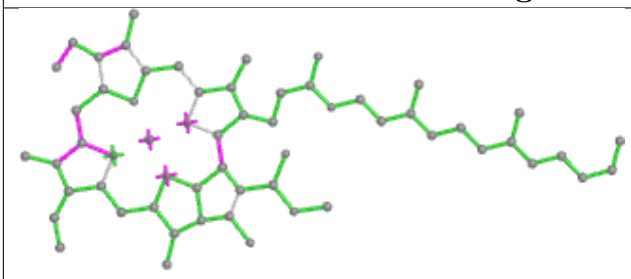


Torsions

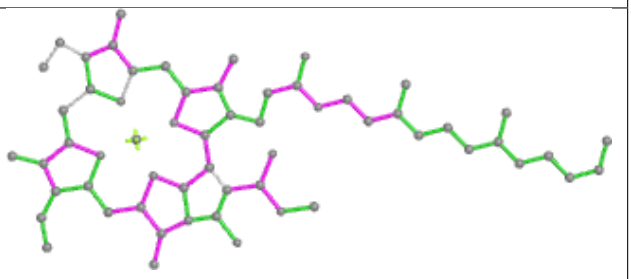


Rings

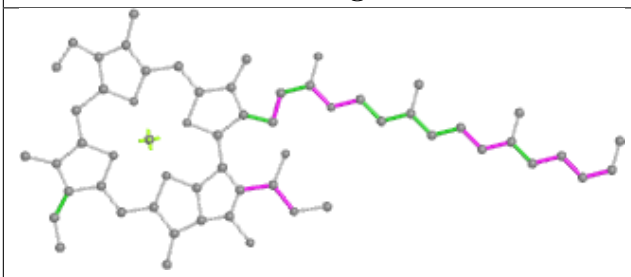
## Ligand CLA B 1219



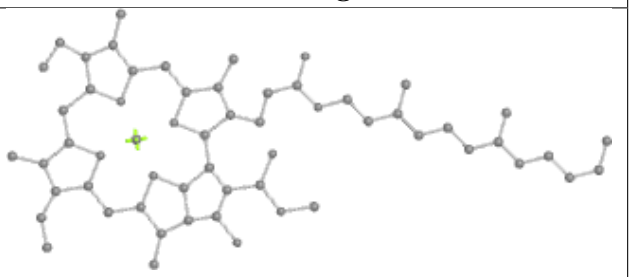
Bond lengths



Bond angles

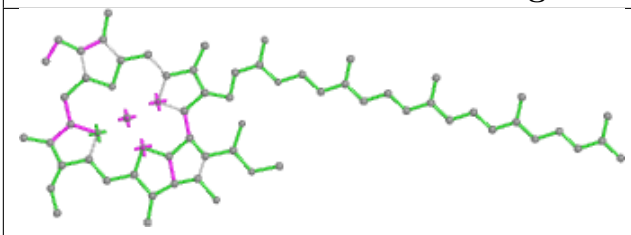


Torsions

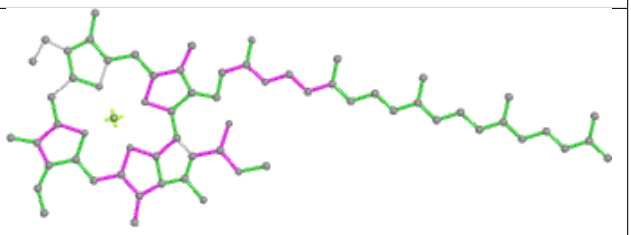


Rings

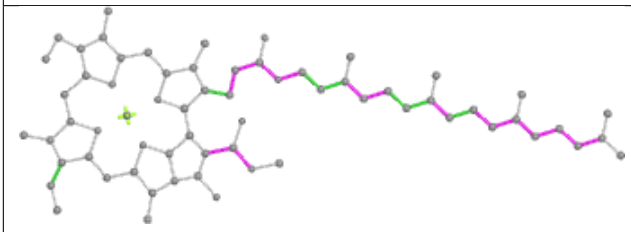
## Ligand CLA 7 603



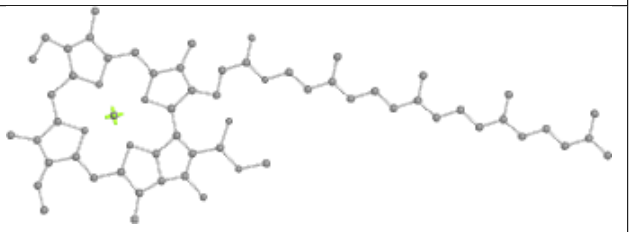
Bond lengths



Bond angles

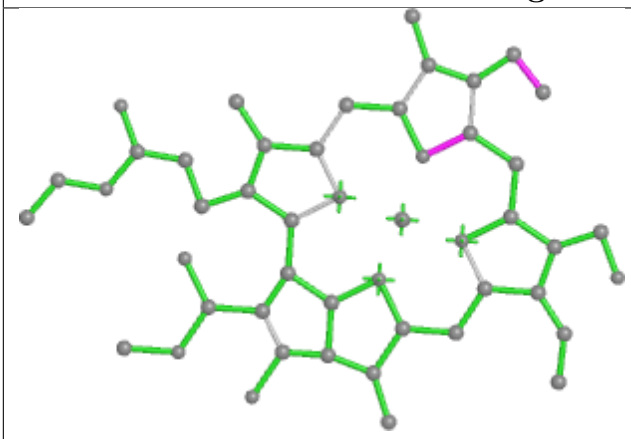


Torsions

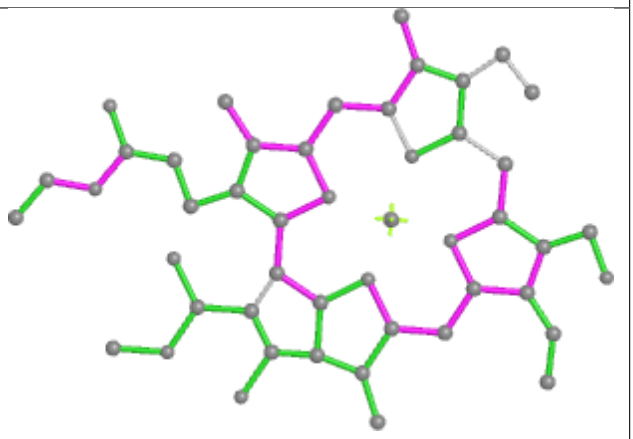


Rings

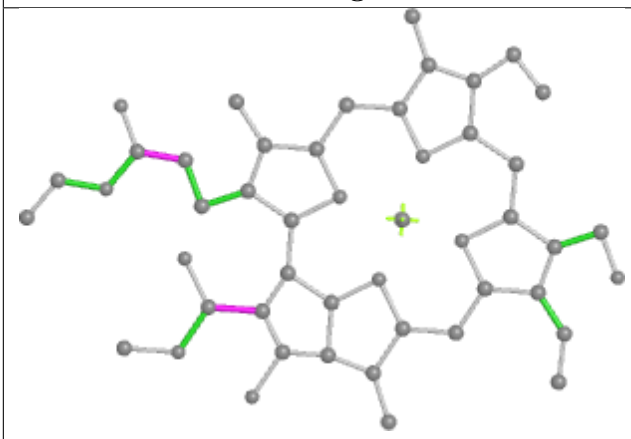
## Ligand CHL 1 610



Bond lengths



Bond angles



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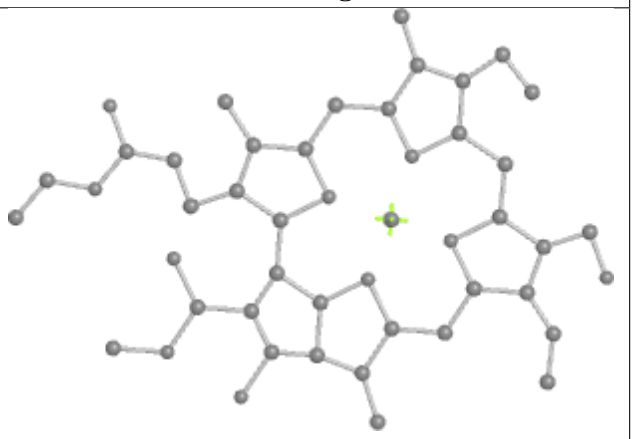
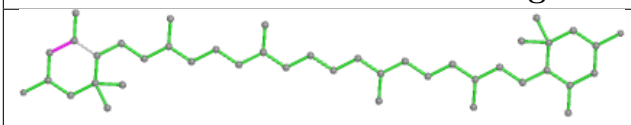
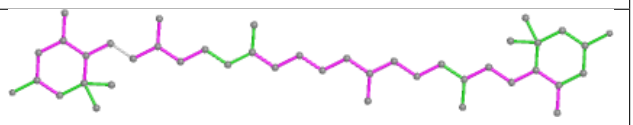


Rings

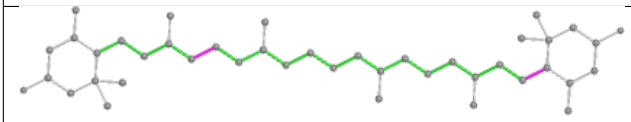
## Ligand LUT 6 501



Bond lengths



Bond angles



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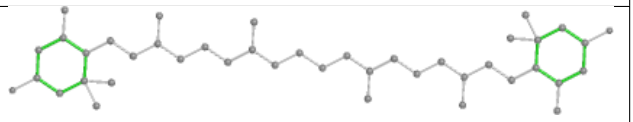
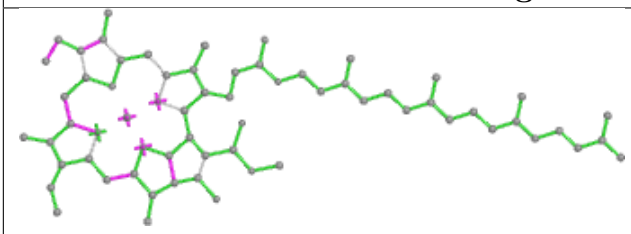
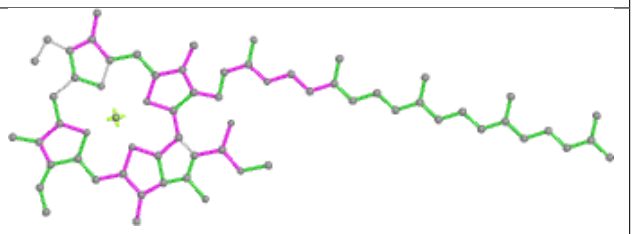


Rings

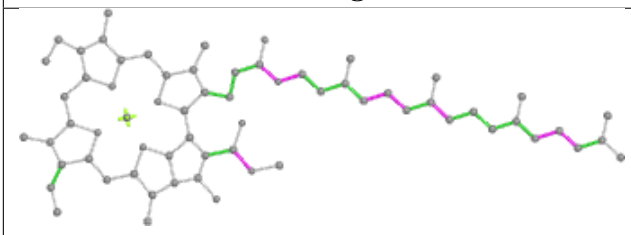
## Ligand CLA B 1226



Bond lengths



Bond angles



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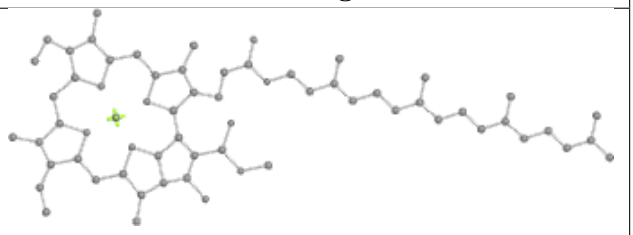
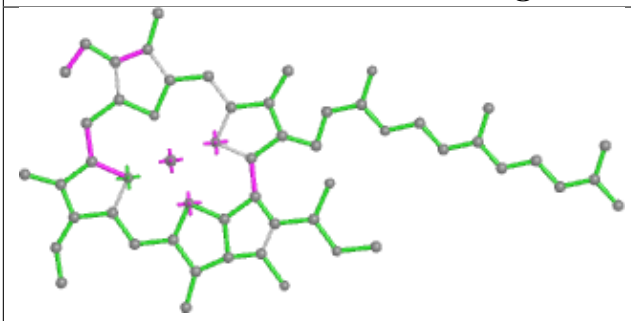
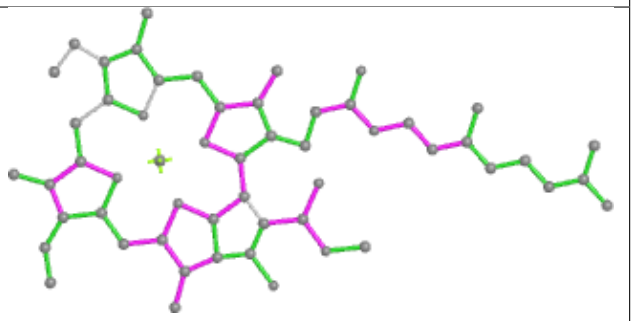


Rings

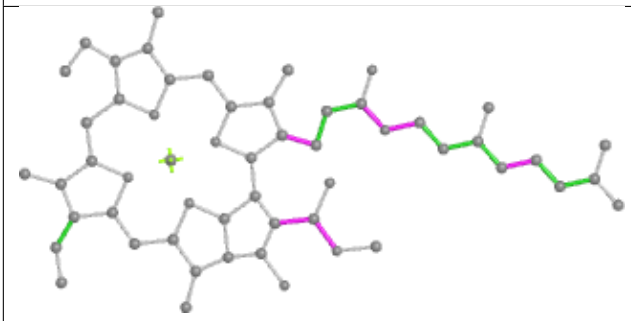
## Ligand CLA H 1701



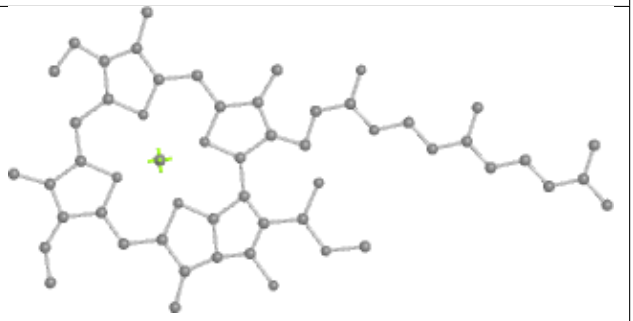
Bond lengths



Bond angles

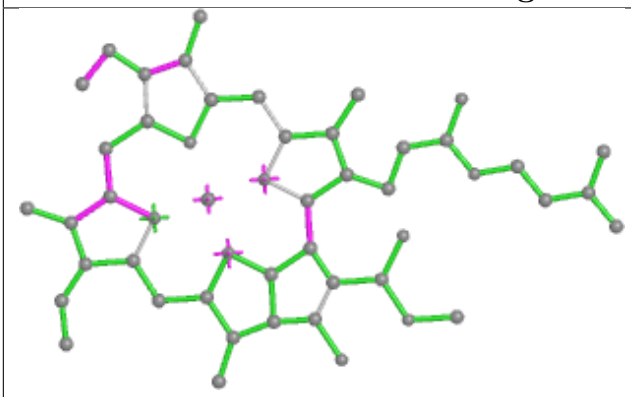


Torsions

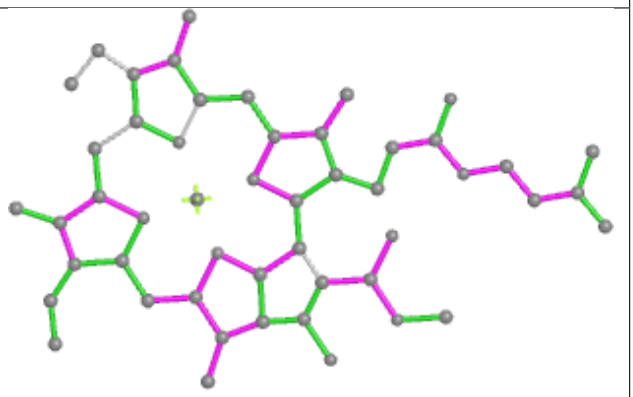


Rings

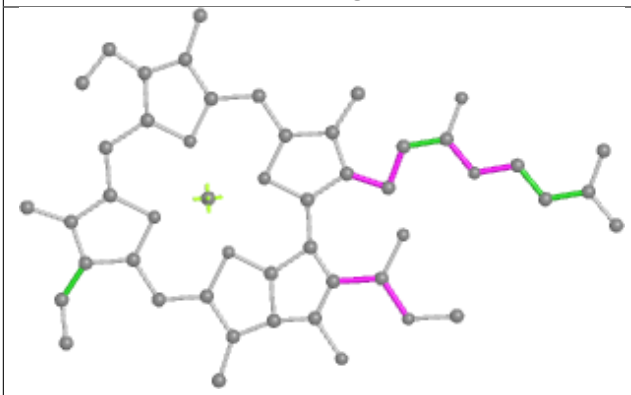
## Ligand CLA L 1501



Bond lengths



Bond angles



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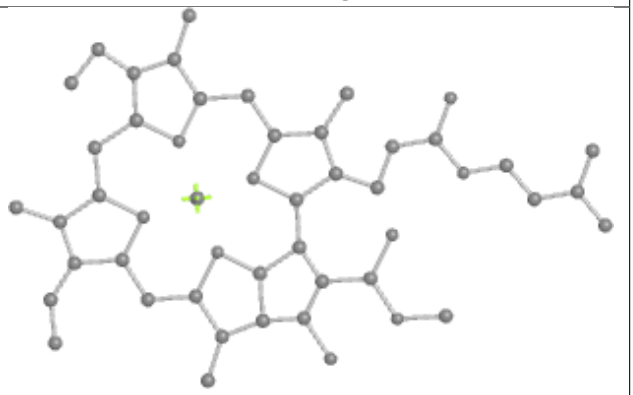
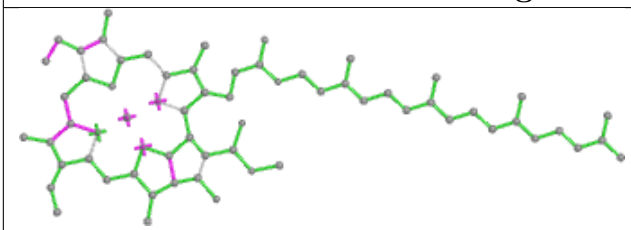
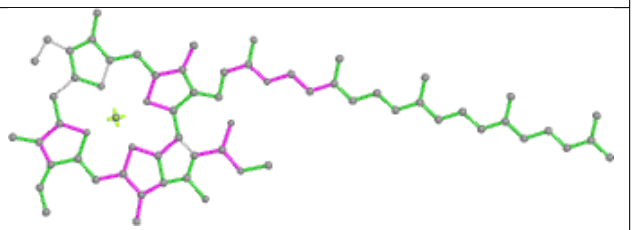


Rings

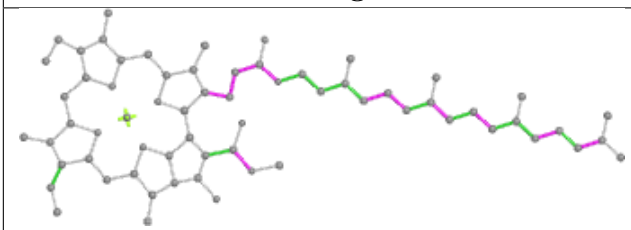
## Ligand CLA B 1209



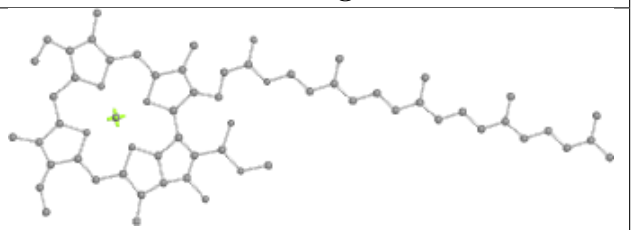
Bond lengths



Bond angles

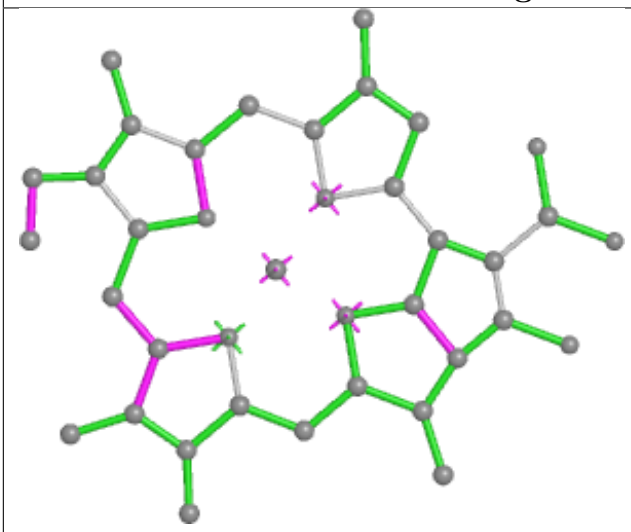


Torsions

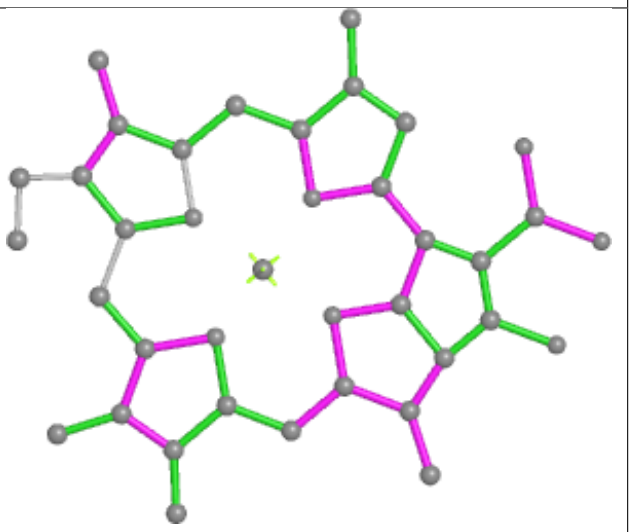


Rings

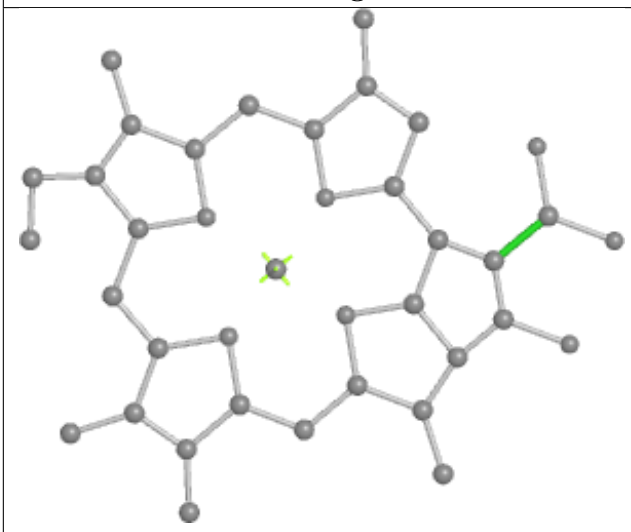
**Ligand CLA O 1801**



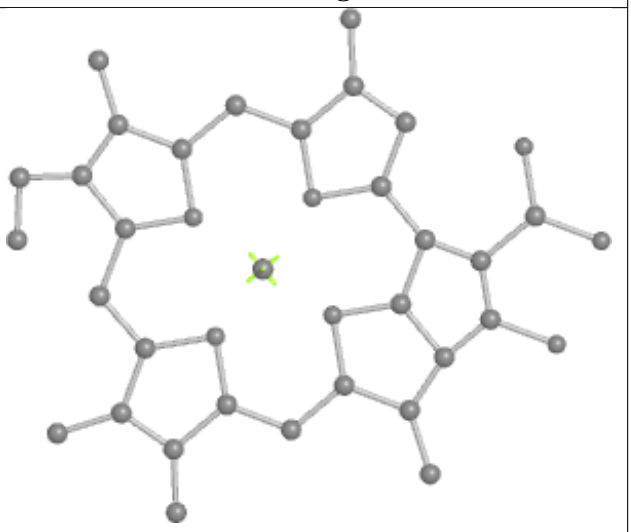
**Bond lengths**



**Bond angles**

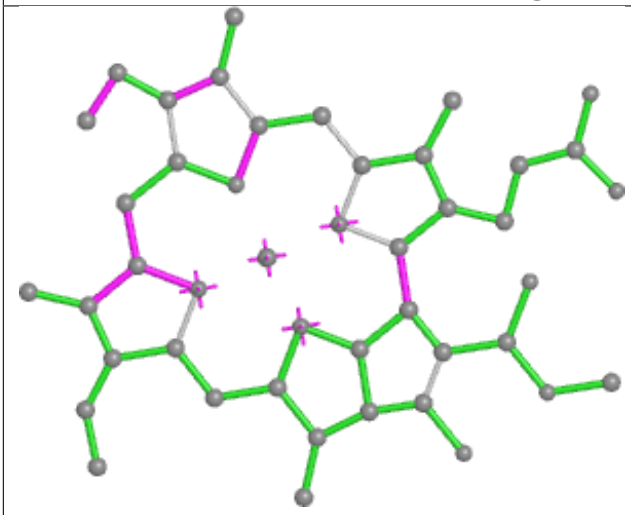


**Torsions**

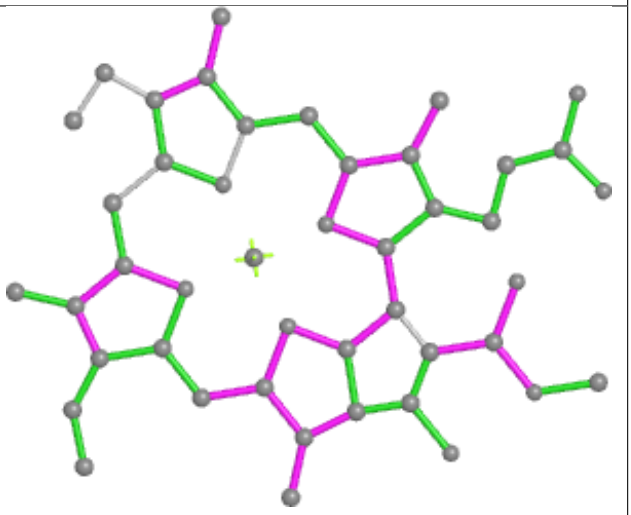


**Rings**

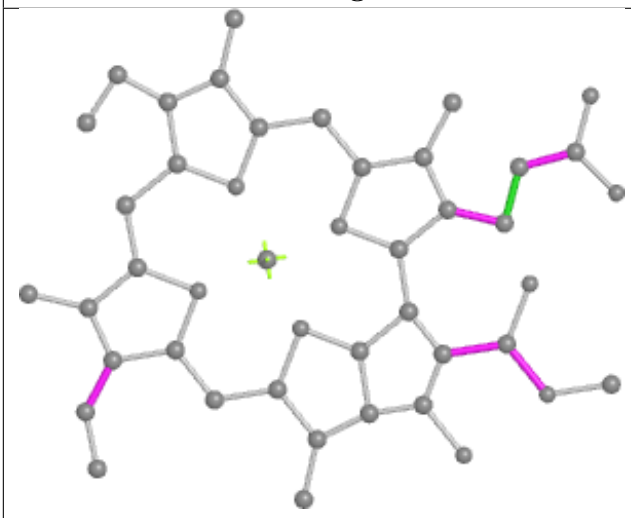
## Ligand CLA 8 620



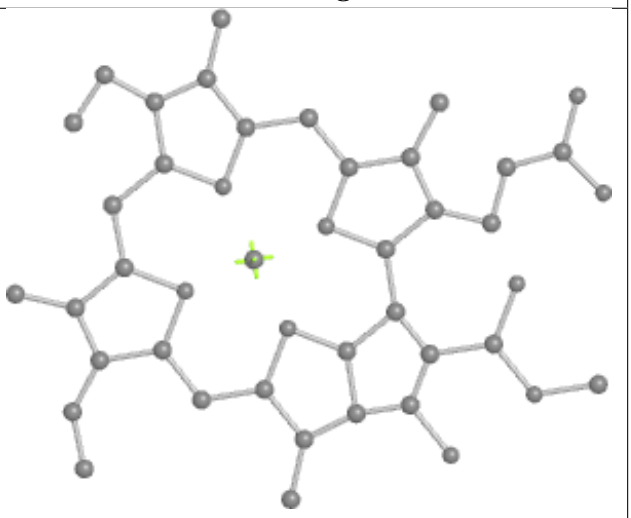
Bond lengths



Bond angles

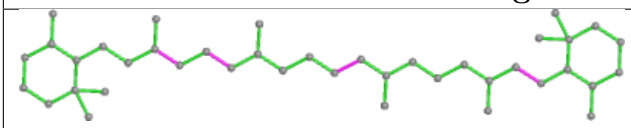


Torsions

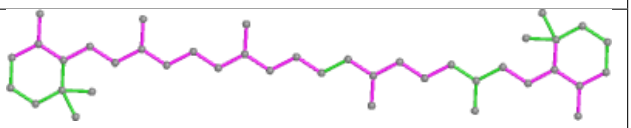


Rings

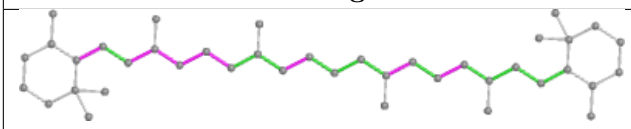
## Ligand BCR A 4004



Bond lengths



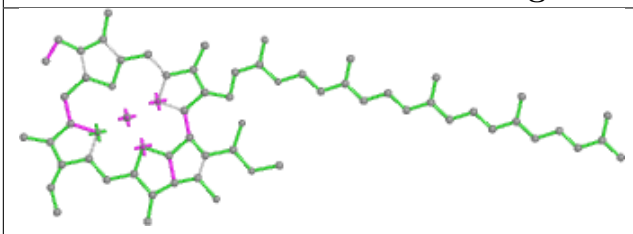
Bond angles



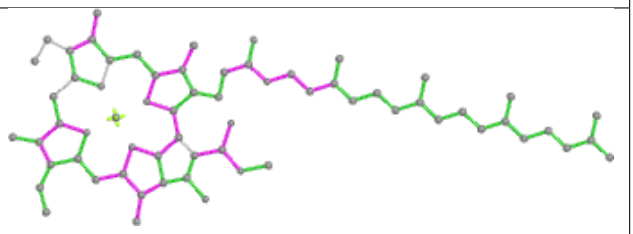
Torsions

Rings

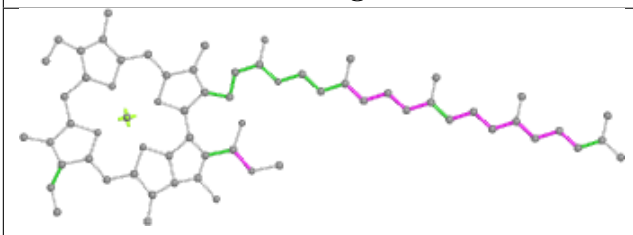
## Ligand CLA 3 605



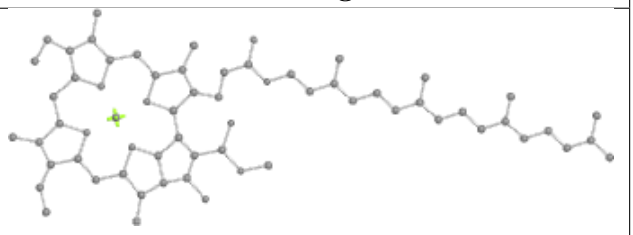
Bond lengths



Bond angles

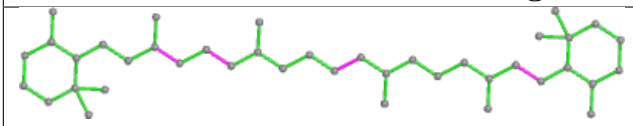


Torsions

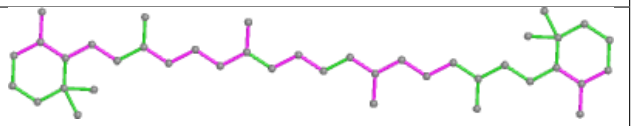


Rings

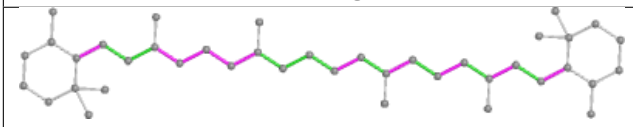
## Ligand BCR 6 503



Bond lengths



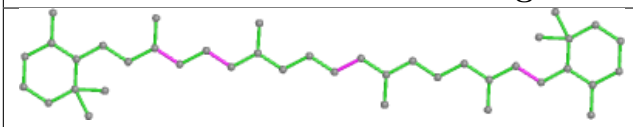
Bond angles



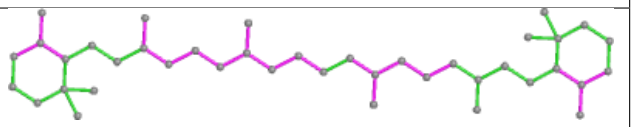
Torsions

Rings

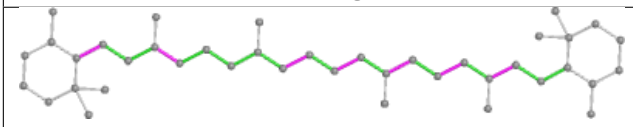
## Ligand BCR L 4002



Bond lengths



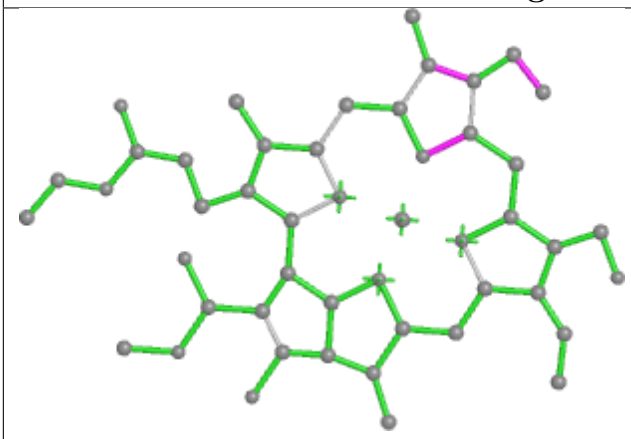
Bond angles



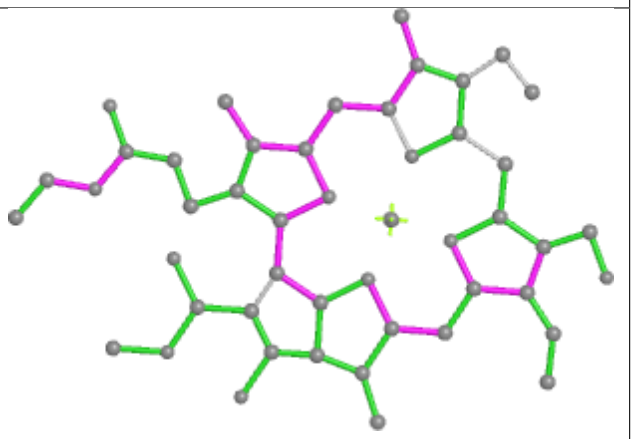
Torsions

Rings

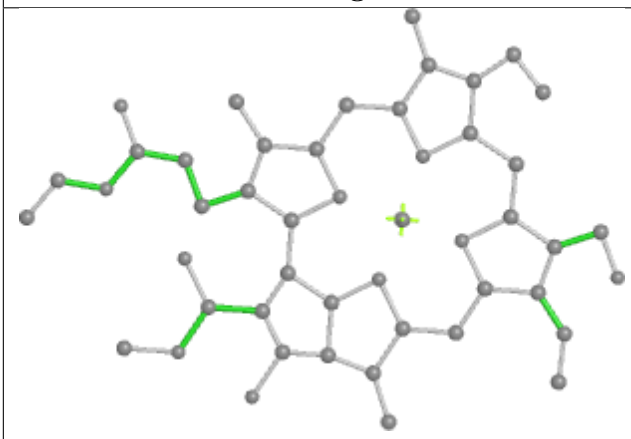
## Ligand CHL 2 610



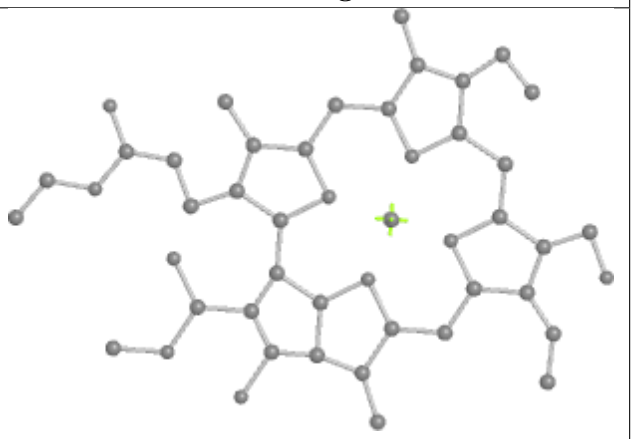
Bond lengths



Bond angles

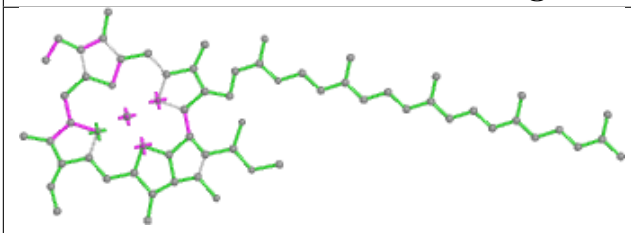


Torsions



Rings

## Ligand CLA 6 606



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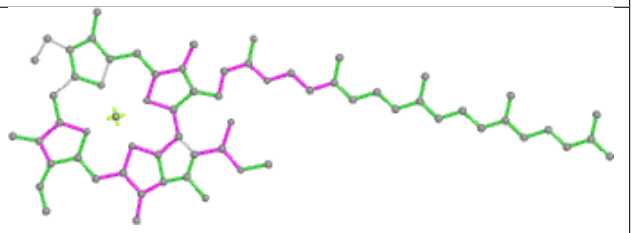
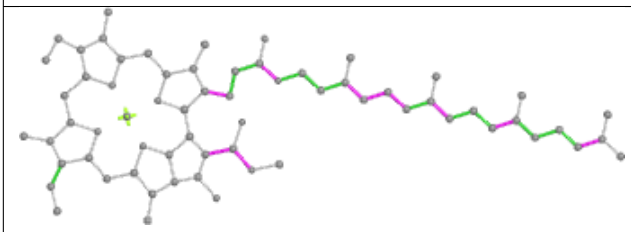


Bond angles



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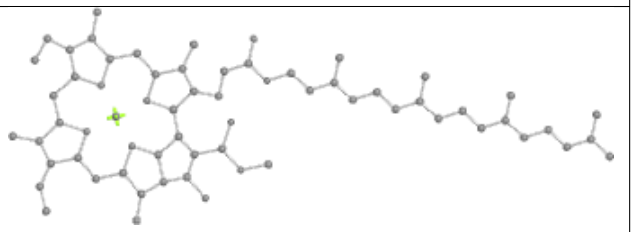
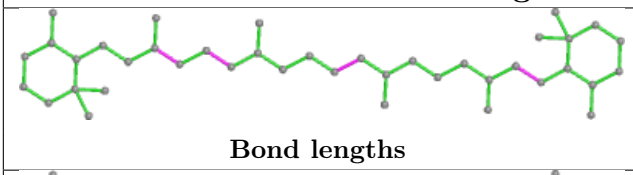


Rings

## Ligand BCR A 4003



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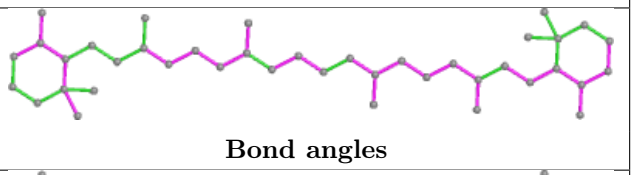
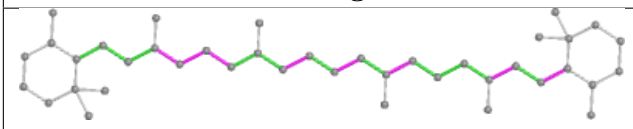
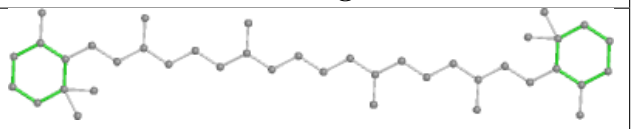


Bond angles

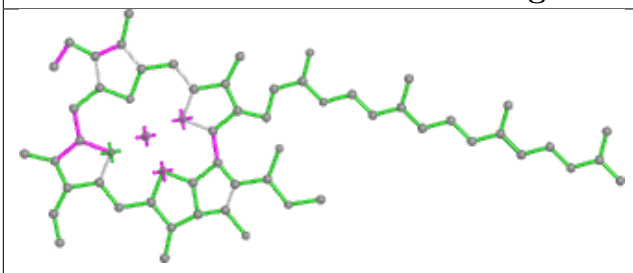


Torsions

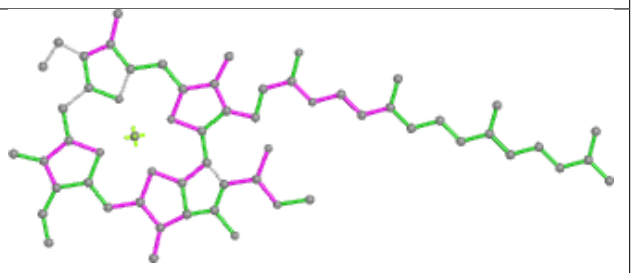


Rings

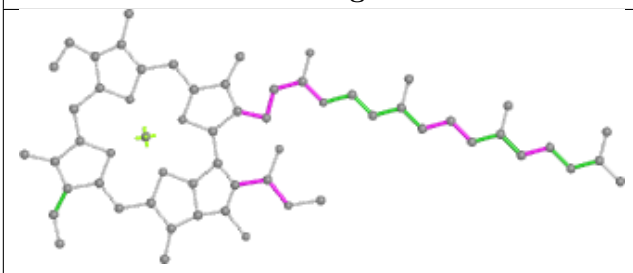
## Ligand CLA 6 601



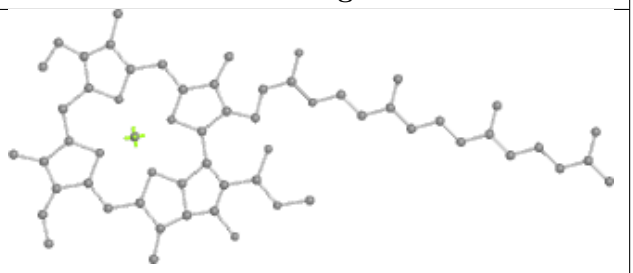
Bond lengths



Bond angles

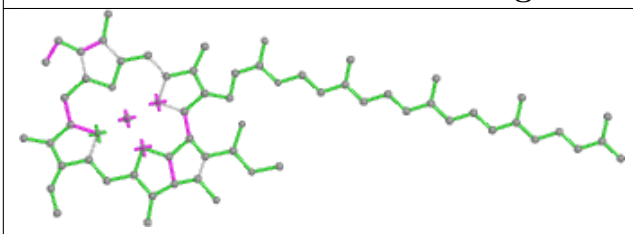


Torsions



Rings

## Ligand CLA A 1132



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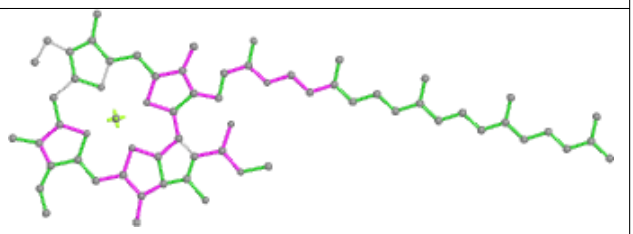
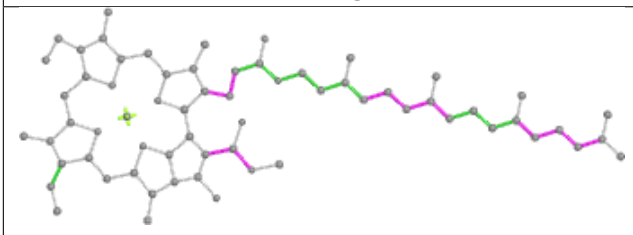


Bond angles



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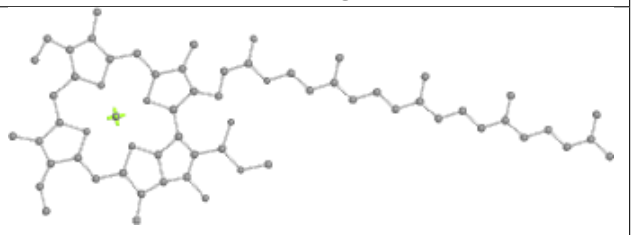
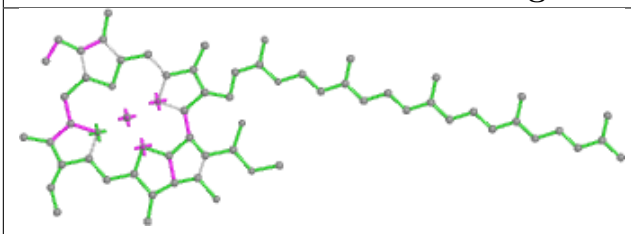


Rings

## Ligand CLA 1 605



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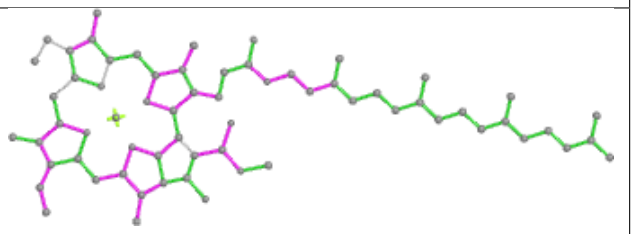
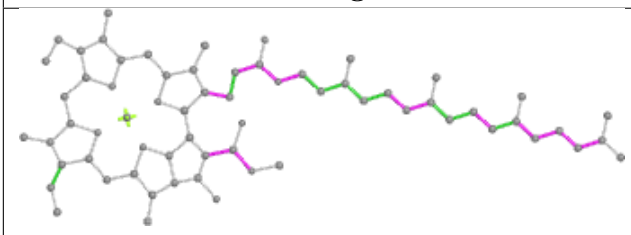


Bond angles



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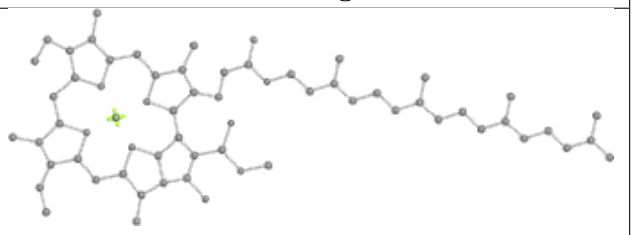
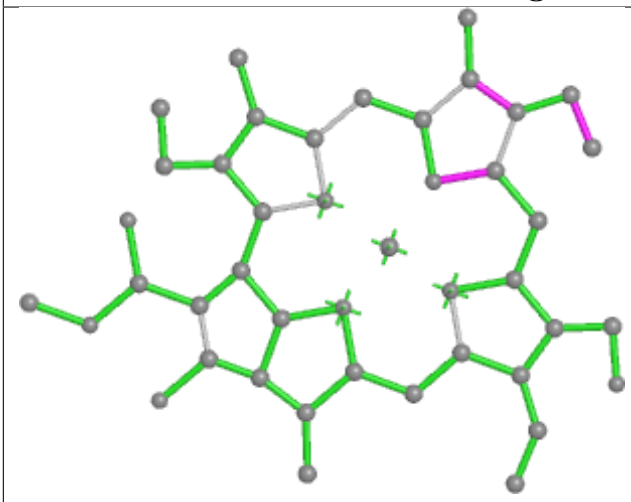


Rings

## Ligand CHL 6 617



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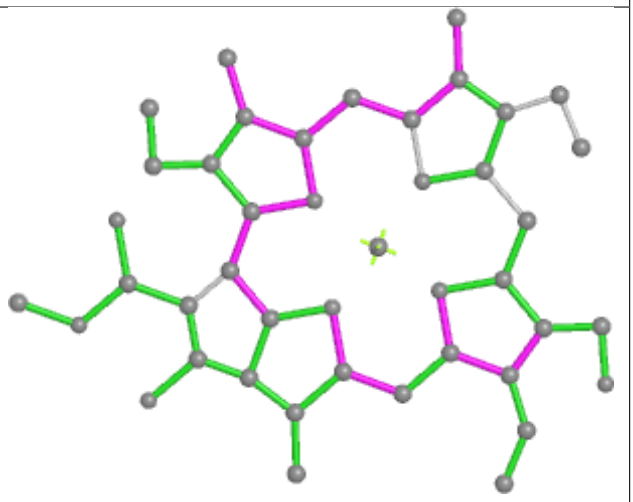
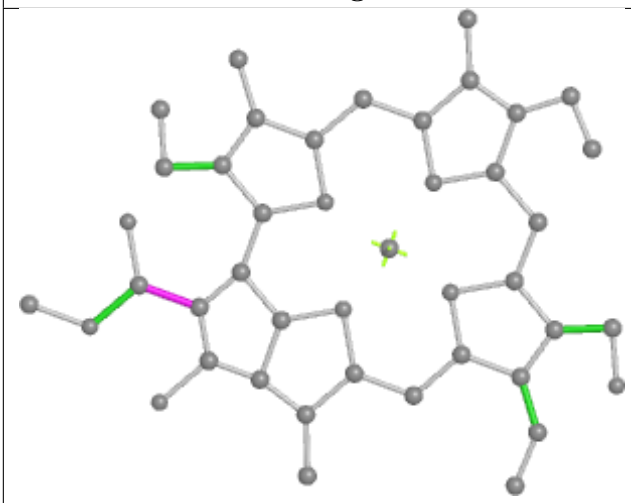


Bond angles



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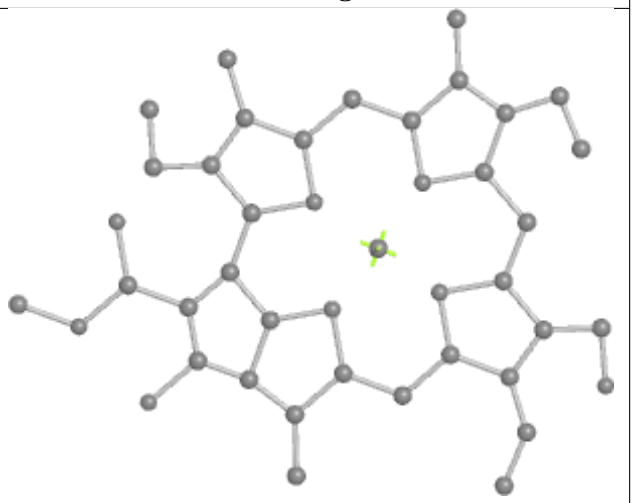
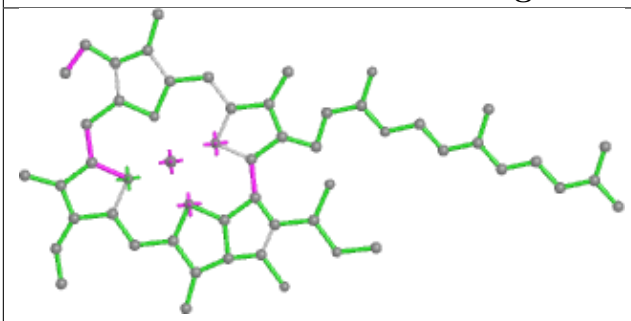


Rings

## Ligand CLA A 1102



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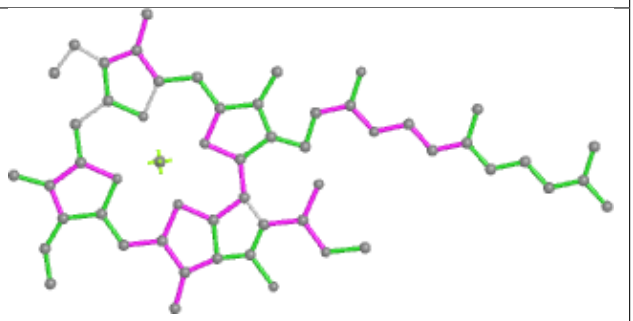
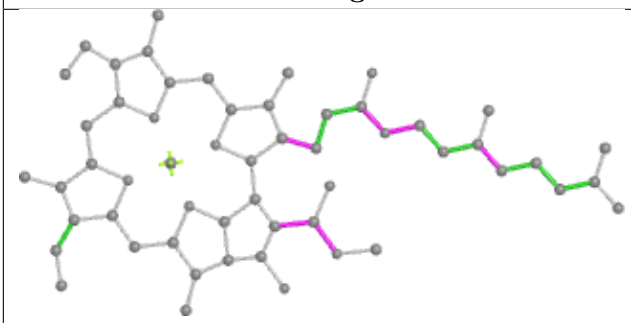


Bond angles



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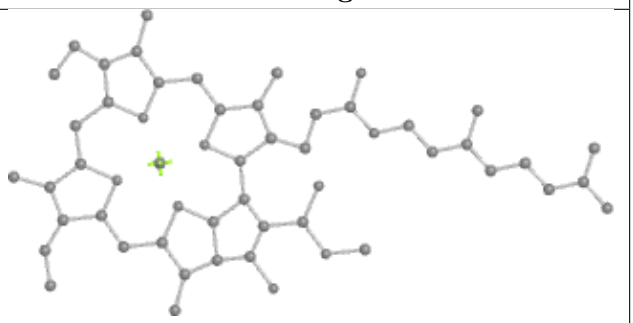
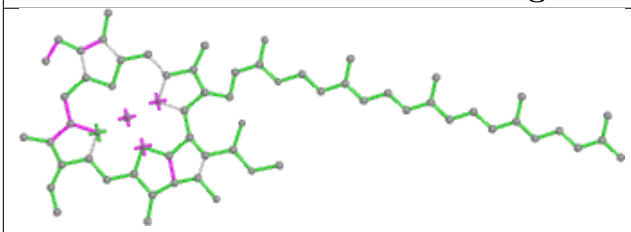


Rings

## Ligand CLA 6 604



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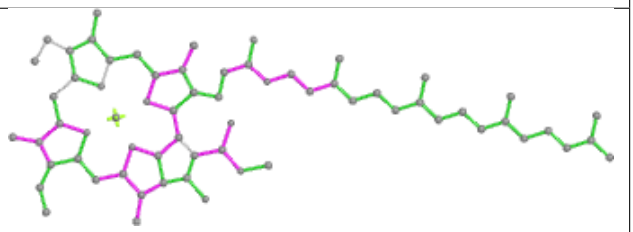
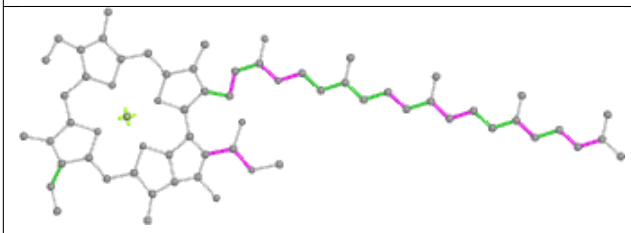
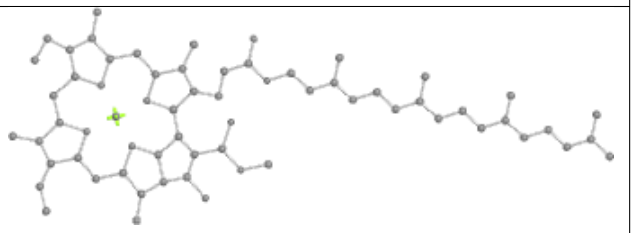


Bond angles

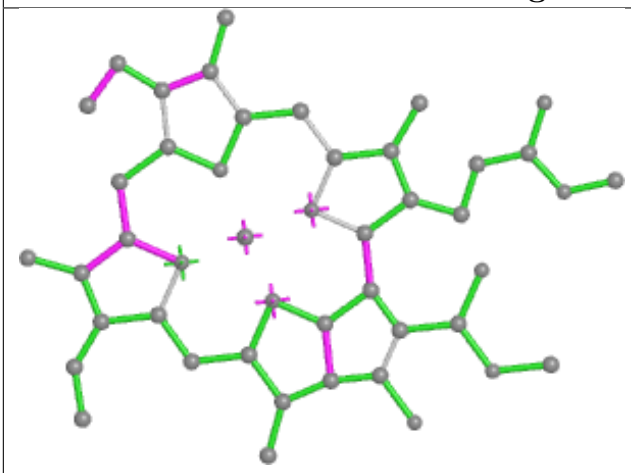


Torsions

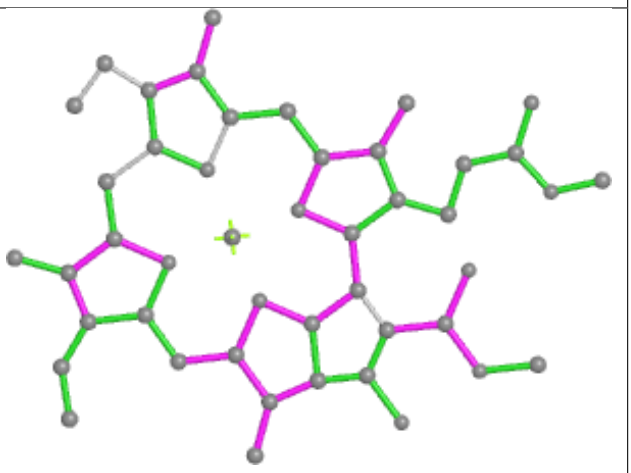


Rings

**Ligand CLA 6 605**



**Bond lengths**



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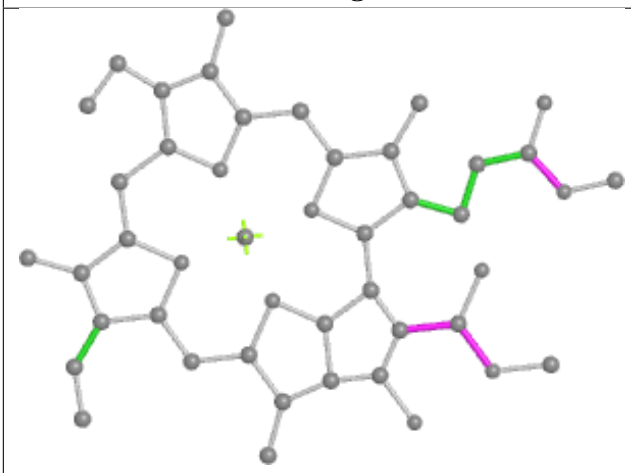
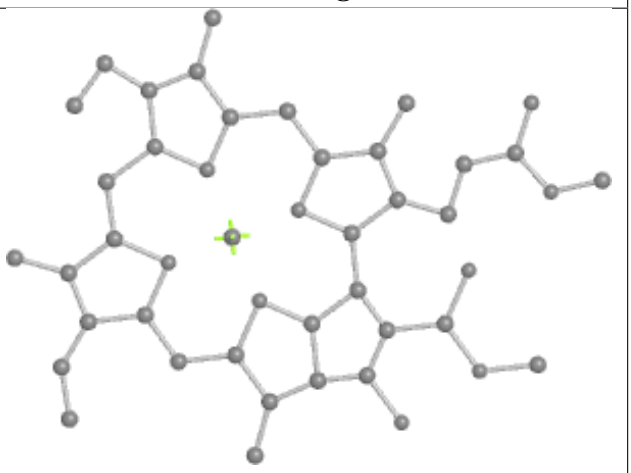
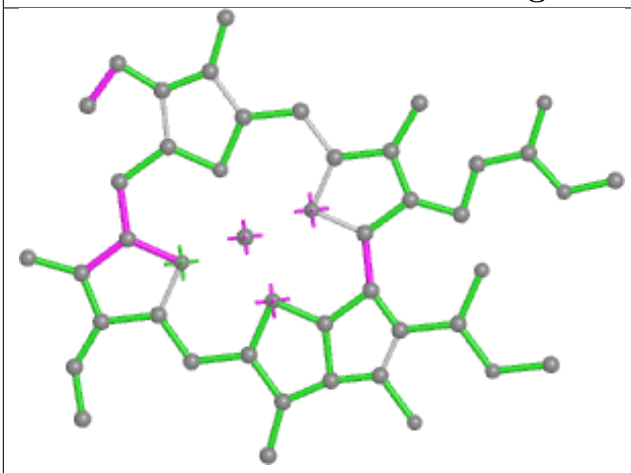


**Torsions**

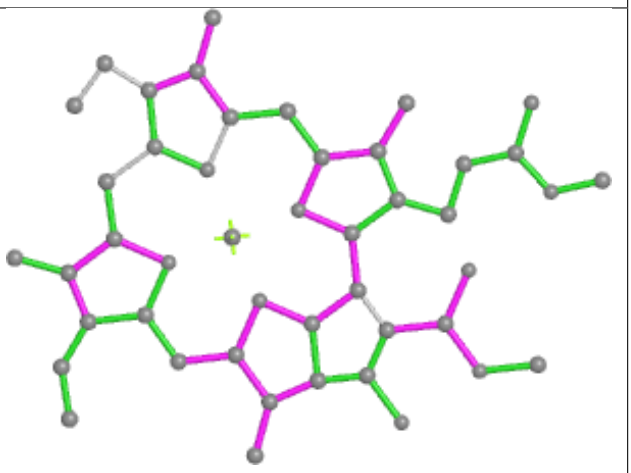


**Rings**

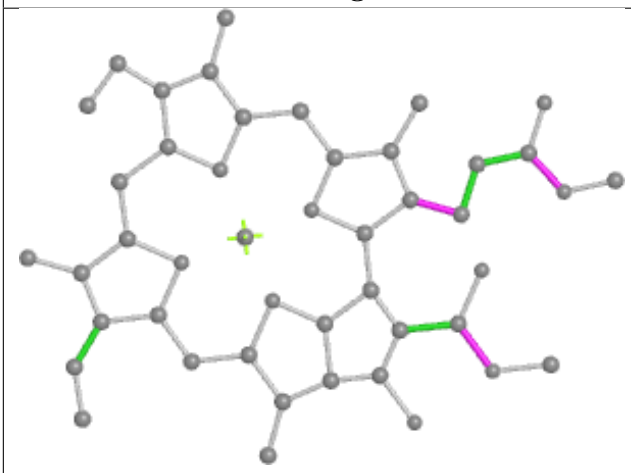
## Ligand CLA 9 609



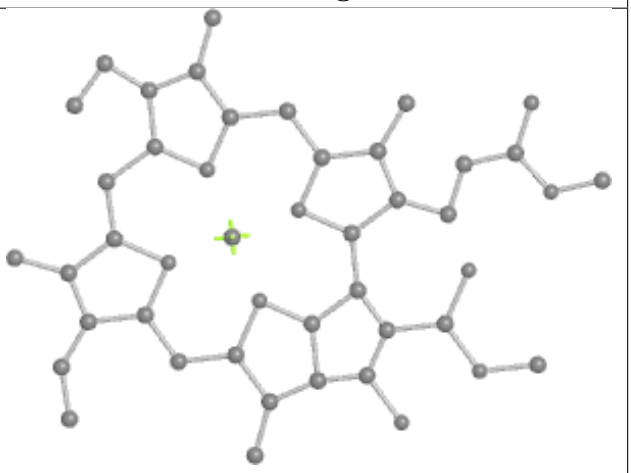
Bond lengths



Bond angles

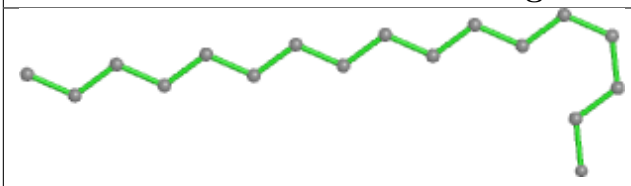


Torsions

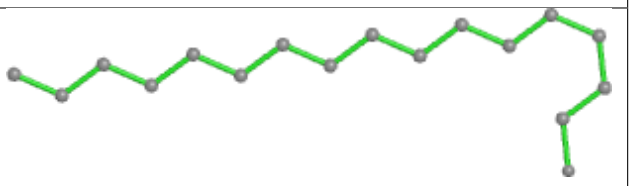


Rings

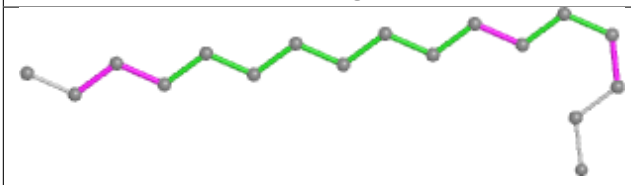
## Ligand PLM a 804



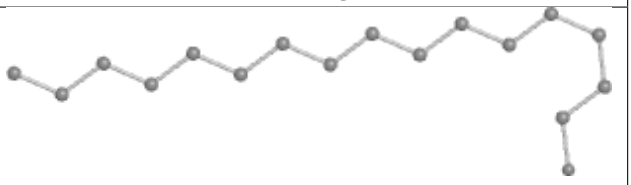
Bond lengths



Bond angles

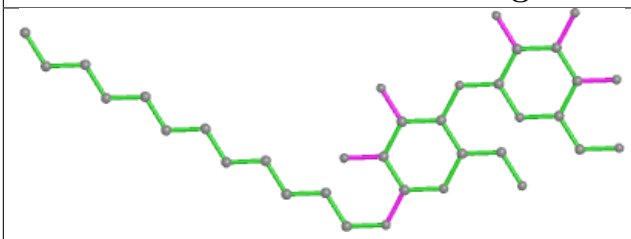


Torsions

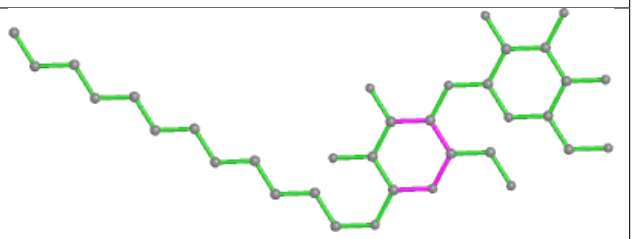


Rings

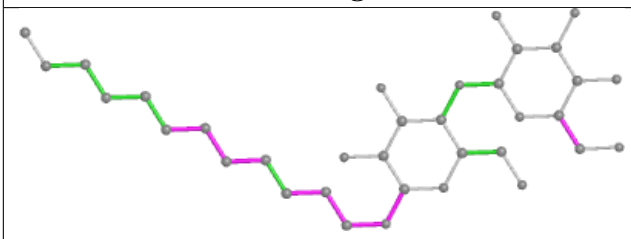
## Ligand LMT A 5008



Bond lengths



Bond angles



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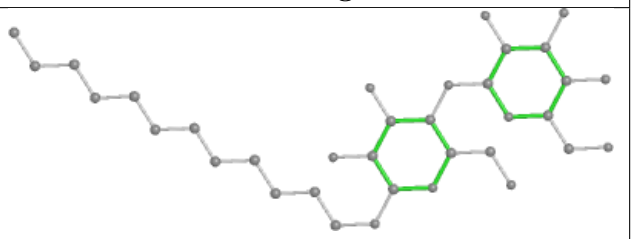
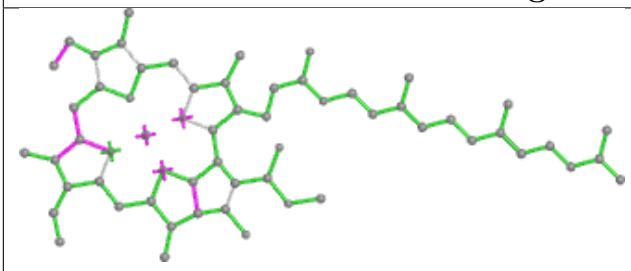
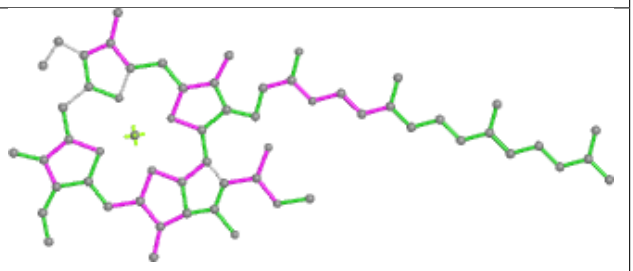


Rings

## Ligand CLA 9 604



Bond lengths



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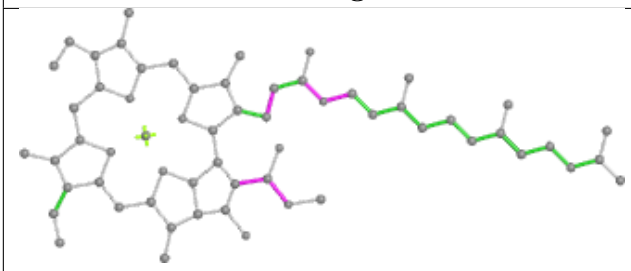

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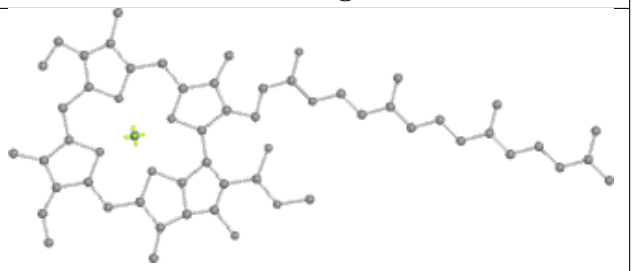
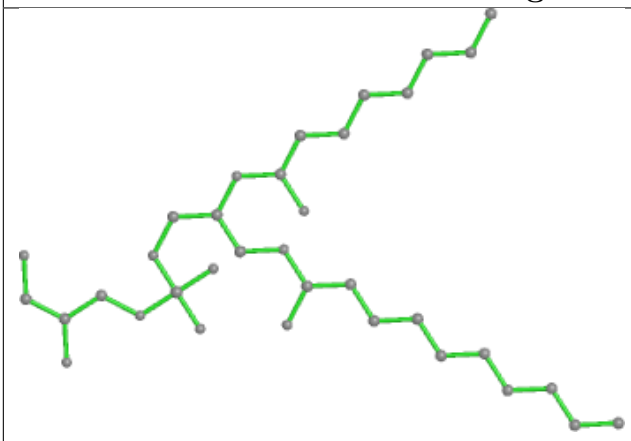


Rings

## Ligand LHG 7 803



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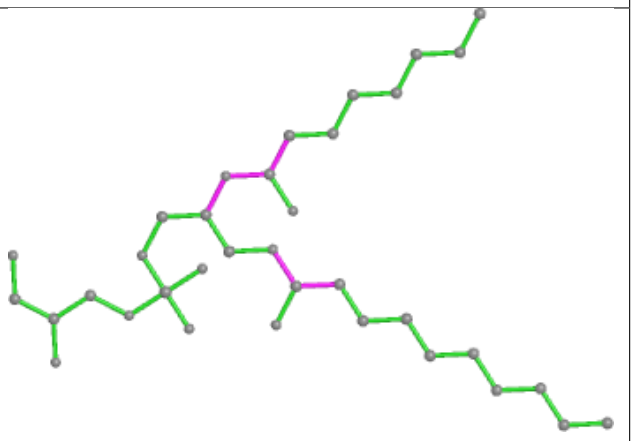

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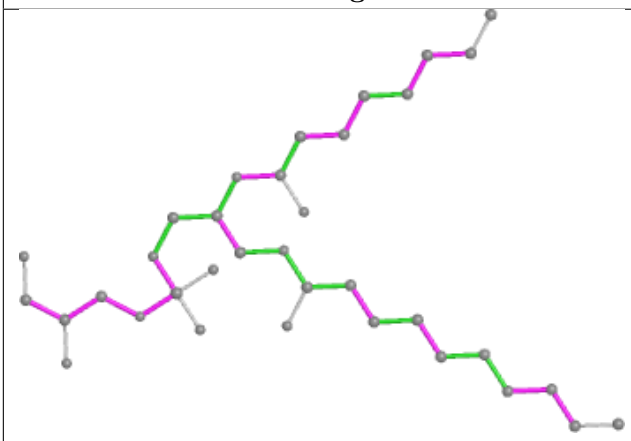

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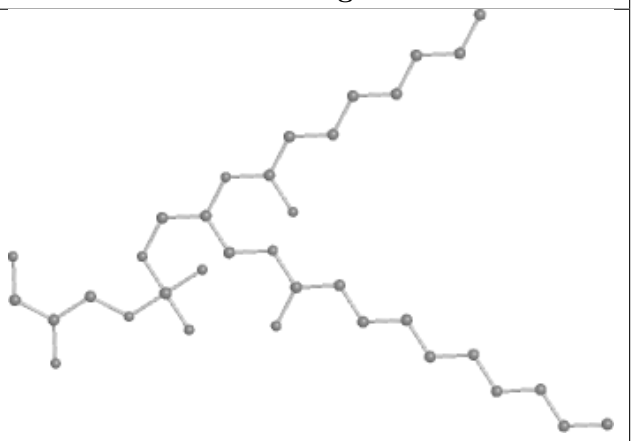
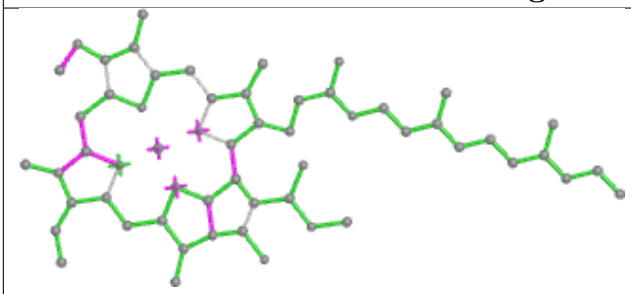


Rings

## Ligand CLA 1 606



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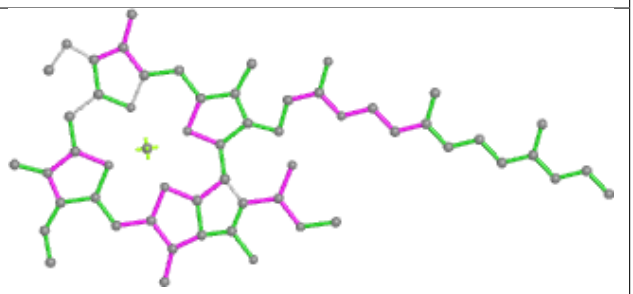

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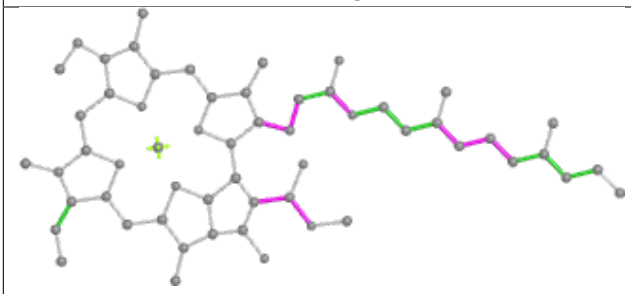

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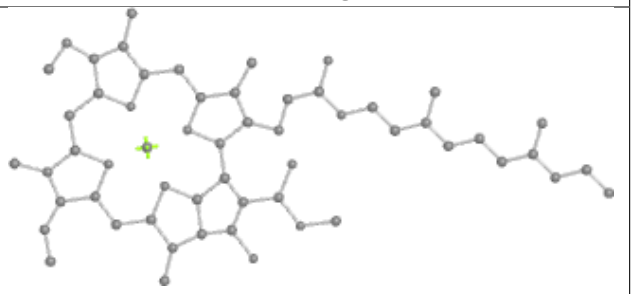

Rings

## Ligand BCR B 4003

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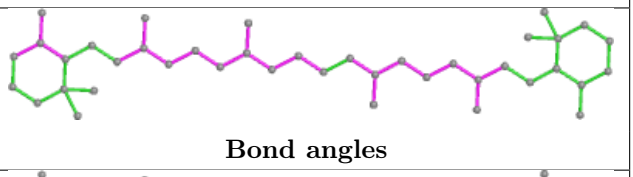

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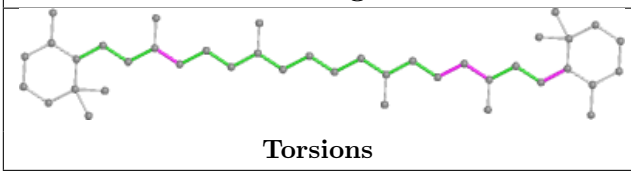

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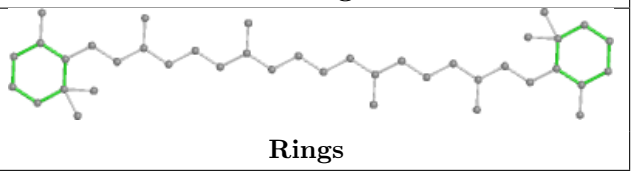
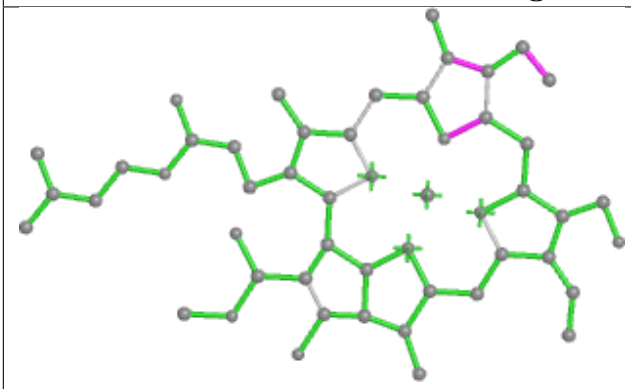


Rings

## Ligand CHL 5 618



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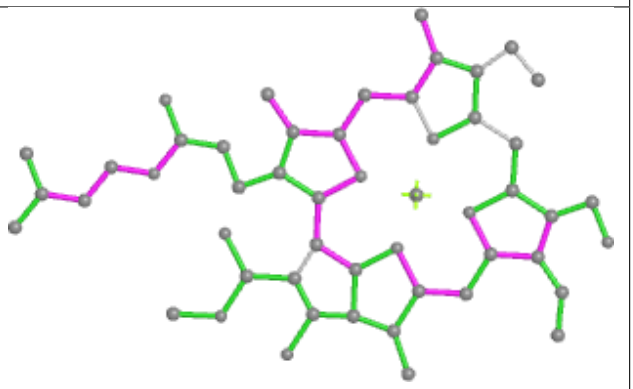

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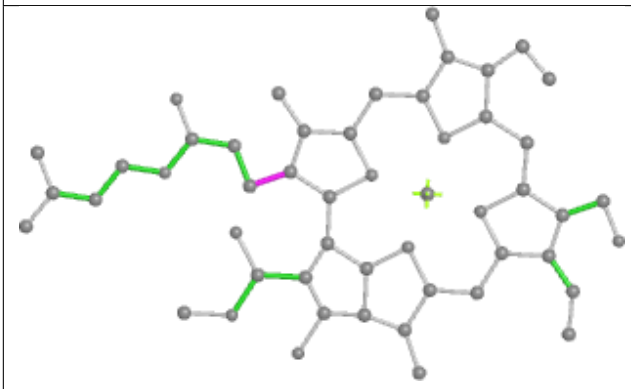

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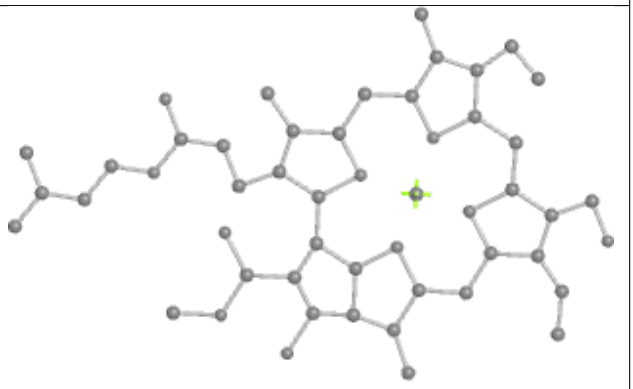
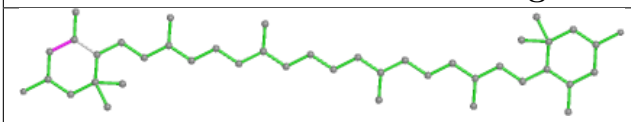


Rings

## Ligand LUT 9 501



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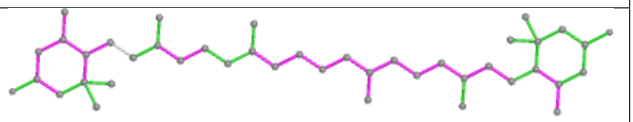
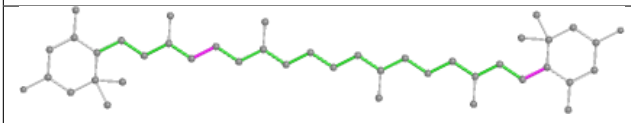


Bond angles



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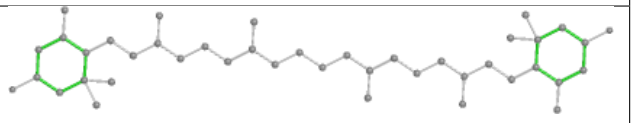
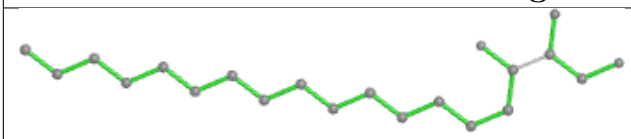


Rings

## Ligand SPH 4 805



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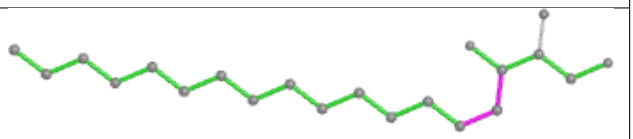
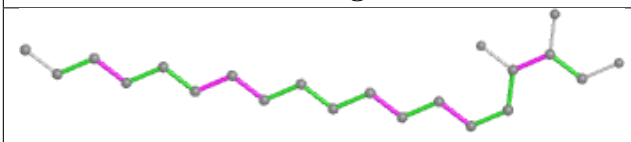


Bond angles



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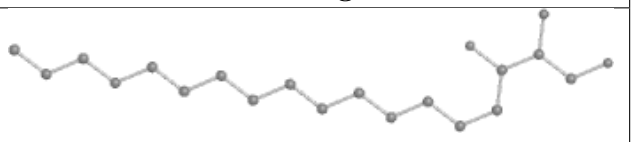
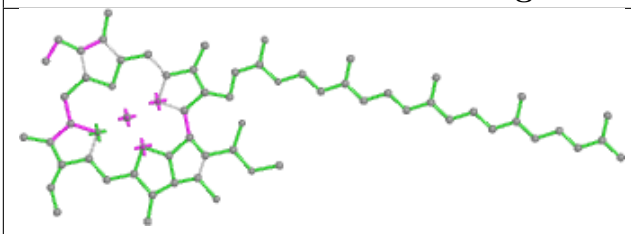


Rings

## Ligand CLA B 1224



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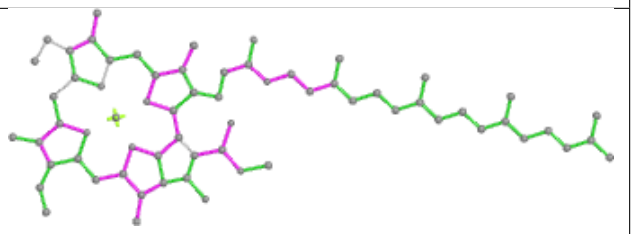
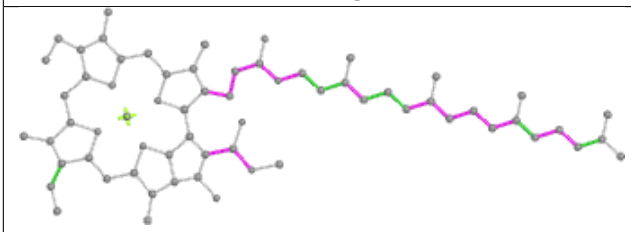


Bond angles



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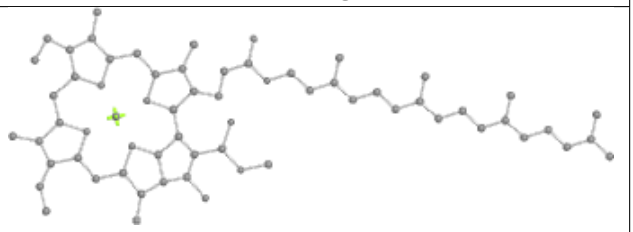
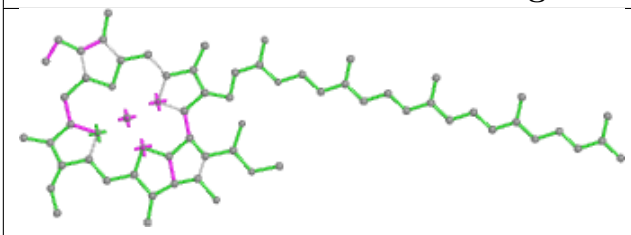


Rings

## Ligand CLA 3 607



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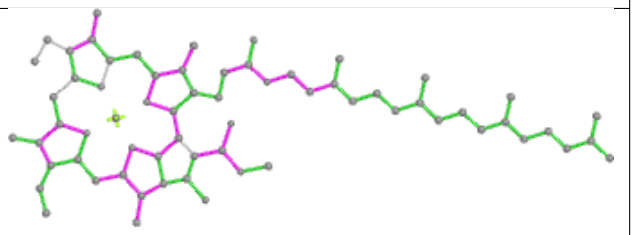
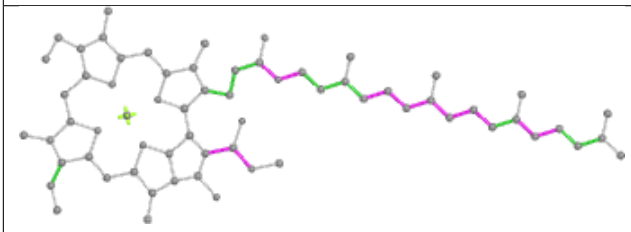


Bond angles



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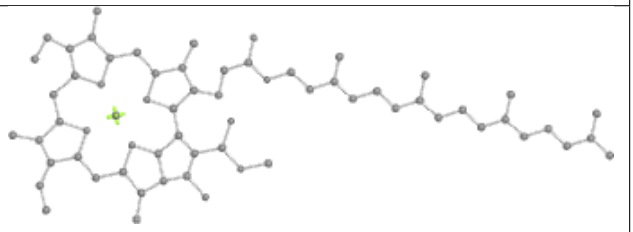
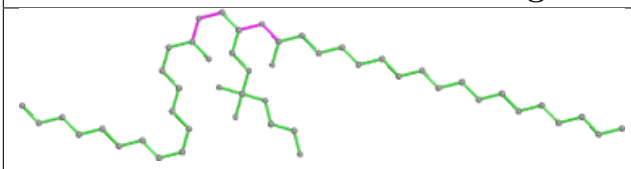


Rings

## Ligand PTY 9 803



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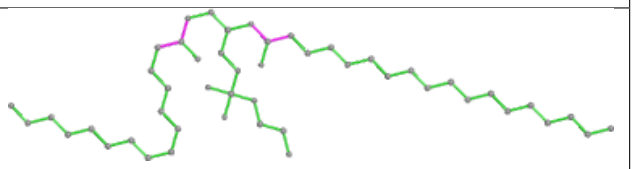

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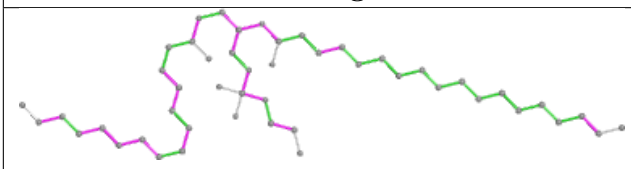

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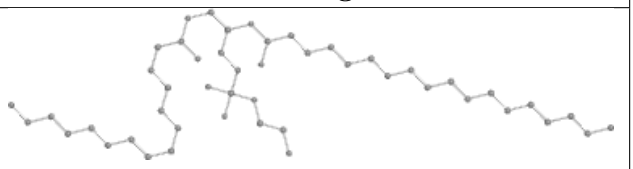
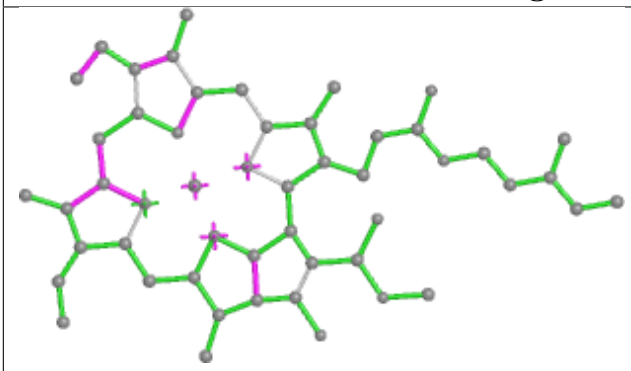


Rings

## Ligand CLA 4 608



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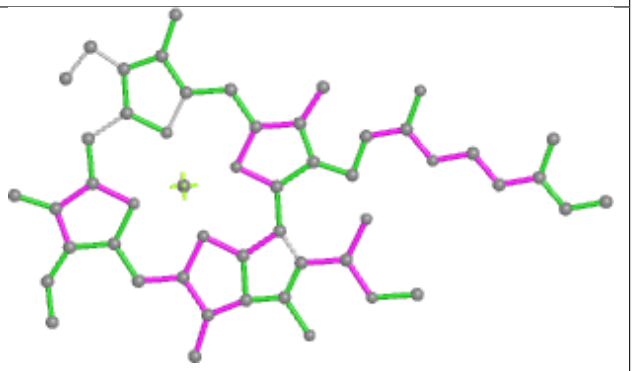
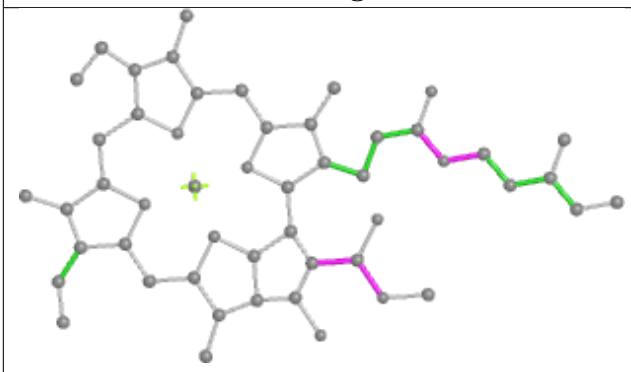


Bond angles



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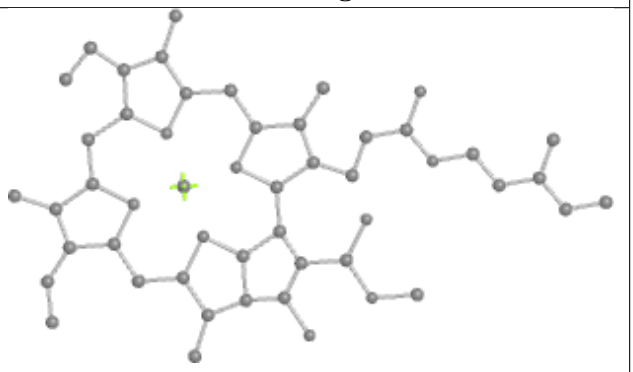
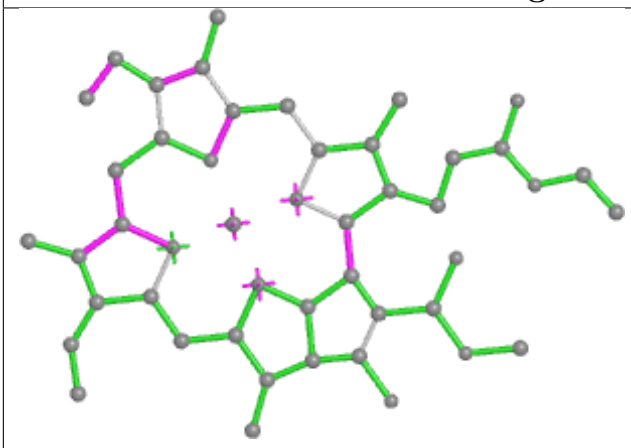


Rings

**Ligand CLA 9 607**



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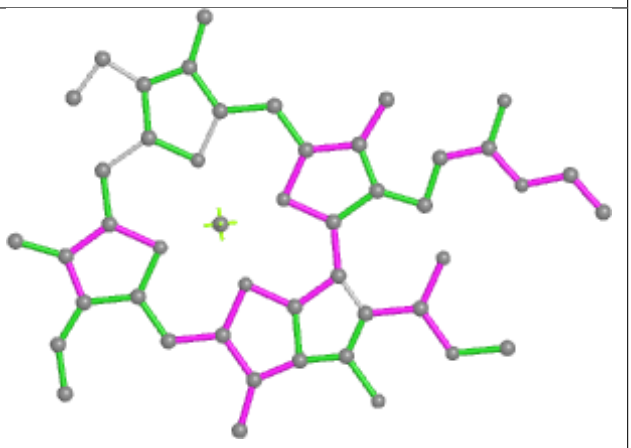
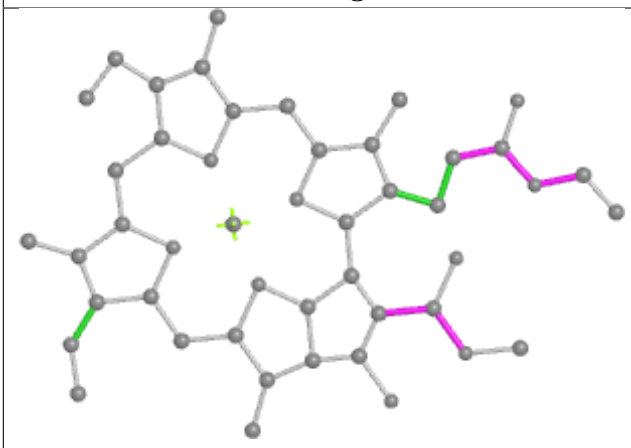


Bond angles



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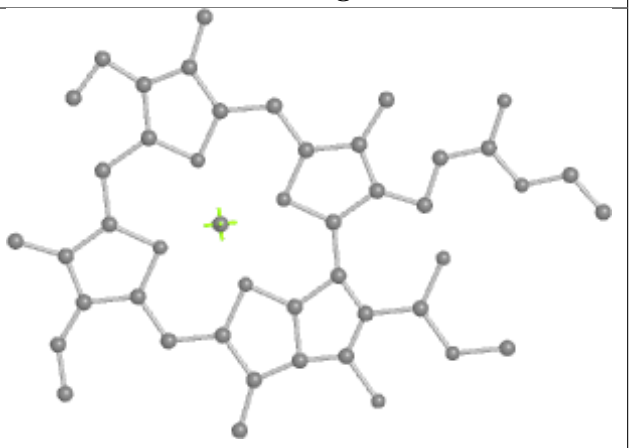
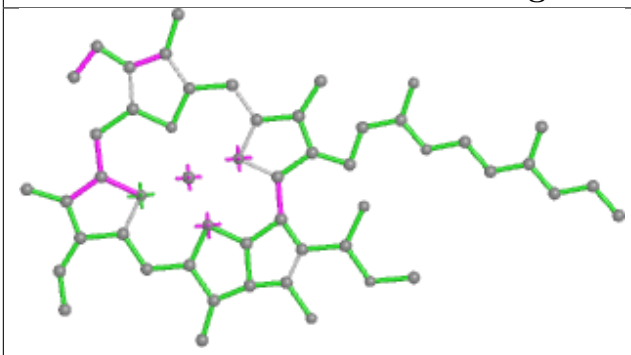
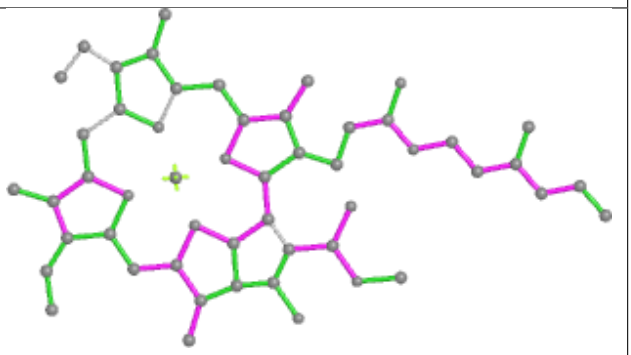


Rings

**Ligand CLA 5 602**



**Bond lengths**



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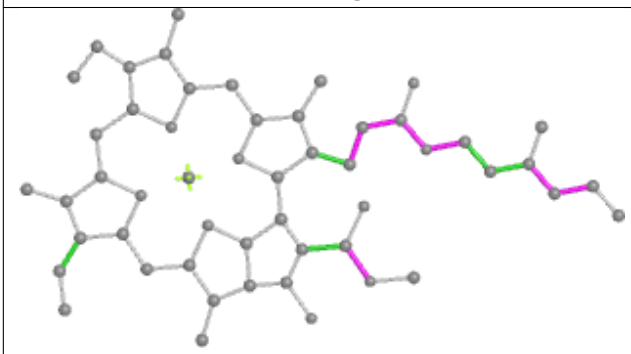

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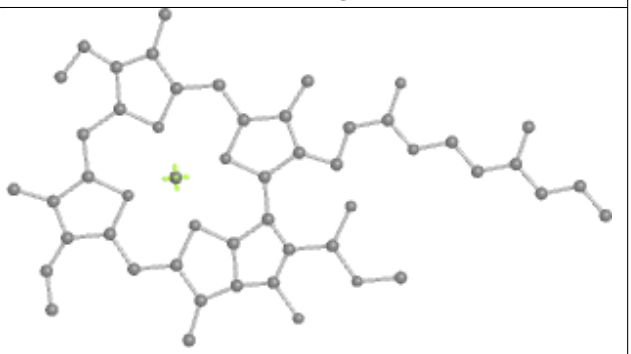
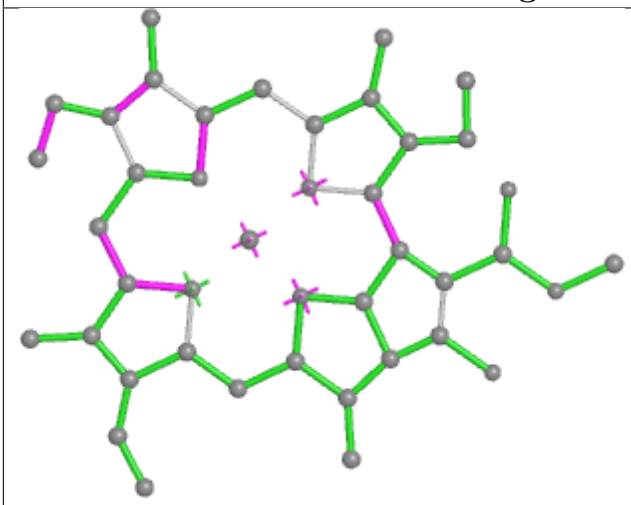


**Rings**

**Ligand CLA J 1901**



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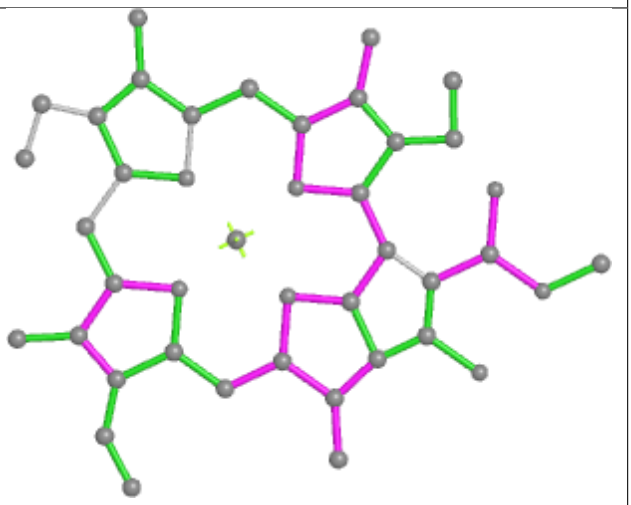
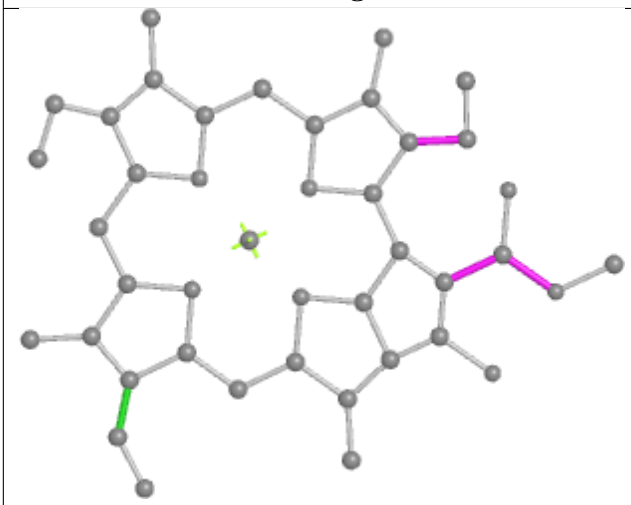


**Bond angles**



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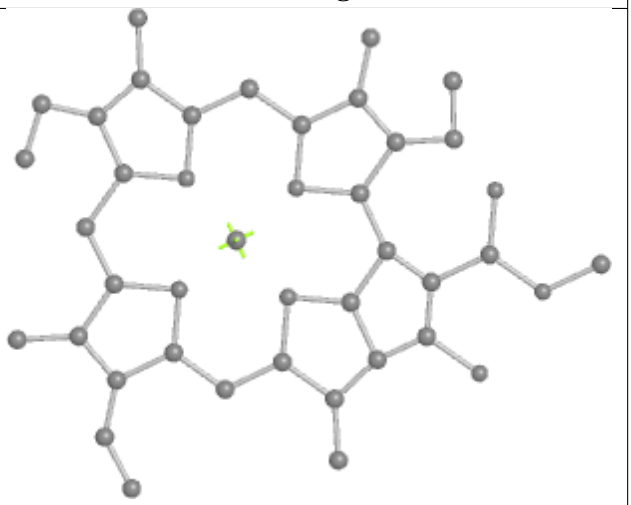
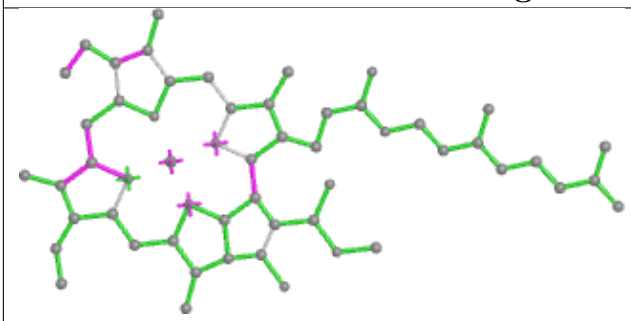
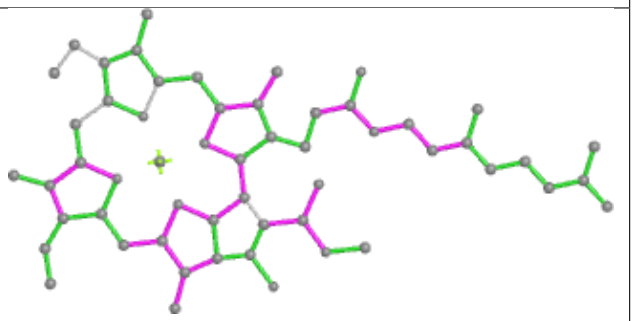


**Rings**

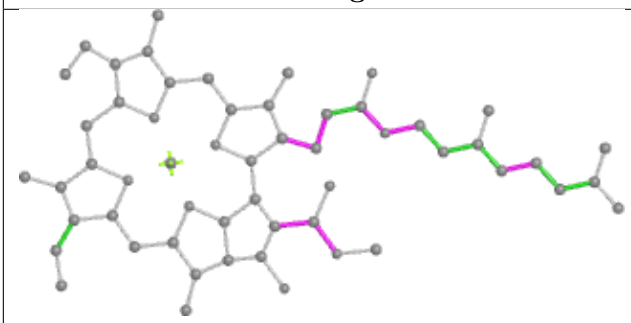
## Ligand CLA A 1140



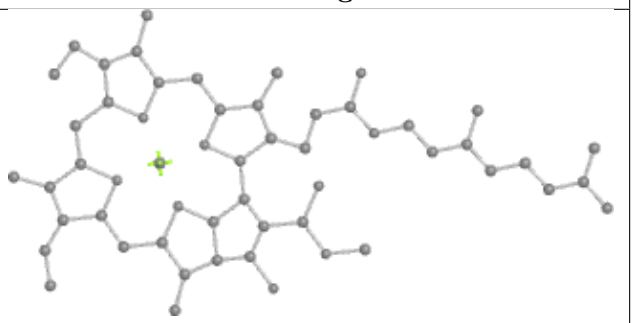
Bond lengths



Bond angles

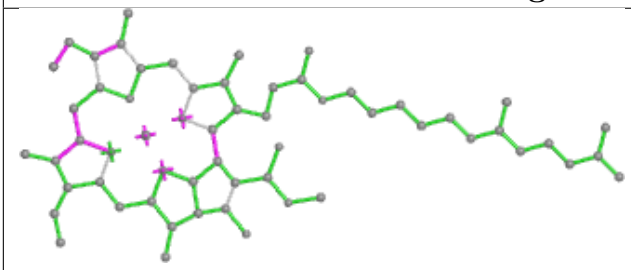


Torsions

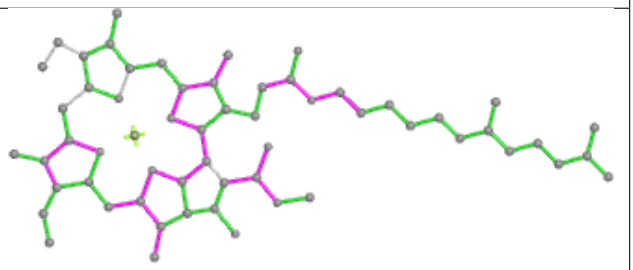


Rings

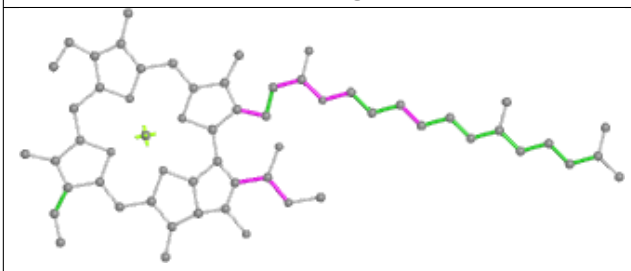
## Ligand CLA 7 607



Bond lengths



Bond angles



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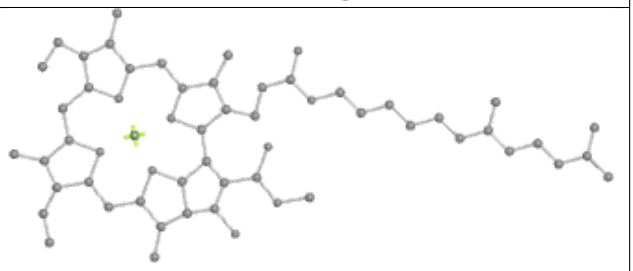
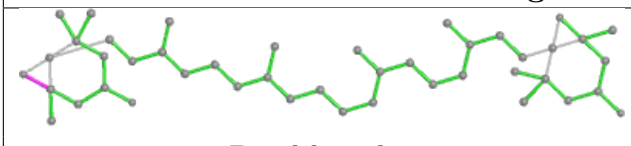


Rings

## Ligand XAT 7 502



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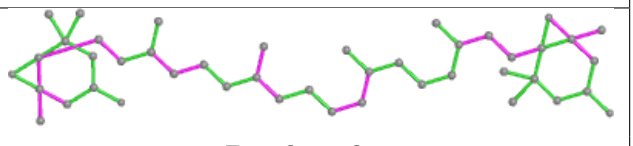
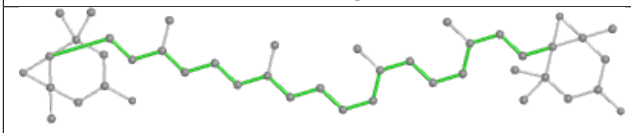
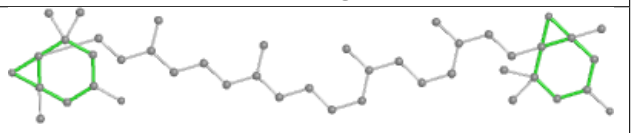


Bond angles

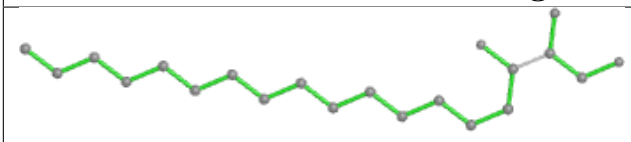


Torsions



Rings

## Ligand SPH 6 806



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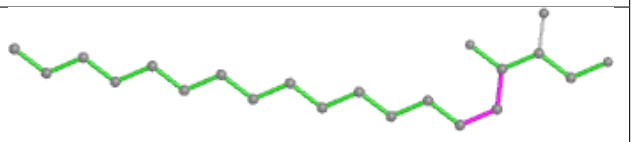
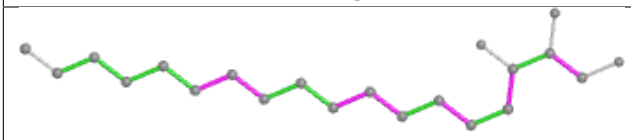


Bond angles



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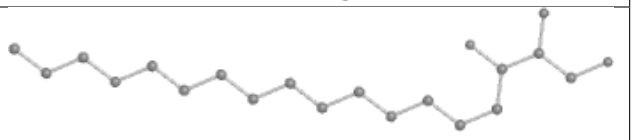
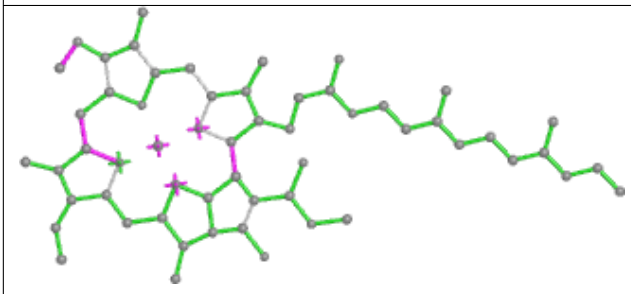
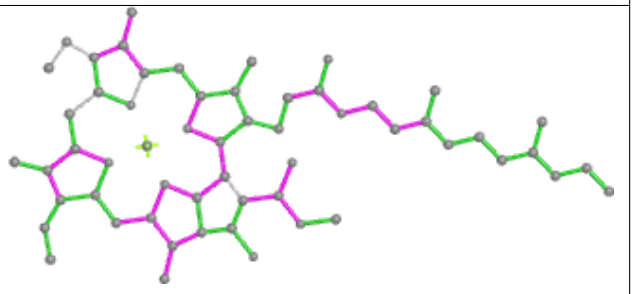


Rings

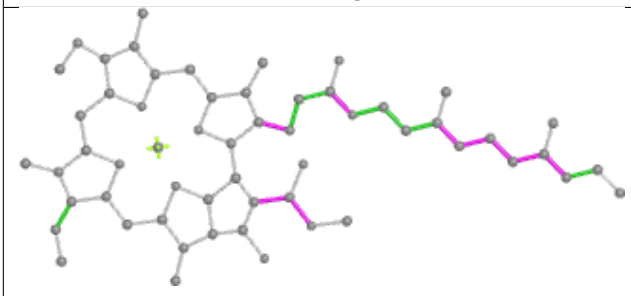
## Ligand CLA 8 606



Bond lengths



Bond angles



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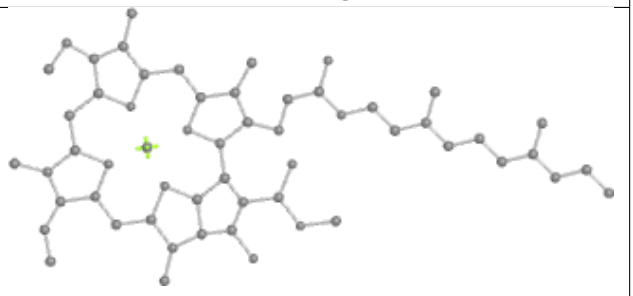
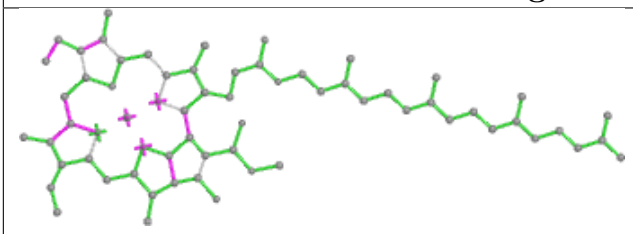
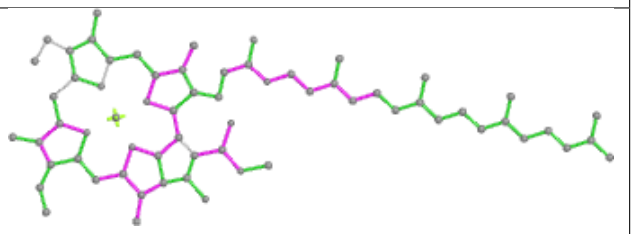


Rings

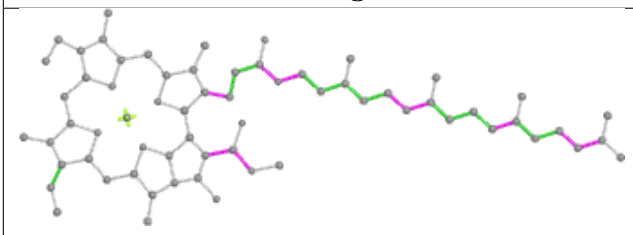
**Ligand CLA 2 621**



Bond lengths



Bond angles



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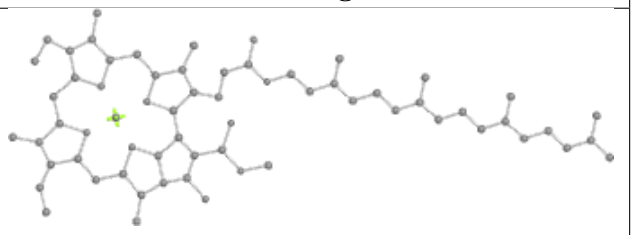
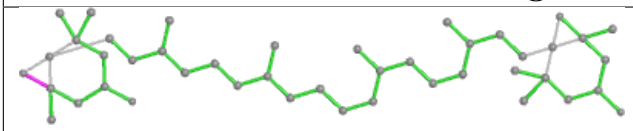


Rings

**Ligand XAT 2 501**



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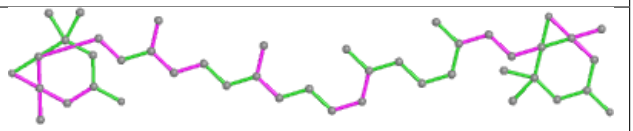
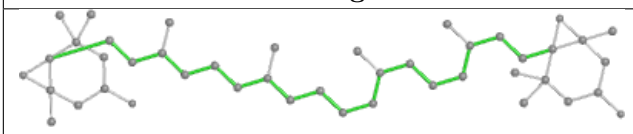


Bond angles



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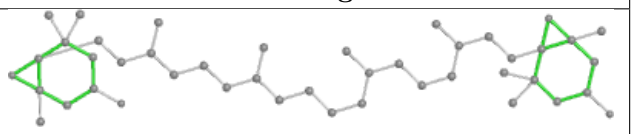
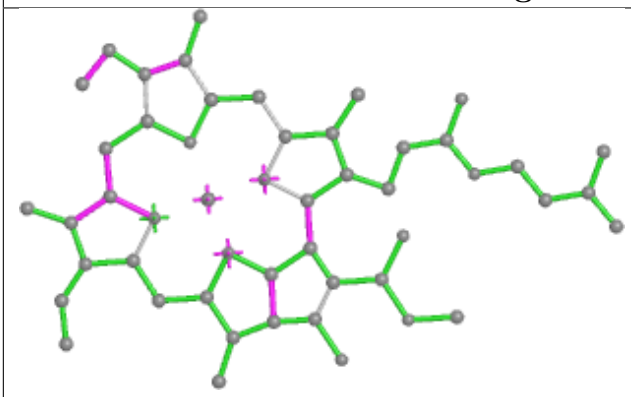


Rings

## Ligand CLA A 1129



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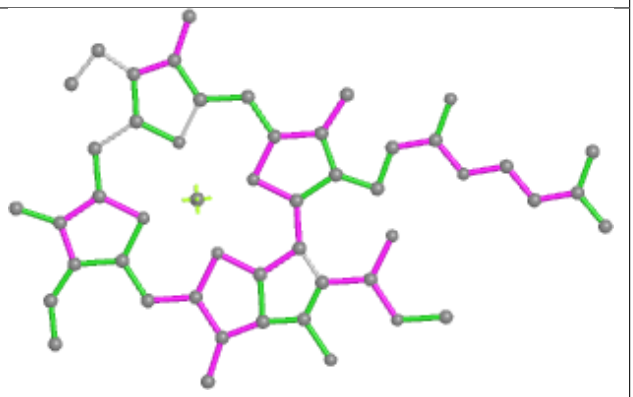
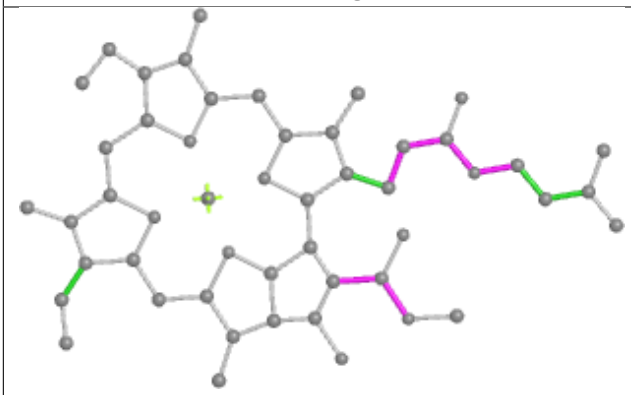
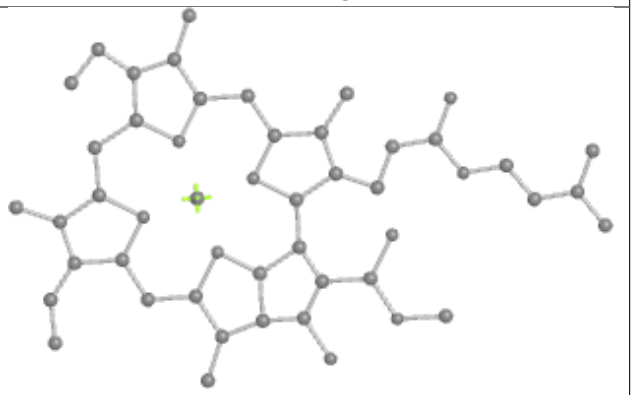


Bond angles

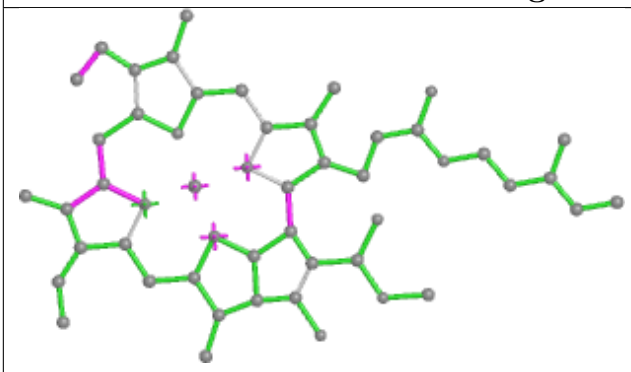


Torsions

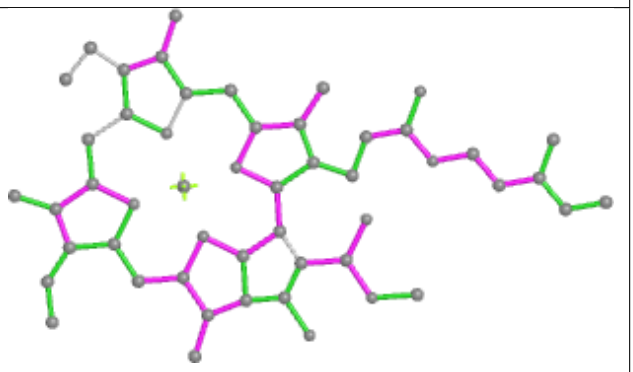


Rings

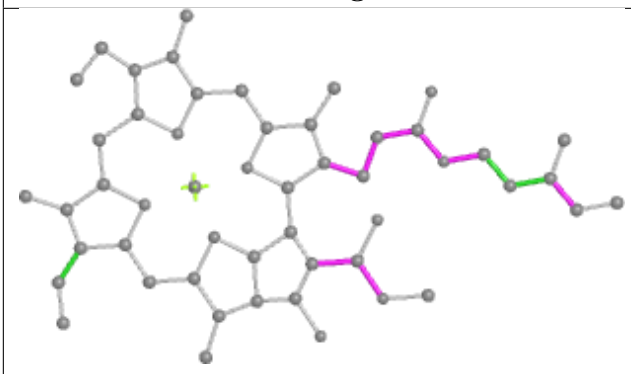
## Ligand CLA 5 609



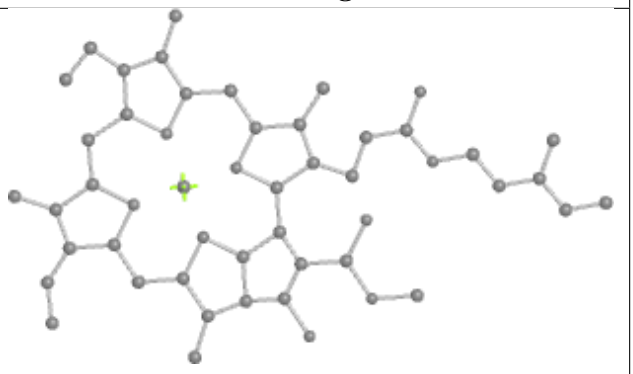
Bond lengths



Bond angles

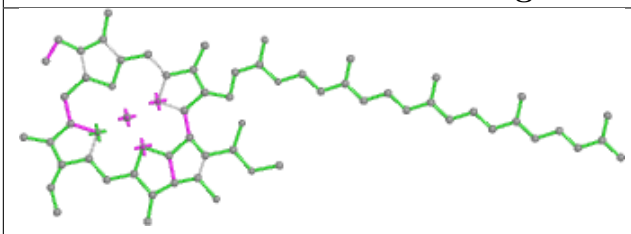


Torsions



Rings

## Ligand CLA B 1228



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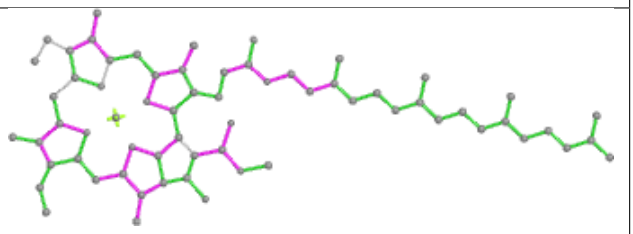
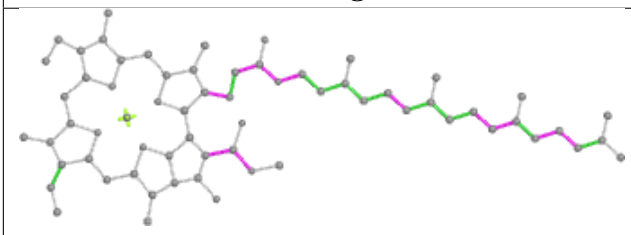


Bond angles



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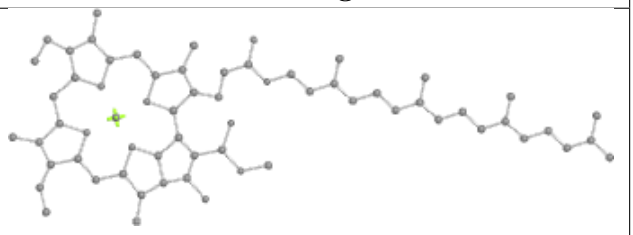
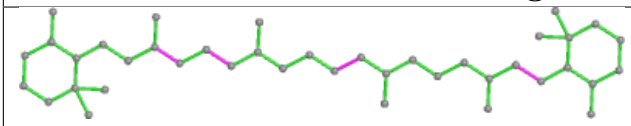


Rings

## Ligand BCR 7 503



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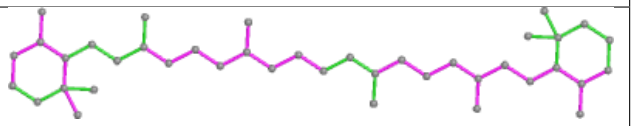
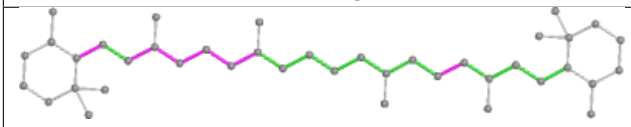


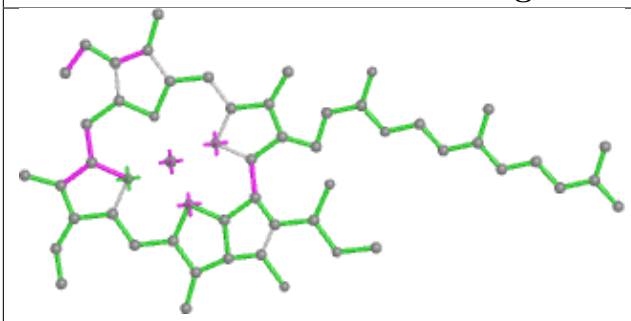
Bond angles



Torsions

Rings

## Ligand CLA A 1124



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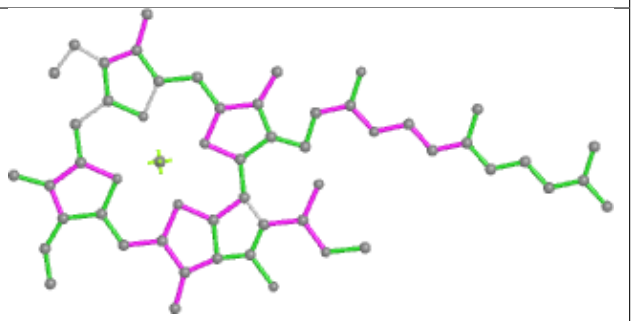
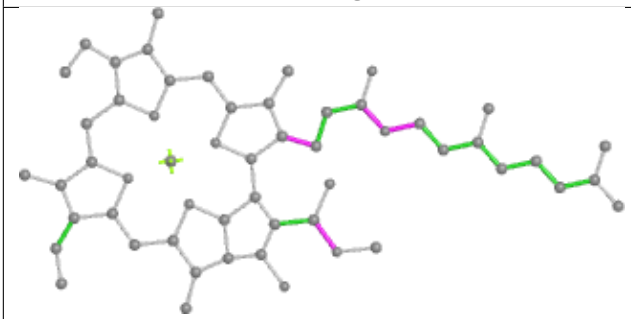
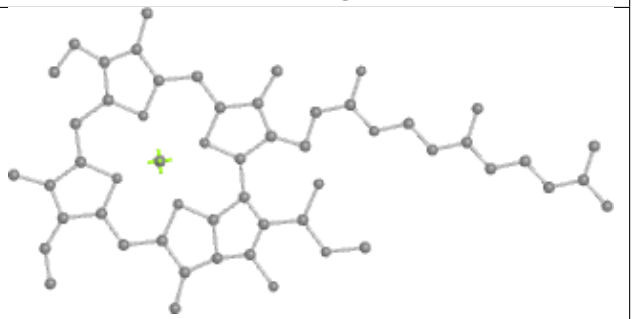


Bond angles

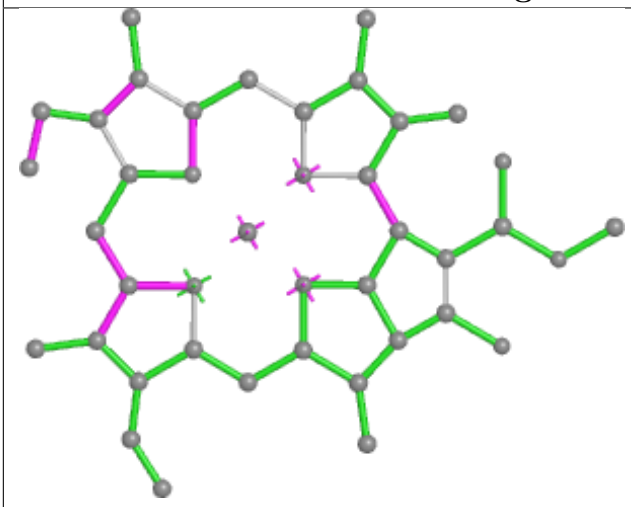


Torsions

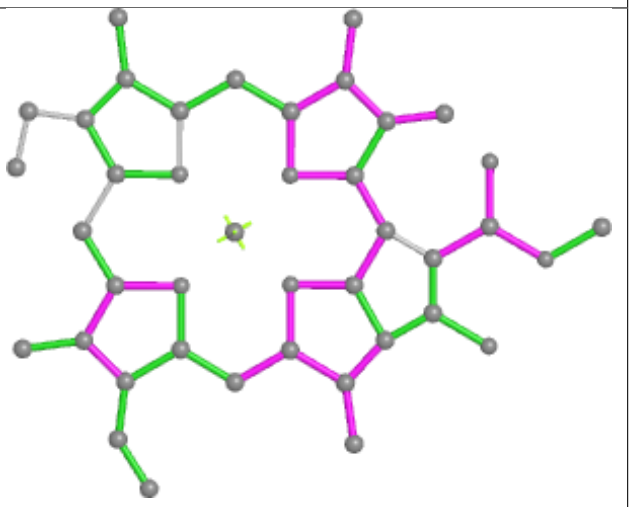


Rings

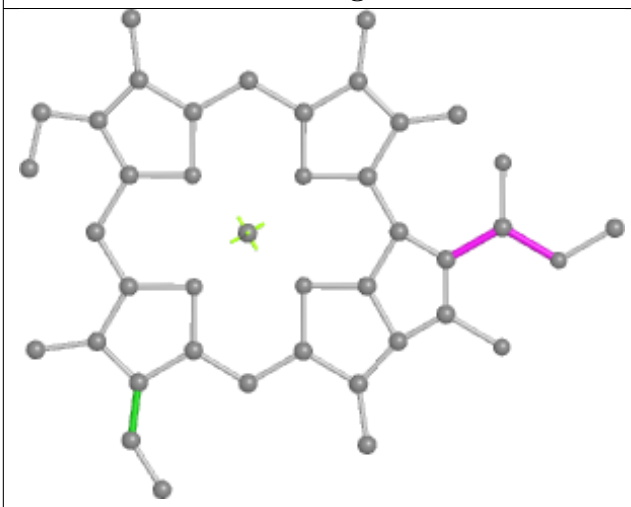
## Ligand CLA O 1803



Bond lengths



Bond angles



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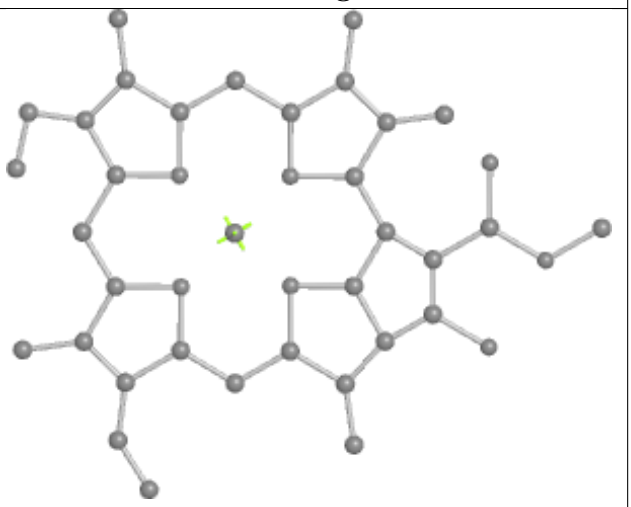
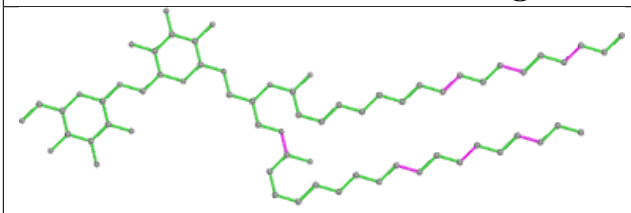
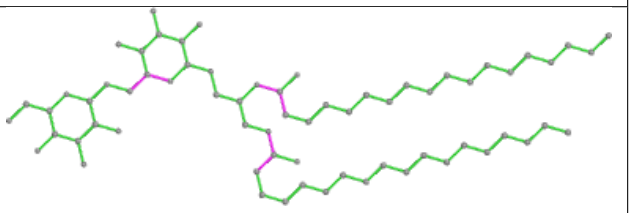


Rings

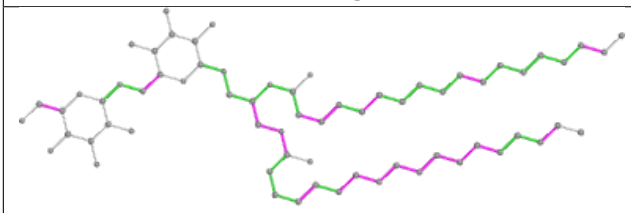
## Ligand DGD B 5003



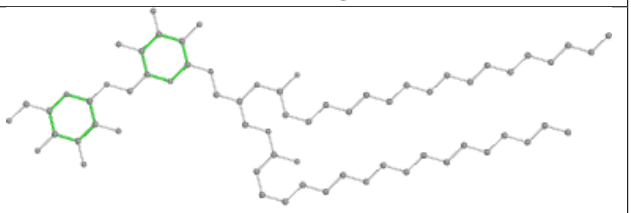
Bond lengths



Bond angles

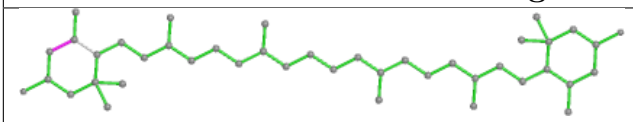


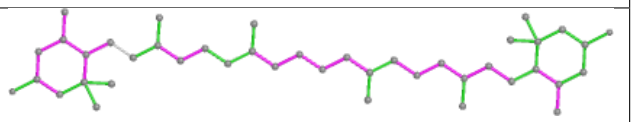
Torsions

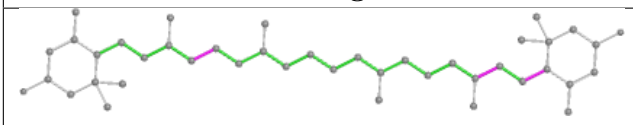


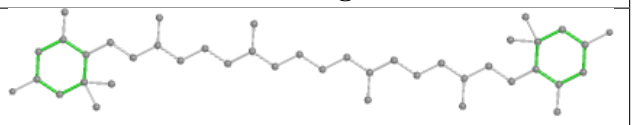
Rings

## Ligand LUT 8 502

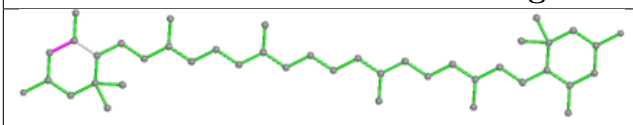

Bond lengths


Bond angles


Torsions


Rings

## Ligand LUT 9 502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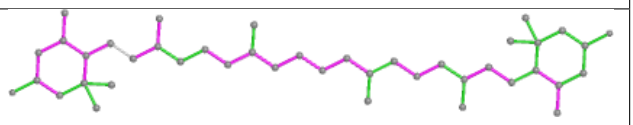
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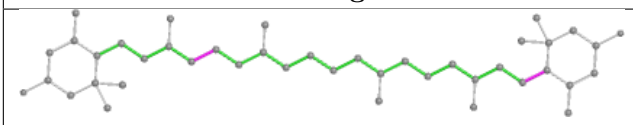
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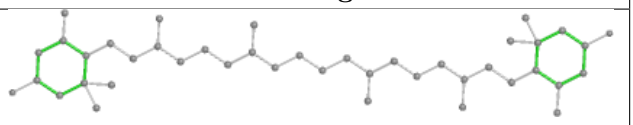
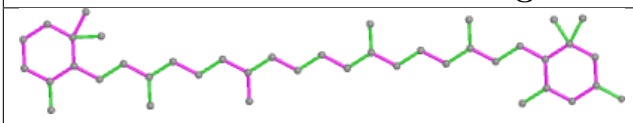

Rings

## Ligand RRX J 4002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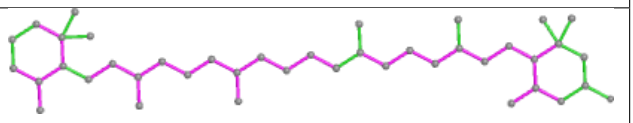
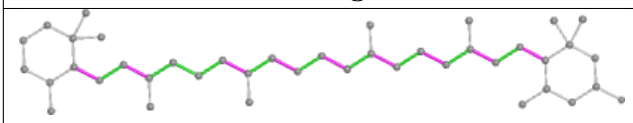

Bond angles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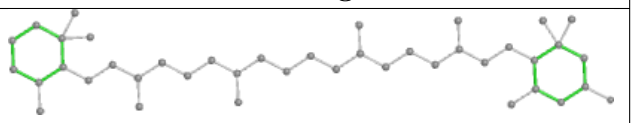
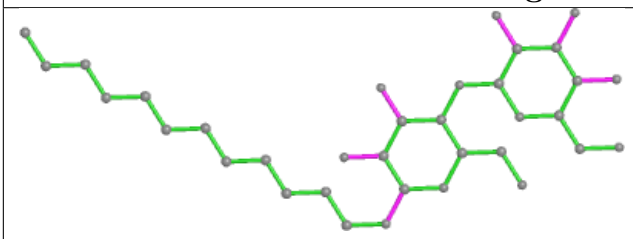

Rings

## Ligand LMT 2 804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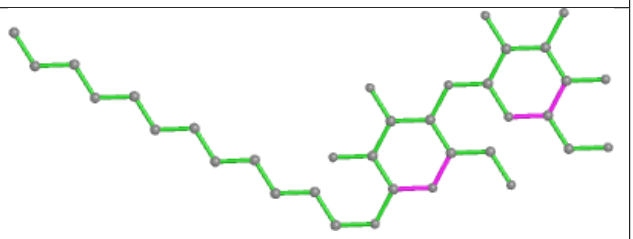
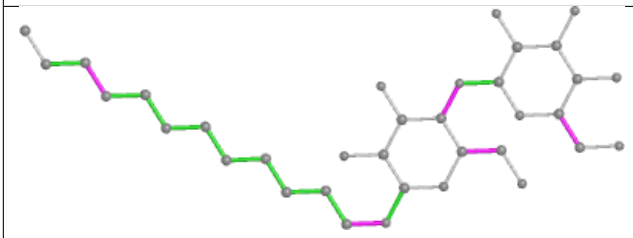
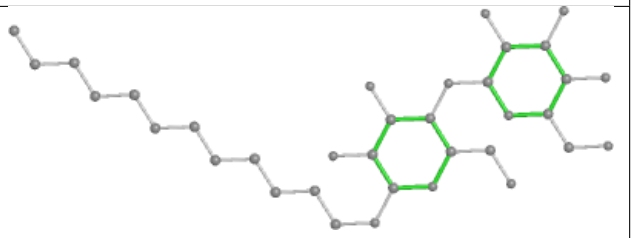
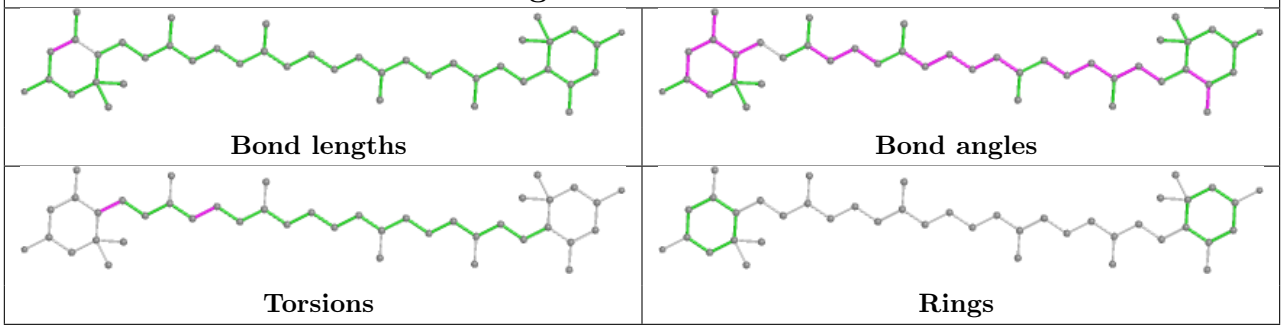

Bond angles

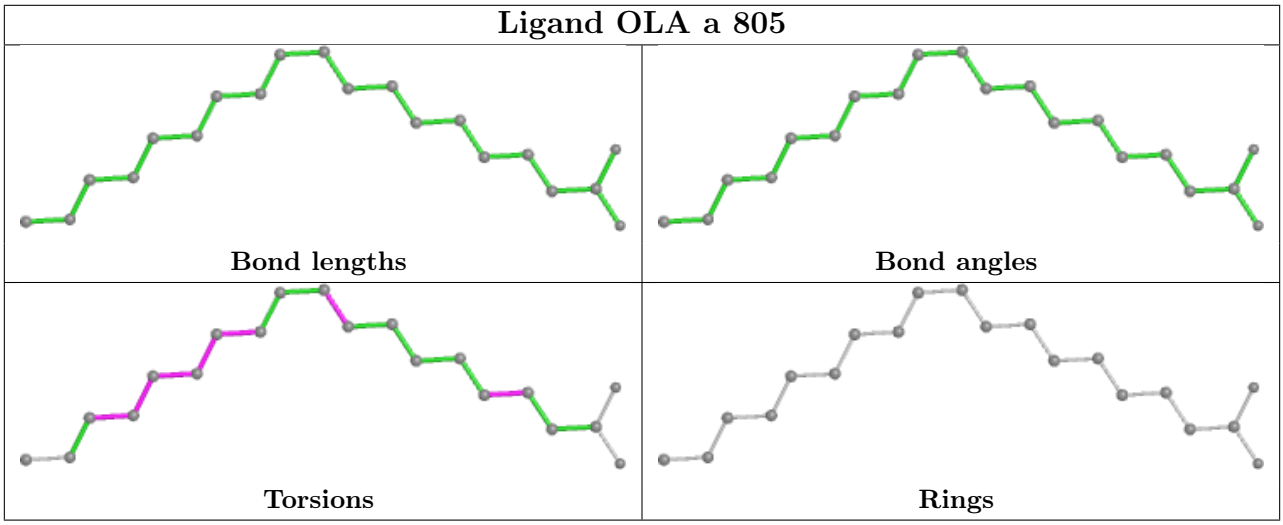

Torsions


Rings

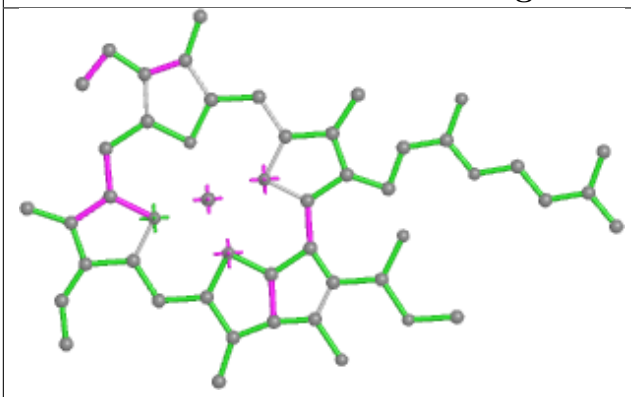
## Ligand LUT 3 502



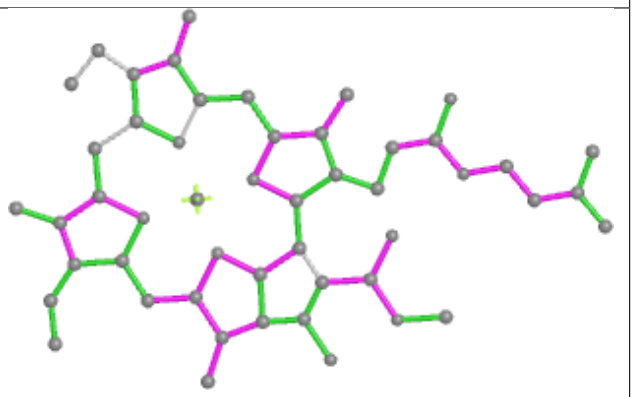

## Ligand OLA a 805



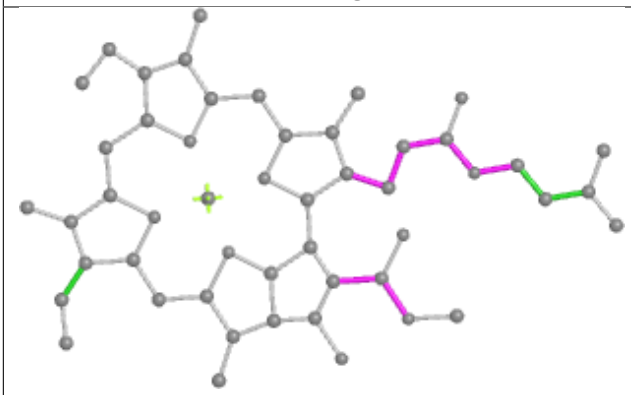
## Ligand CLA B 1227



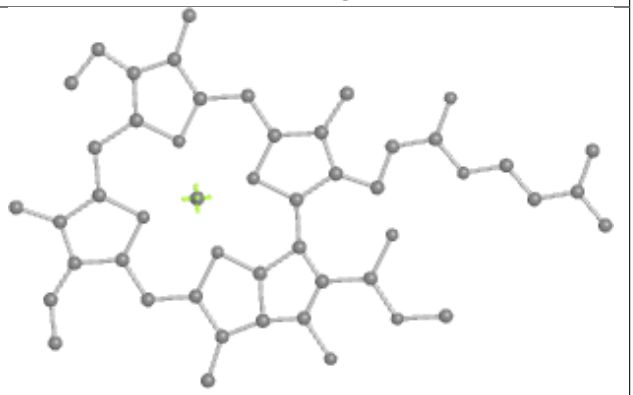
Bond lengths



Bond angles

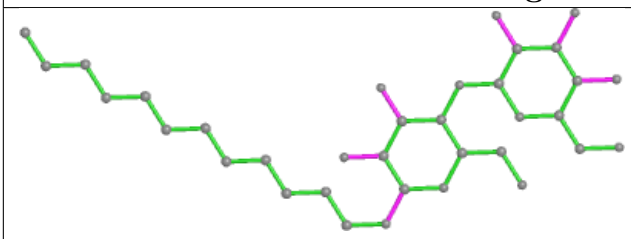


Torsions



Rings

## Ligand LMT 1 804



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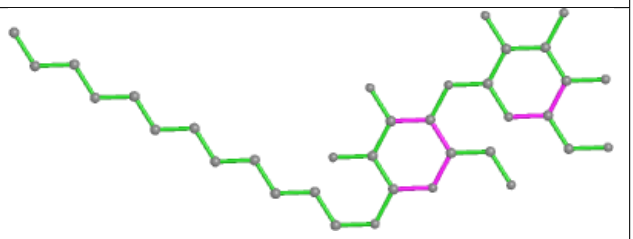
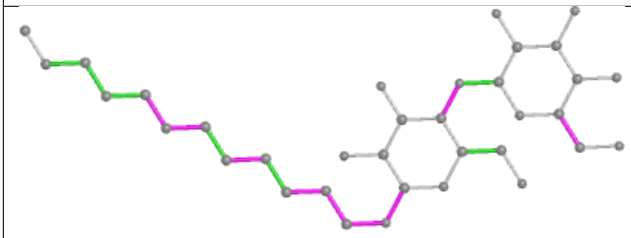


Bond angles



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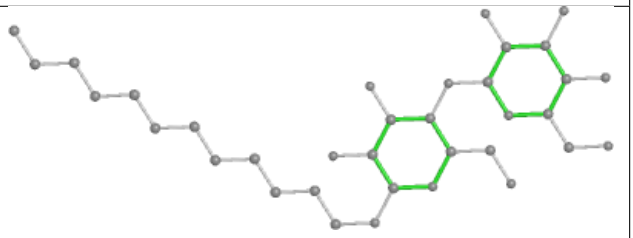
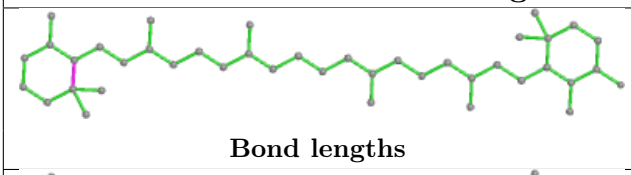


Rings

## Ligand ECH M 4001



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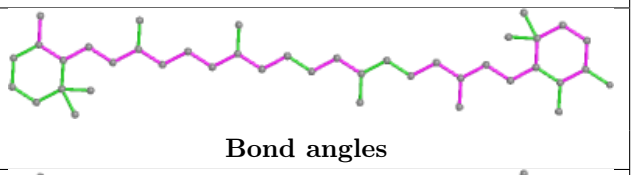
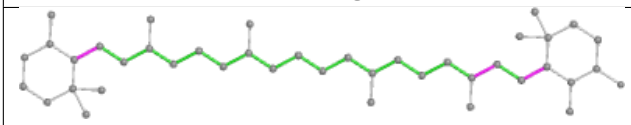


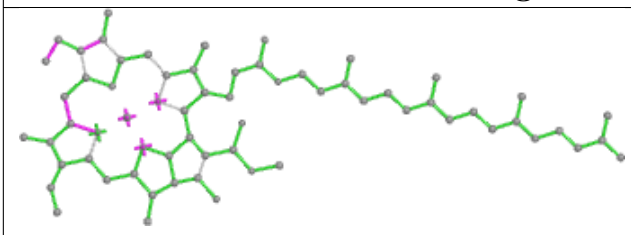
Bond angles



Torsions

Rings

## Ligand CLA A 1127



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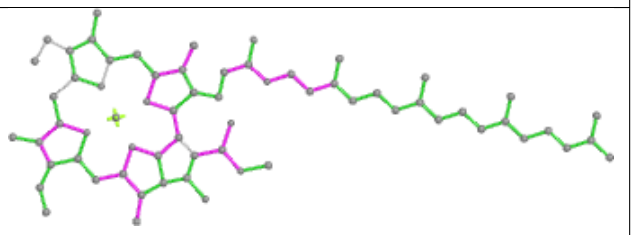
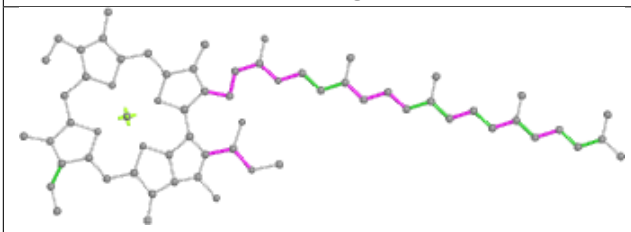
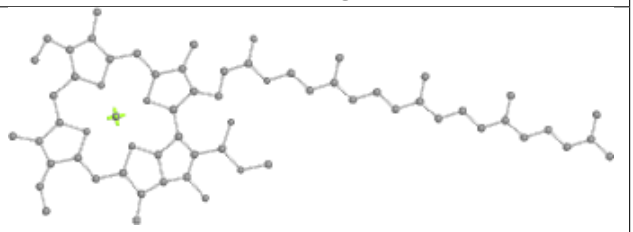


Bond angles

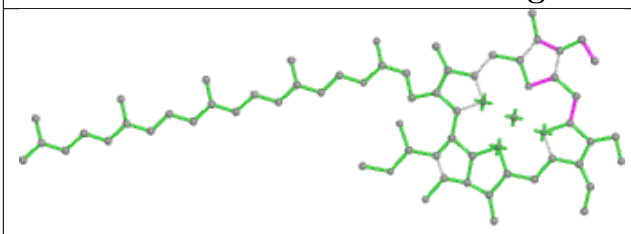


Torsions

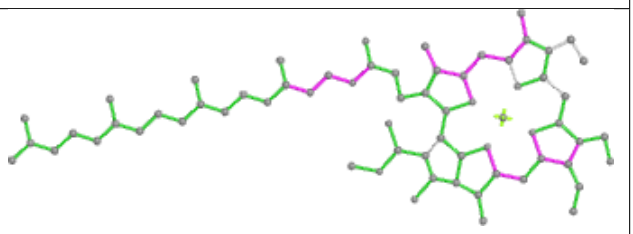


Rings

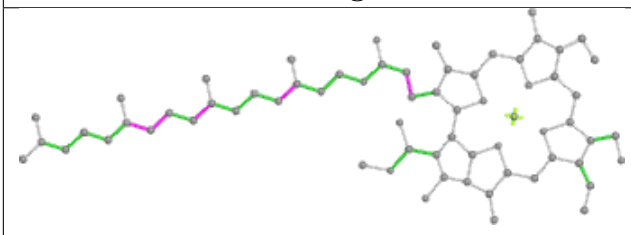
## Ligand CHL 8 603



Bond lengths



Bond angles



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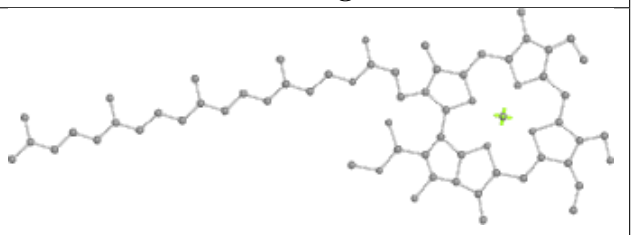
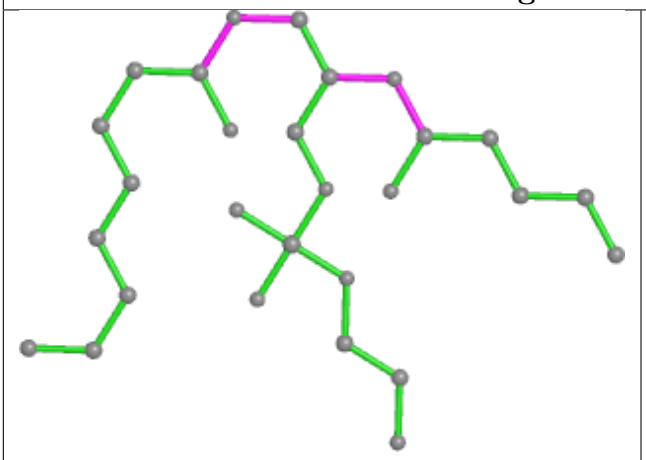
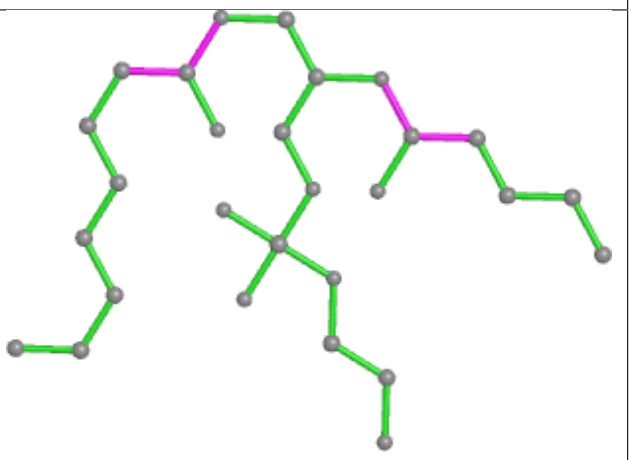


Rings

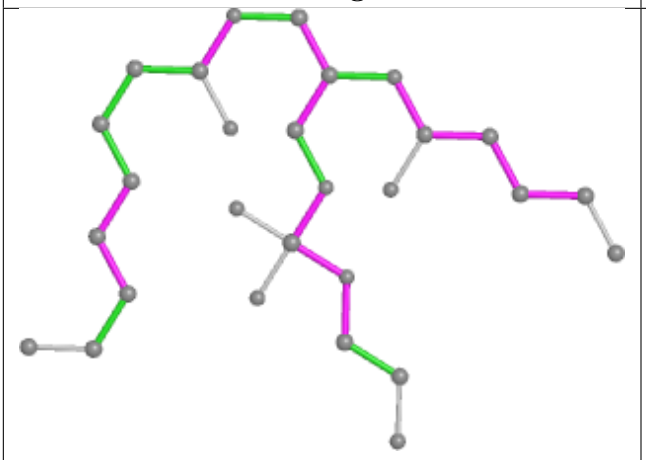
## Ligand PTY J 5001



Bond lengths



Bond angles



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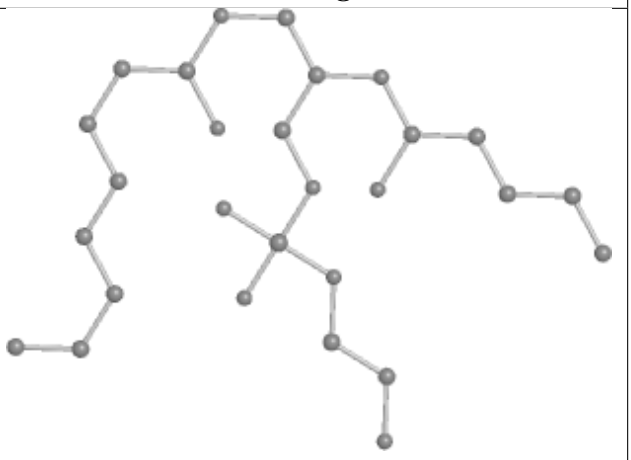
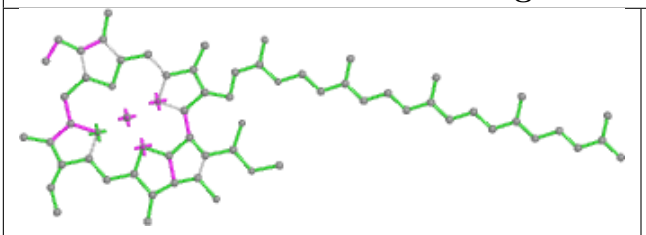


Rings

## Ligand CLA A 1138



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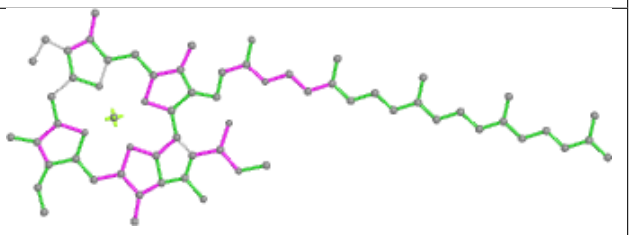
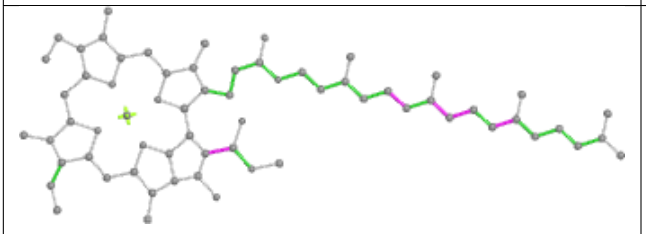
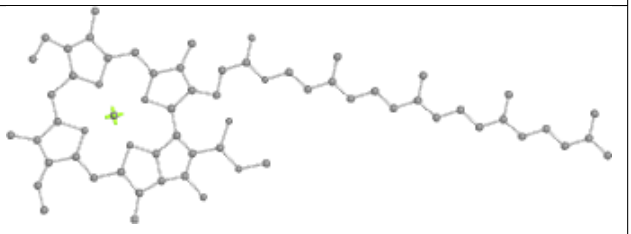


Bond angles

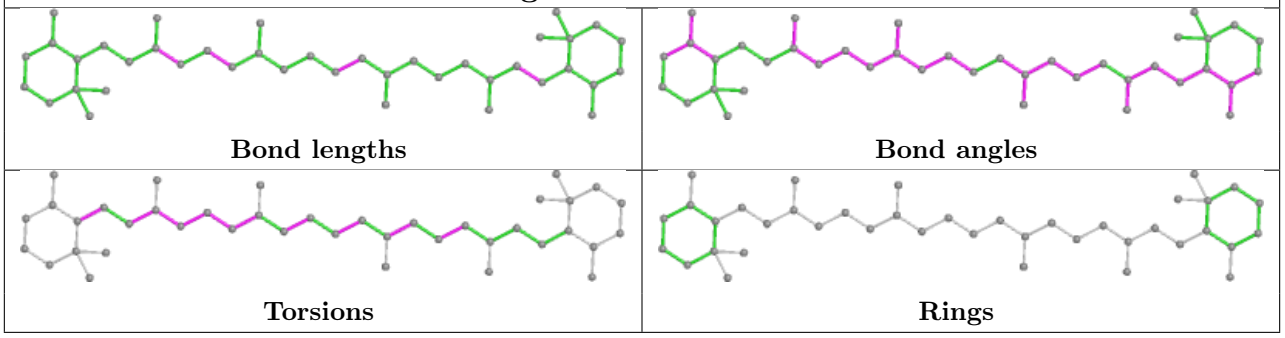


Torsions

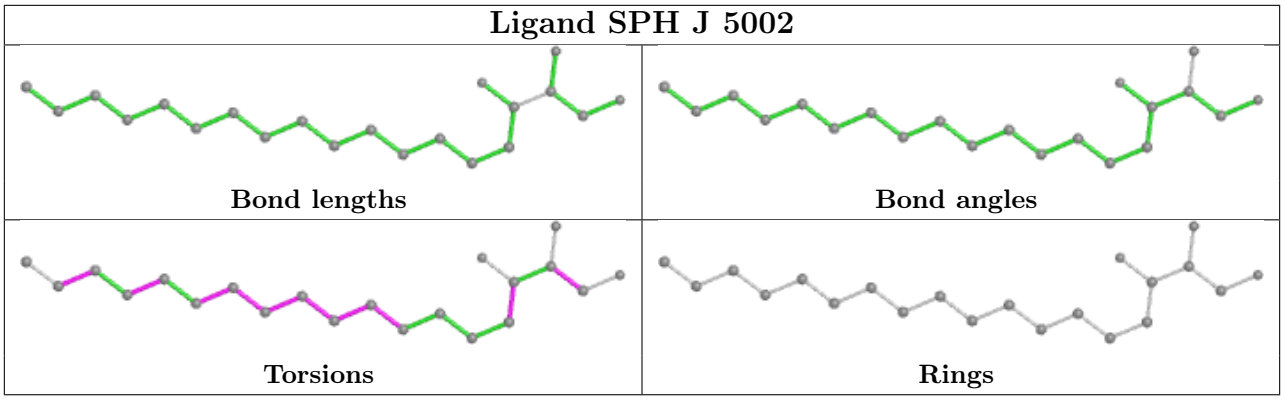


Rings

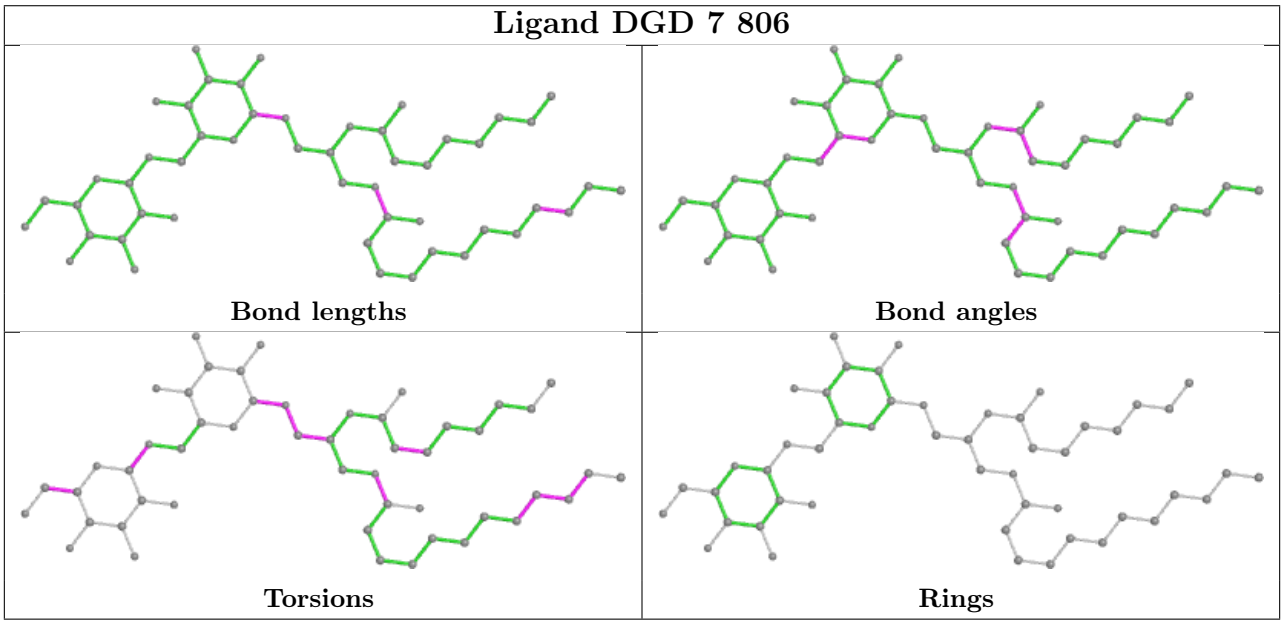
## Ligand BCR I 4001



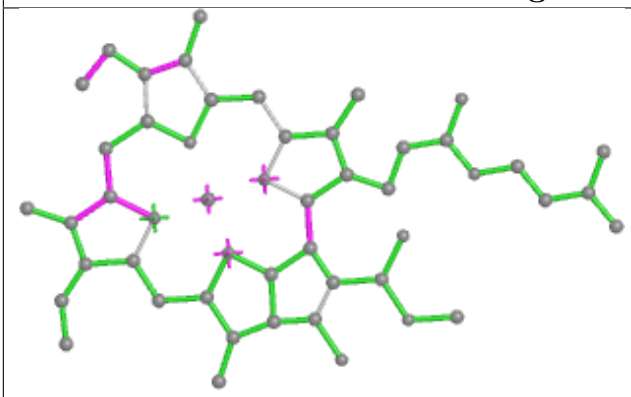

## Ligand SPH J 5002



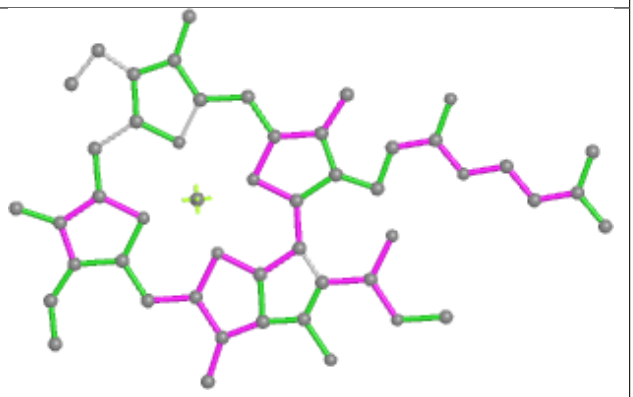

## Ligand DGD 7 806



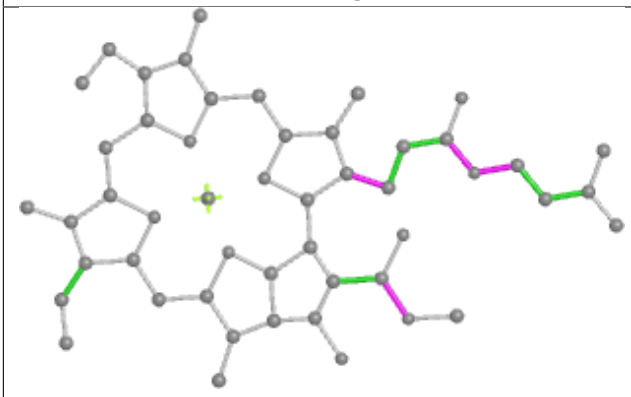
**Ligand CLA 4 616**



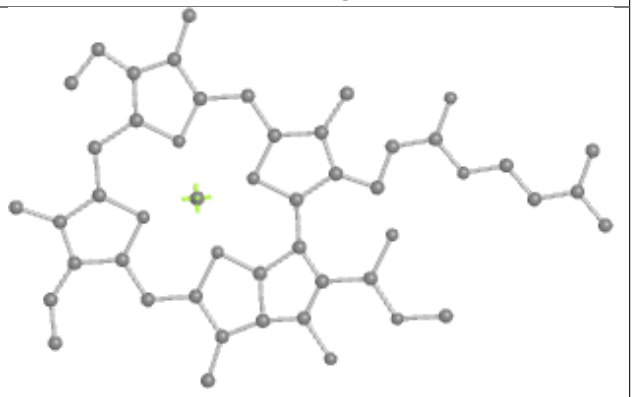
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

| Ligand CHL 6 613 | |
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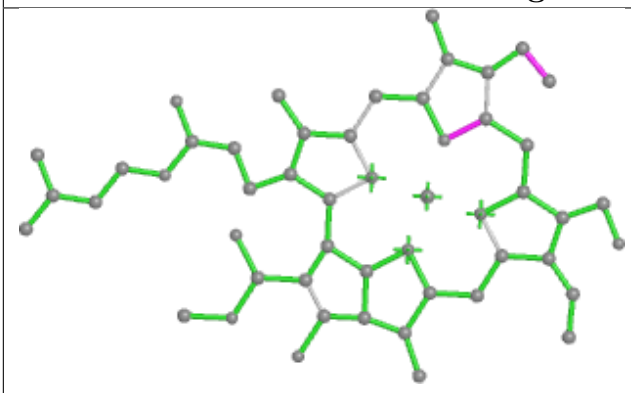
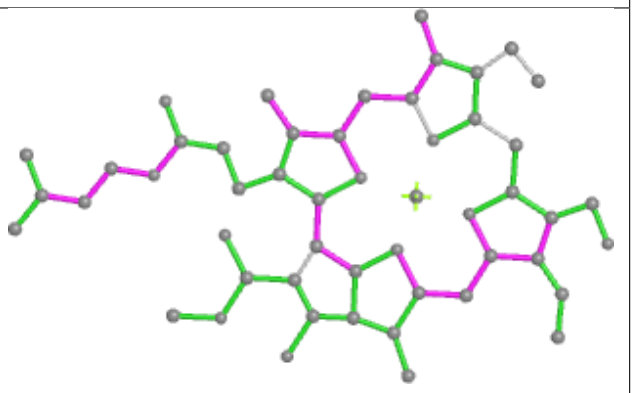
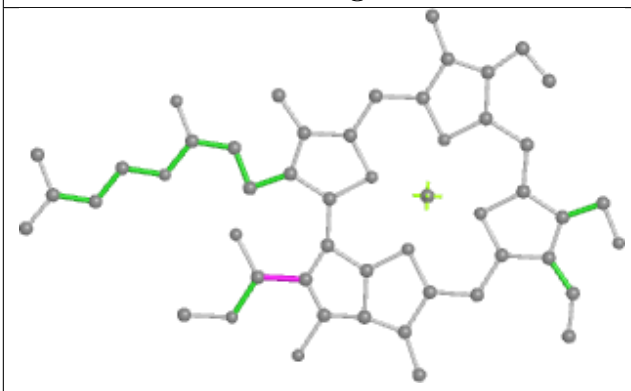
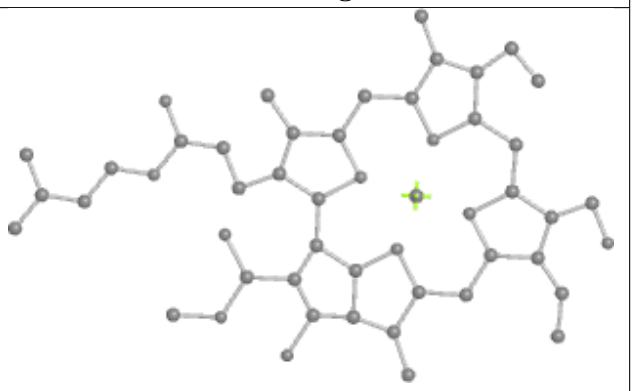
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

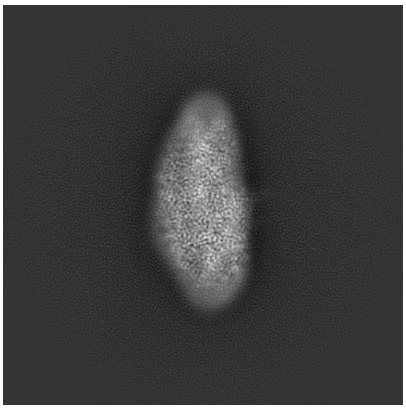
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11588. These allow visual inspection of the internal detail of the map and identification of artifacts.

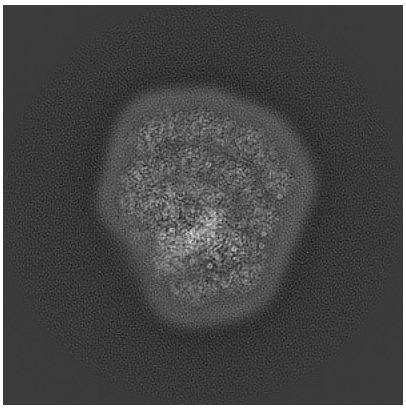
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

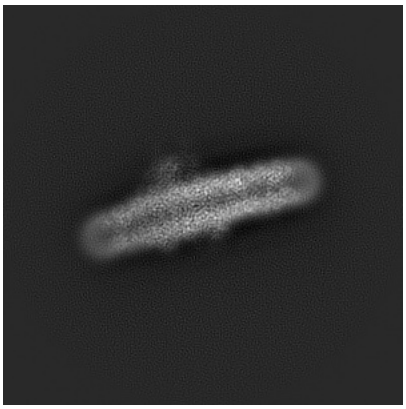
### 6.1.1 Primary map



X

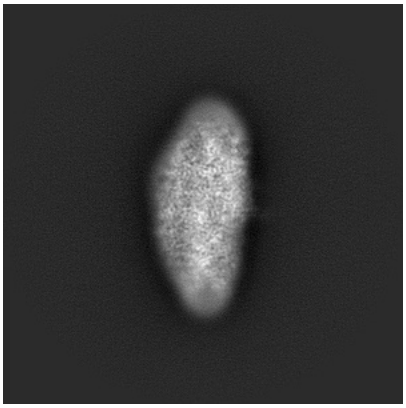


Y

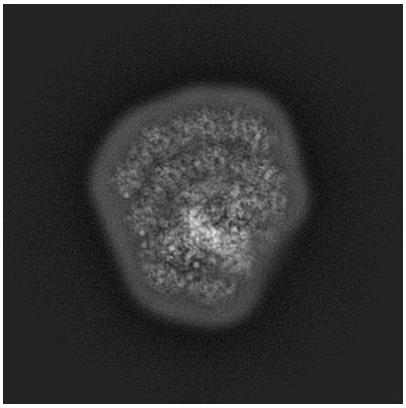


Z

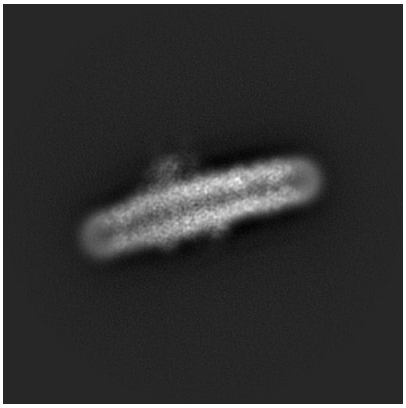
### 6.1.2 Raw map



X



Y

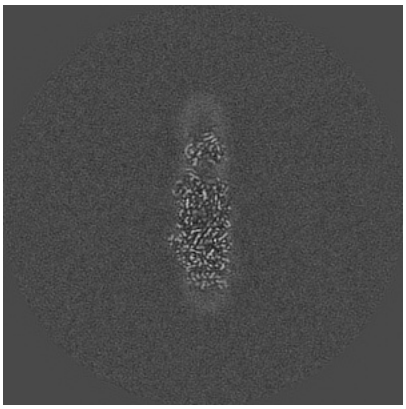


Z

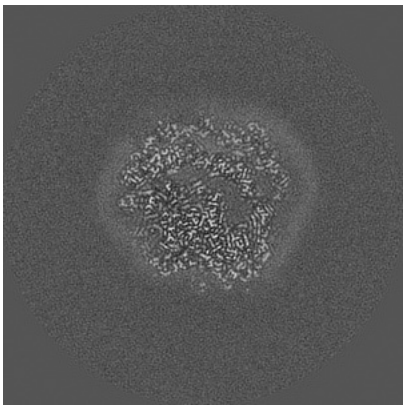
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

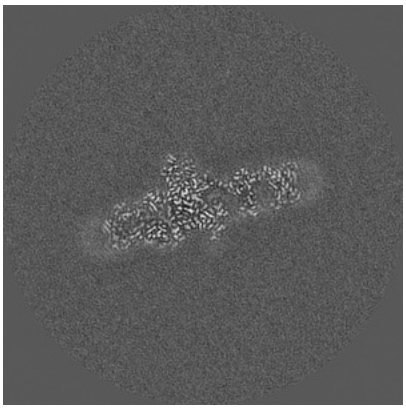
### 6.2.1 Primary map



X Index: 240

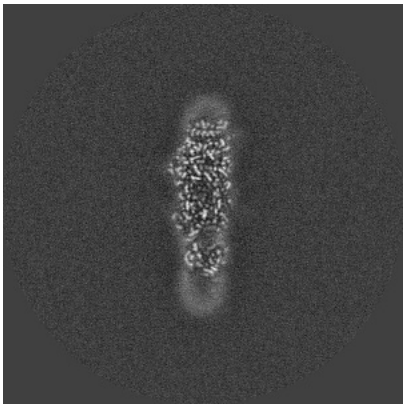


Y Index: 240

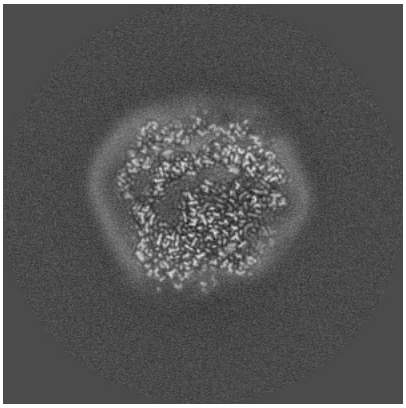


Z Index: 240

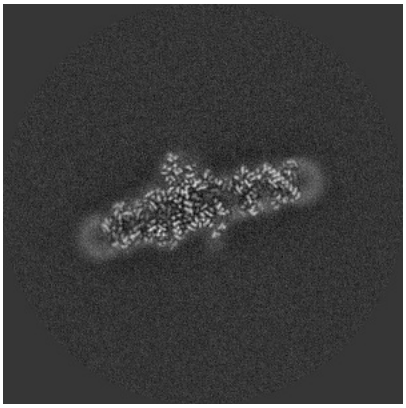
### 6.2.2 Raw map



X Index: 240



Y Index: 240

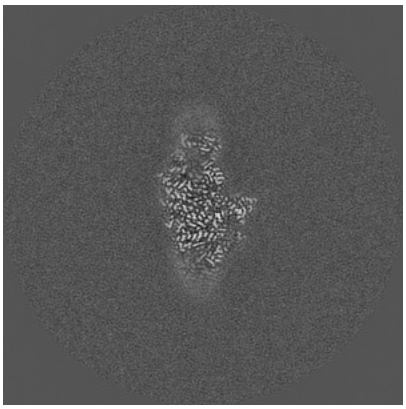


Z Index: 240

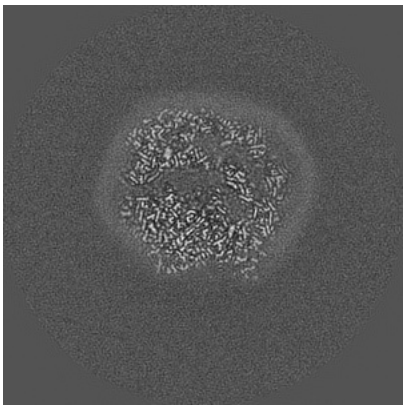
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

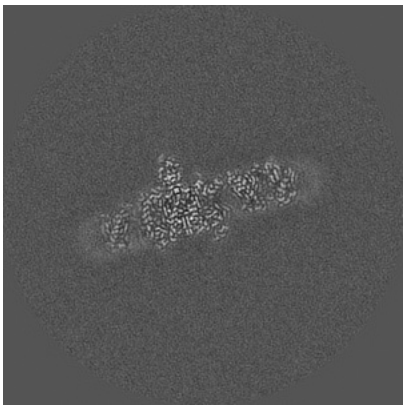
### 6.3.1 Primary map



X Index: 208

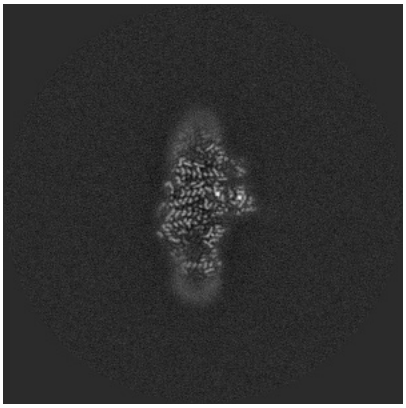


Y Index: 248

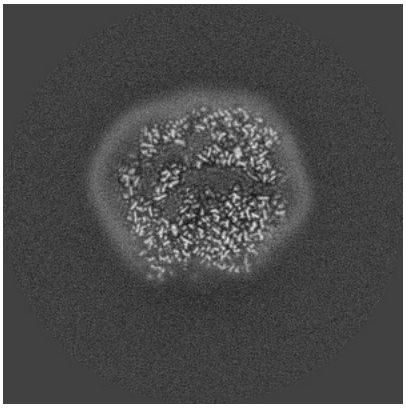


Z Index: 227

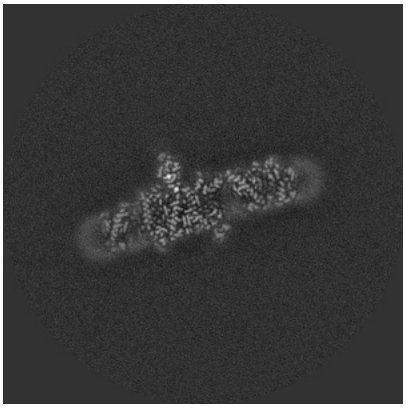
### 6.3.2 Raw map



X Index: 207



Y Index: 248

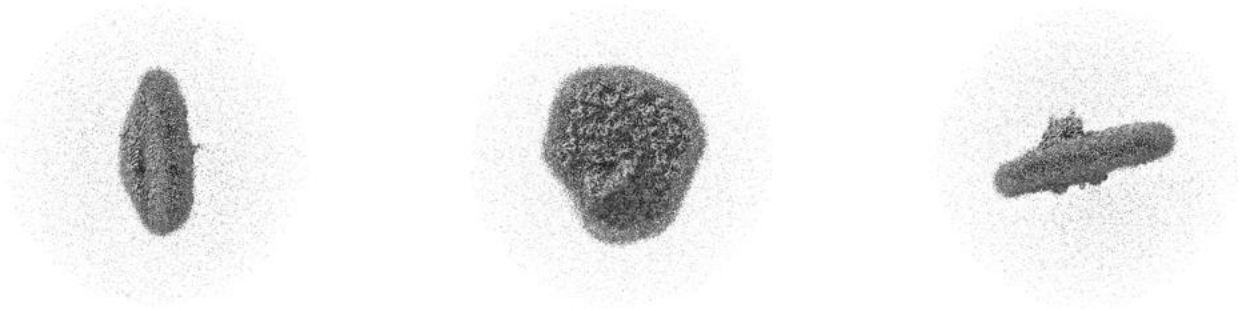


Z Index: 253

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

## 6.4 Orthogonal surface views (i)

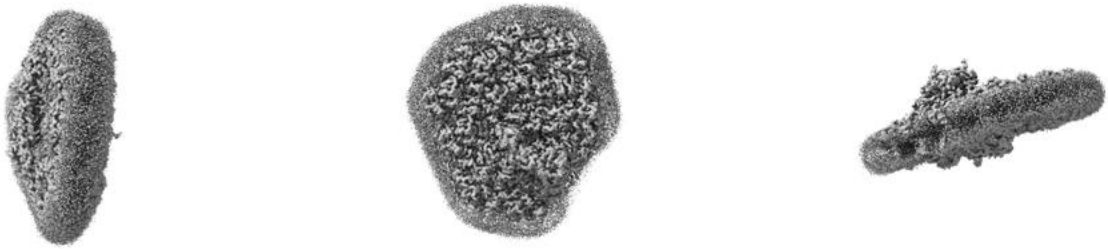
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



X Y Z

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

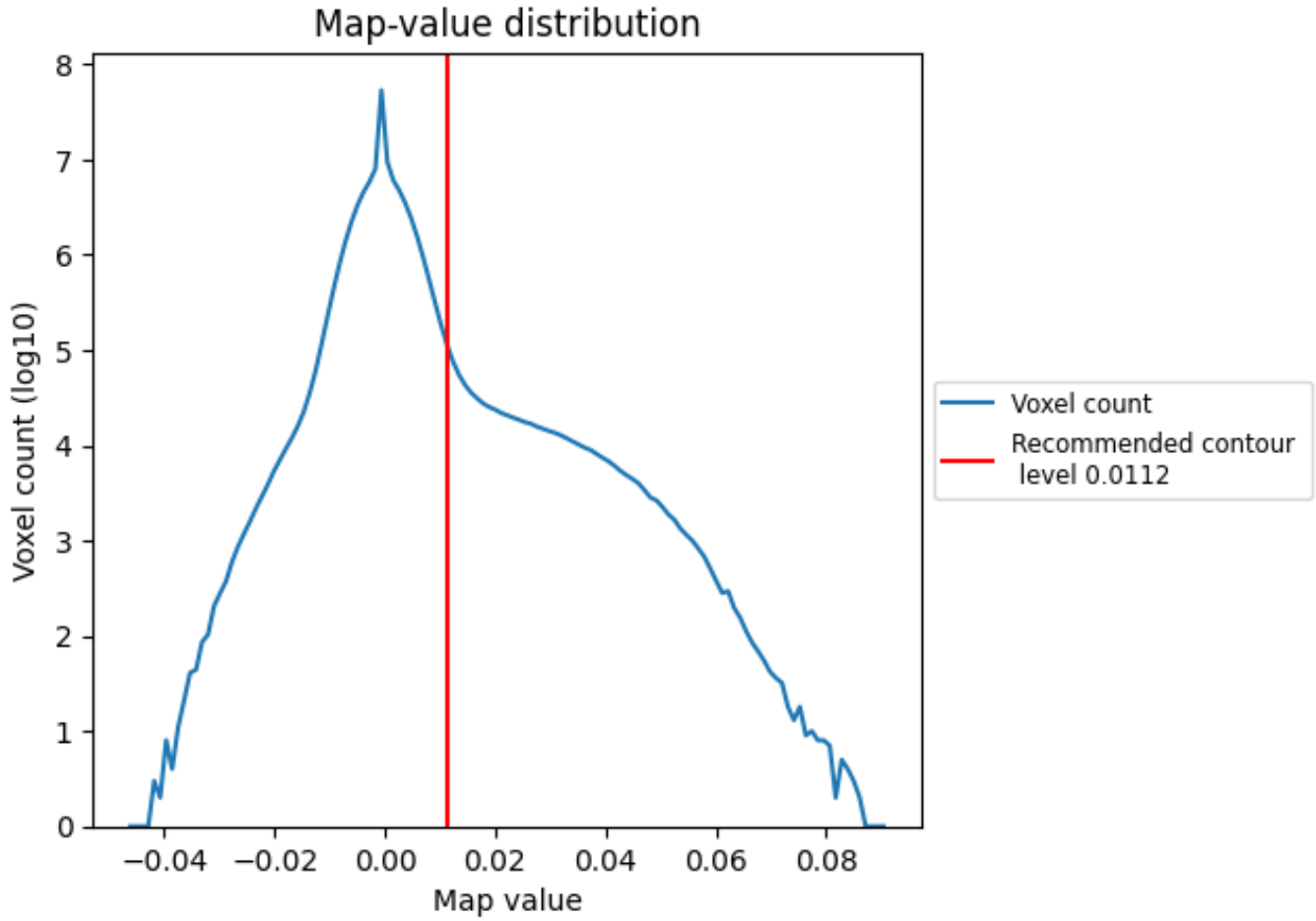
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

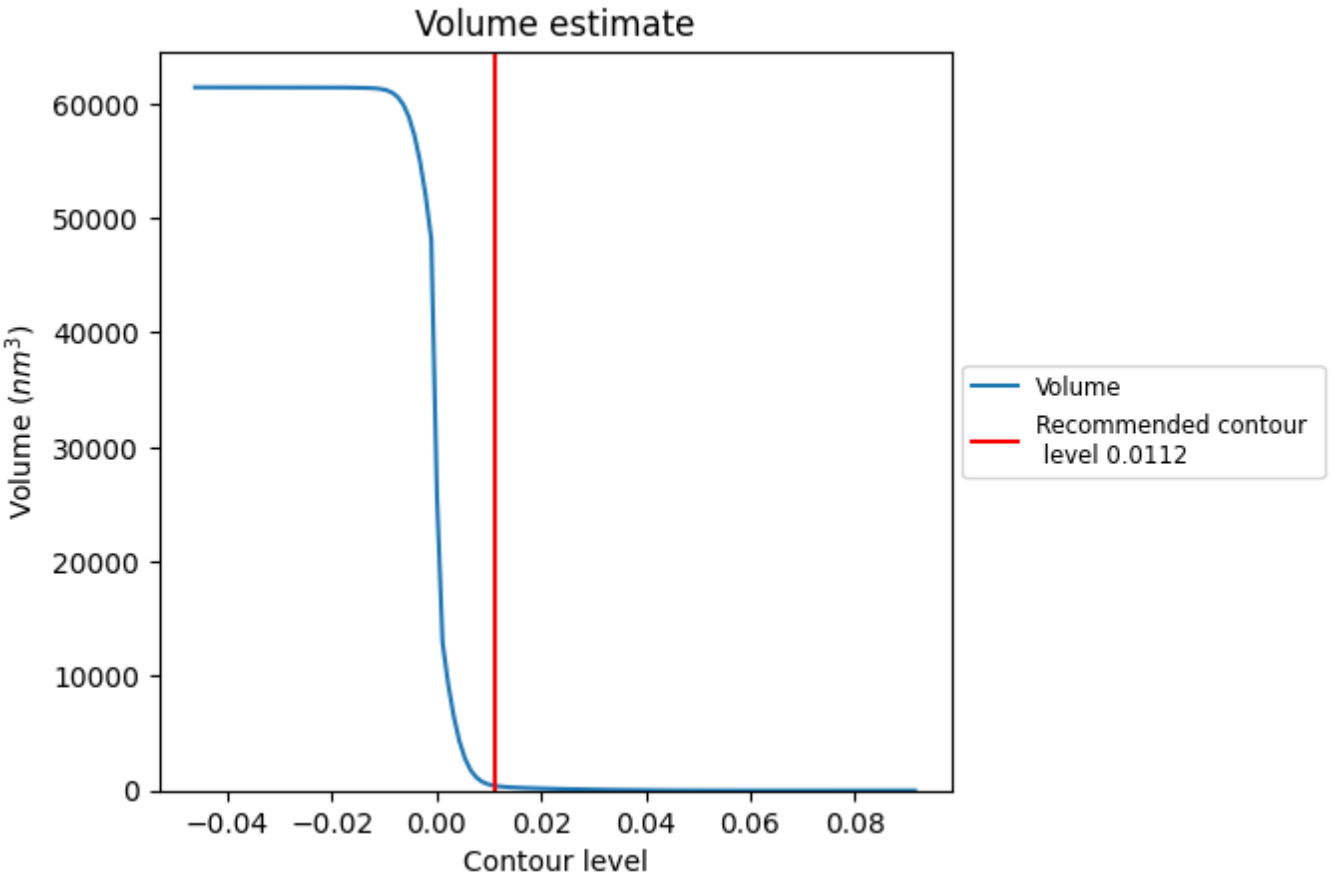
This section contains the results of statistical analysis of the map.

## 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.

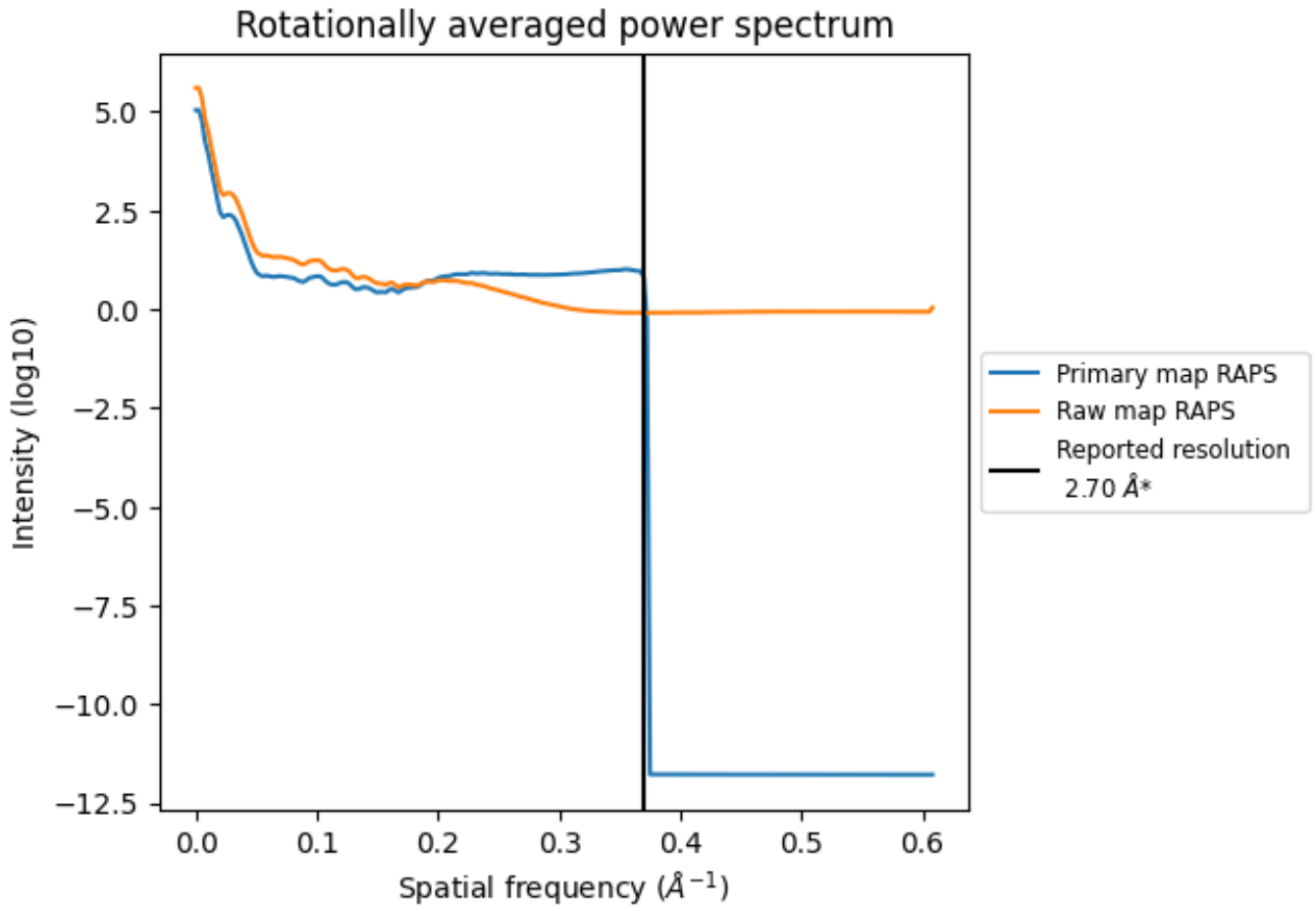
## 7.2 Volume estimate




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)

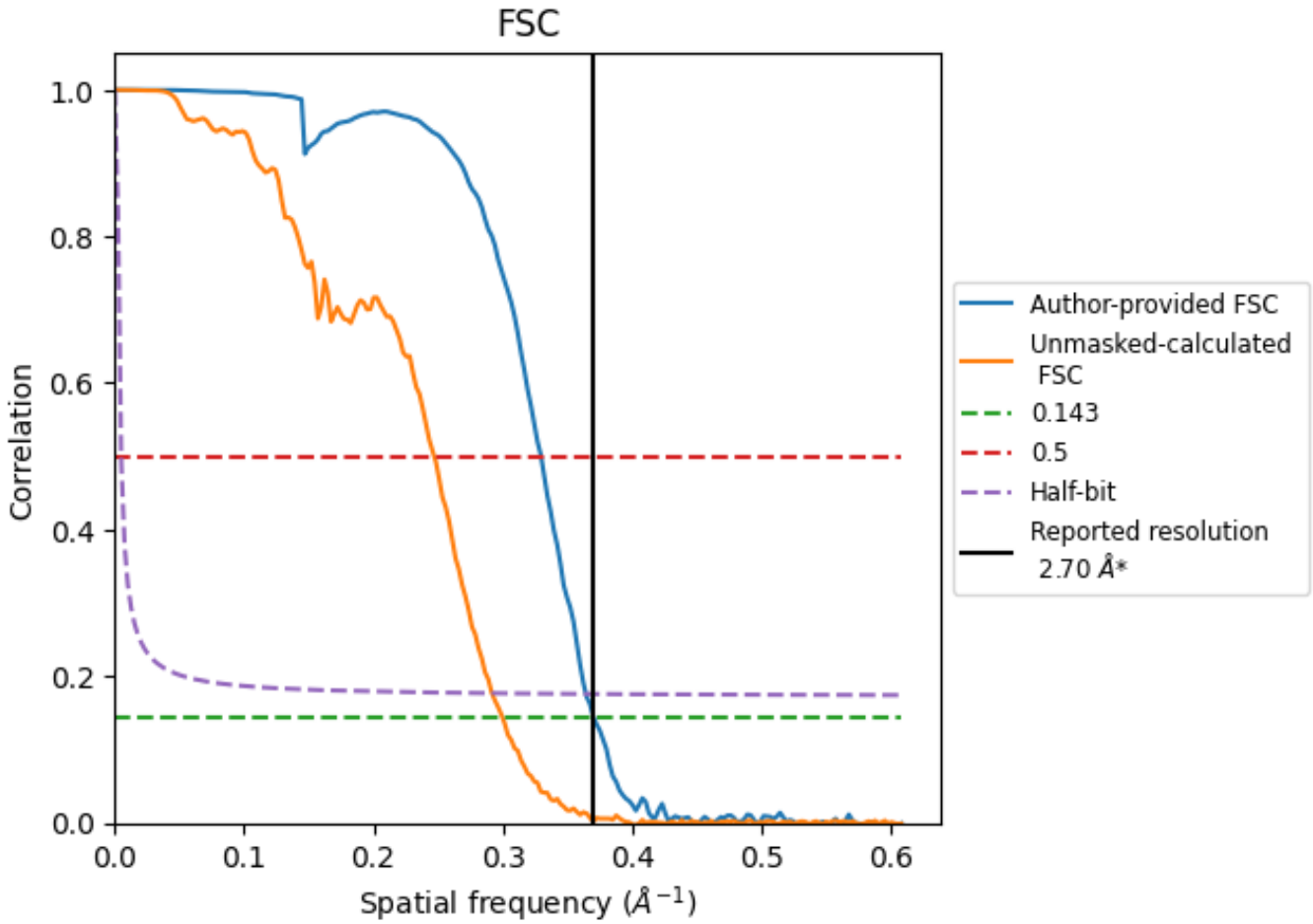



*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

# 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 0.370 Å$^{-1}$

## 8.2 Resolution estimates (i)

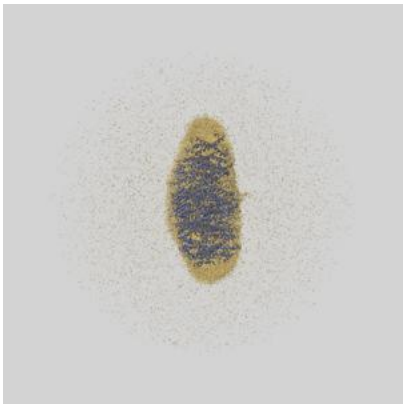
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.70 | - | - |
| Author-provided FSC curve | 2.70 | 3.03 | 2.74 |
| Unmasked-calculated* | 3.33 | 4.05 | 3.43 |

*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 3.33 differs from the reported value 2.7 by more than 10 %

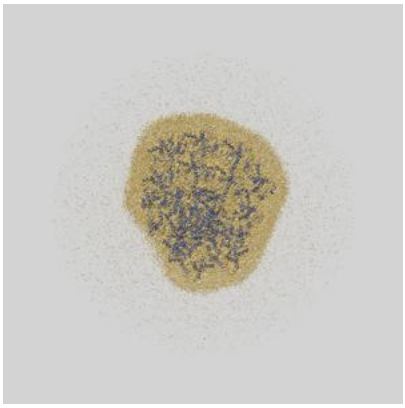
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11588 and PDB model 6ZZX. Per-residue inclusion information can be found in section 3 on page 55.

## 9.1 Map-model overlay



X

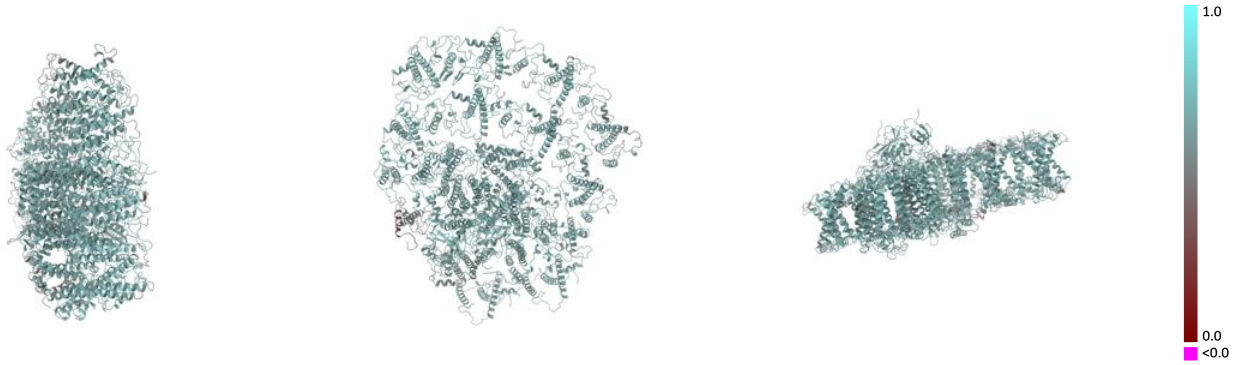


Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

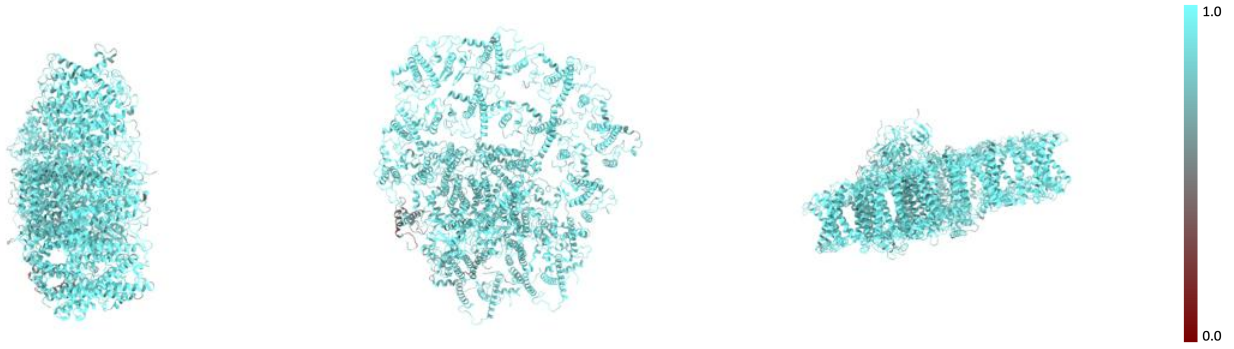
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

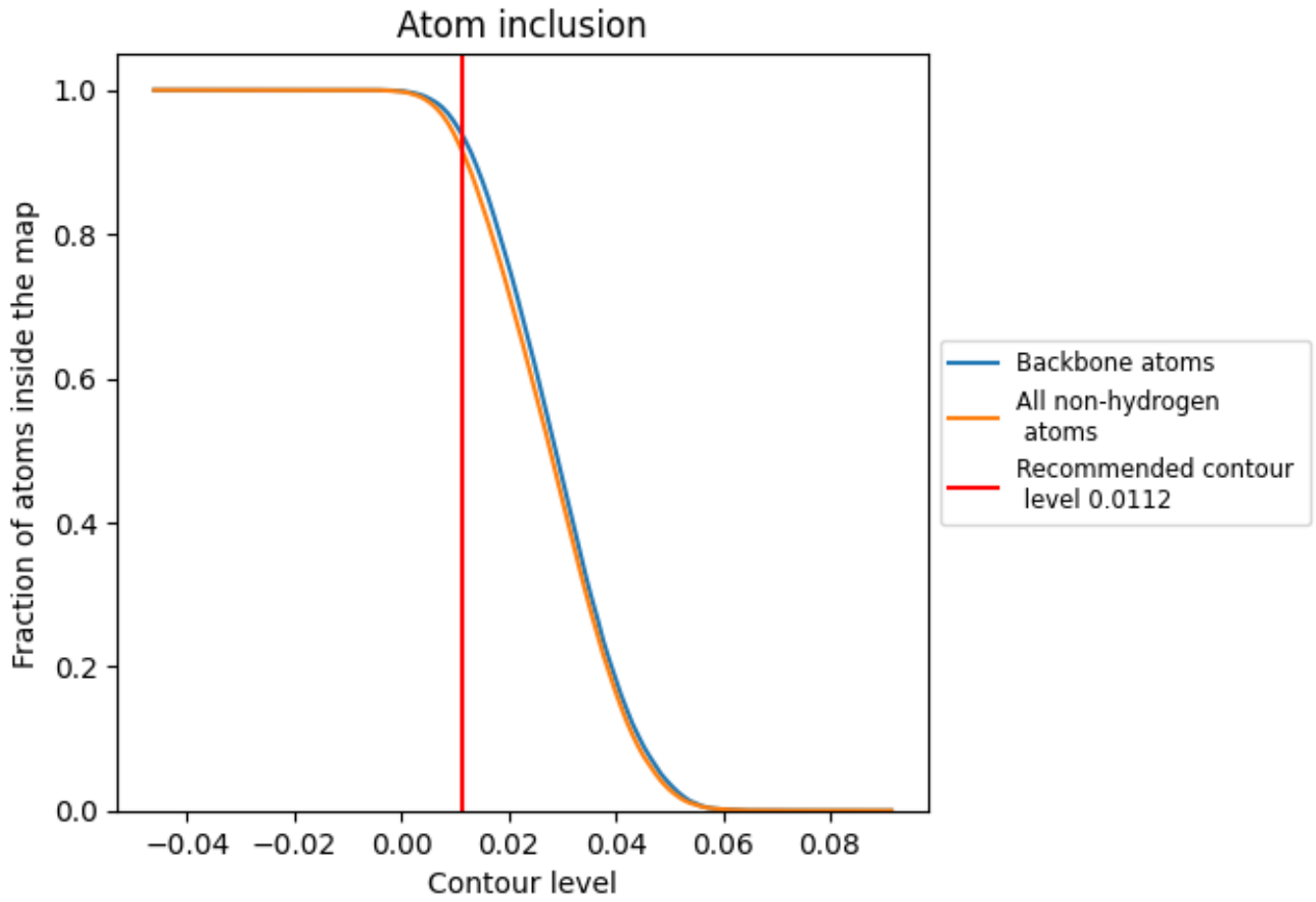
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0112).

## 9.4 Atom inclusion (i)




At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.0112) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9178 | 0.6210 |
| 1 | 0.9057 | 0.6130 |
| 2 | 0.8860 | 0.6000 |
| 3 | 0.9372 | 0.6350 |
| 4 | 0.8972 | 0.5980 |
| 5 | 0.9342 | 0.6190 |
| 6 | 0.9202 | 0.6190 |
| 7 | 0.9087 | 0.6200 |
| 8 | 0.9053 | 0.6190 |
| 9 | 0.9165 | 0.6190 |
| A | 0.9562 | 0.6480 |
| B | 0.9600 | 0.6500 |
| C | 0.9784 | 0.6530 |
| D | 0.9321 | 0.6250 |
| E | 0.9309 | 0.6160 |
| F | 0.9121 | 0.6210 |
| G | 0.8992 | 0.6170 |
| H | 0.7476 | 0.5440 |
| I | 0.9008 | 0.6100 |
| J | 0.9023 | 0.6260 |
| K | 0.8957 | 0.6010 |
| L | 0.8824 | 0.5930 |
| M | 0.9638 | 0.6330 |
| O | 0.5450 | 0.4140 |
| a | 0.8547 | 0.5770 |