



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 02:53 PM JST

PDB ID : 6KIF
EMDB ID : EMD-9994
Title : Structure of cyanobacterial photosystem I-IsiA-flavodoxin supercomplex
Authors : Cao, P.; Cao, D.F.; Si, L.; Su, X.D.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2019-07-18
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

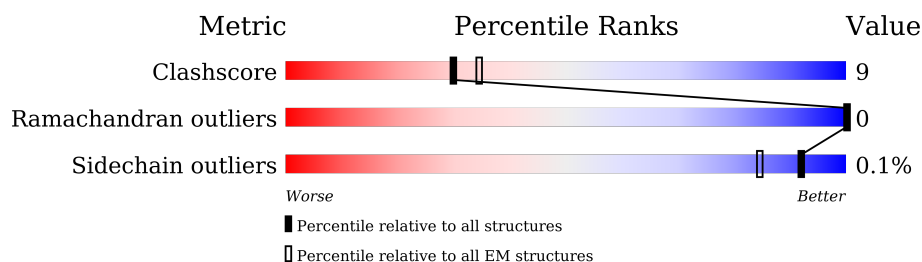
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 763 | 82% 16% . |
| 1 | G | 763 | 82% 16% . |
| 1 | e | 763 | 98% . |
| 2 | B | 734 | 82% 17% |
| 2 | H | 734 | 83% 17% |
| 2 | f | 734 | 100% |
| 3 | C | 81 | 80% 19% . |
| 3 | N | 81 | 79% 20% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | g | 81 | 99% |
| 4 | D | 141 | 81% 19% |
| 4 | O | 141 | 81% 19% |
| 4 | h | 141 | 100% |
| 5 | E | 75 | 11% 81% 13% 5% |
| 5 | Q | 75 | 12% 84% 11% 5% |
| 5 | i | 75 | 12% 95% 5% |
| 6 | F | 159 | 75% 11% 14% |
| 6 | R | 159 | 76% 9% 14% |
| 6 | j | 159 | 86% 14% |
| 7 | I | 38 | 8% 76% 24% |
| 7 | S | 38 | 5% 84% 16% |
| 7 | k | 38 | 8% 100% |
| 8 | J | 41 | 5% 80% 20% |
| 8 | T | 41 | 5% 80% 20% |
| 8 | l | 41 | 5% 100% |
| 9 | K | 84 | 19% 70% 23% 7% |
| 9 | U | 84 | 23% 69% 24% 7% |
| 9 | m | 84 | 15% 93% 7% |
| 10 | L | 166 | 80% 19% |
| 10 | V | 166 | 80% 19% |
| 10 | n | 166 | 99% |
| 11 | M | 29 | 79% 21% |
| 11 | W | 29 | 86% 14% |
| 11 | o | 29 | 100% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 12 | P | 172 | |
| 12 | X | 172 | |
| 12 | p | 172 | |
| 13 | 1 | 342 | |
| 13 | 2 | 342 | |
| 13 | 3 | 342 | |
| 13 | 4 | 342 | |
| 13 | 5 | 342 | |
| 13 | 6 | 342 | |
| 13 | Y | 342 | |
| 13 | Z | 342 | |
| 13 | a | 342 | |
| 13 | b | 342 | |
| 13 | c | 342 | |
| 13 | d | 342 | |
| 13 | q | 342 | |
| 13 | r | 342 | |
| 13 | s | 342 | |
| 13 | t | 342 | |
| 13 | u | 342 | |
| 13 | v | 342 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | 1 | 501 | X | - | - | - |
| 14 | CLA | 1 | 502 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | 1 | 503 | X | - | - | - |
| 14 | CLA | 1 | 504 | X | - | - | - |
| 14 | CLA | 1 | 505 | X | - | - | - |
| 14 | CLA | 1 | 506 | X | - | - | - |
| 14 | CLA | 1 | 507 | X | - | - | - |
| 14 | CLA | 1 | 508 | X | - | - | - |
| 14 | CLA | 1 | 509 | X | - | - | - |
| 14 | CLA | 1 | 510 | X | - | - | - |
| 14 | CLA | 1 | 511 | X | - | - | - |
| 14 | CLA | 1 | 512 | X | - | - | - |
| 14 | CLA | 1 | 513 | X | - | - | - |
| 14 | CLA | 1 | 516 | X | - | - | - |
| 14 | CLA | 1 | 517 | X | - | - | - |
| 14 | CLA | 1 | 518 | X | - | - | - |
| 14 | CLA | 1 | 519 | X | - | - | - |
| 14 | CLA | 2 | 501 | X | - | - | - |
| 14 | CLA | 2 | 502 | X | - | - | - |
| 14 | CLA | 2 | 503 | X | - | - | - |
| 14 | CLA | 2 | 504 | X | - | - | - |
| 14 | CLA | 2 | 505 | X | - | - | - |
| 14 | CLA | 2 | 506 | X | - | - | - |
| 14 | CLA | 2 | 507 | X | - | - | - |
| 14 | CLA | 2 | 508 | X | - | - | - |
| 14 | CLA | 2 | 509 | X | - | - | - |
| 14 | CLA | 2 | 510 | X | - | - | - |
| 14 | CLA | 2 | 511 | X | - | - | - |
| 14 | CLA | 2 | 512 | X | - | - | - |
| 14 | CLA | 2 | 513 | X | - | - | - |
| 14 | CLA | 2 | 518 | X | - | - | - |
| 14 | CLA | 2 | 519 | X | - | - | - |
| 14 | CLA | 3 | 501 | X | - | - | - |
| 14 | CLA | 3 | 502 | X | - | - | - |
| 14 | CLA | 3 | 503 | X | - | - | - |
| 14 | CLA | 3 | 504 | X | - | - | - |
| 14 | CLA | 3 | 505 | X | - | - | - |
| 14 | CLA | 3 | 506 | X | - | - | - |
| 14 | CLA | 3 | 507 | X | - | - | - |
| 14 | CLA | 3 | 508 | X | - | - | - |
| 14 | CLA | 3 | 509 | X | - | - | - |
| 14 | CLA | 3 | 510 | X | - | - | - |
| 14 | CLA | 3 | 511 | X | - | - | - |
| 14 | CLA | 3 | 512 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | 3 | 513 | X | - | - | - |
| 14 | CLA | 3 | 516 | X | - | - | - |
| 14 | CLA | 3 | 517 | X | - | - | - |
| 14 | CLA | 3 | 518 | X | - | - | - |
| 14 | CLA | 3 | 519 | X | - | - | - |
| 14 | CLA | 4 | 501 | X | - | - | - |
| 14 | CLA | 4 | 502 | X | - | - | - |
| 14 | CLA | 4 | 503 | X | - | - | - |
| 14 | CLA | 4 | 504 | X | - | - | - |
| 14 | CLA | 4 | 505 | X | - | - | - |
| 14 | CLA | 4 | 506 | X | - | - | - |
| 14 | CLA | 4 | 507 | X | - | - | - |
| 14 | CLA | 4 | 508 | X | - | - | - |
| 14 | CLA | 4 | 509 | X | - | - | - |
| 14 | CLA | 4 | 510 | X | - | - | - |
| 14 | CLA | 4 | 511 | X | - | - | - |
| 14 | CLA | 4 | 512 | X | - | - | - |
| 14 | CLA | 4 | 513 | X | - | - | - |
| 14 | CLA | 4 | 516 | X | - | - | - |
| 14 | CLA | 4 | 517 | X | - | - | - |
| 14 | CLA | 4 | 518 | X | - | - | - |
| 14 | CLA | 4 | 519 | X | - | - | - |
| 14 | CLA | 5 | 501 | X | - | - | - |
| 14 | CLA | 5 | 502 | X | - | - | - |
| 14 | CLA | 5 | 503 | X | - | - | - |
| 14 | CLA | 5 | 504 | X | - | - | - |
| 14 | CLA | 5 | 505 | X | - | - | - |
| 14 | CLA | 5 | 506 | X | - | - | - |
| 14 | CLA | 5 | 507 | X | - | - | - |
| 14 | CLA | 5 | 508 | X | - | - | - |
| 14 | CLA | 5 | 509 | X | - | - | - |
| 14 | CLA | 5 | 510 | X | - | - | - |
| 14 | CLA | 5 | 511 | X | - | - | - |
| 14 | CLA | 5 | 512 | X | - | - | - |
| 14 | CLA | 5 | 513 | X | - | - | - |
| 14 | CLA | 5 | 516 | X | - | - | - |
| 14 | CLA | 5 | 517 | X | - | - | - |
| 14 | CLA | 5 | 518 | X | - | - | - |
| 14 | CLA | 5 | 519 | X | - | - | - |
| 14 | CLA | 6 | 501 | X | - | - | - |
| 14 | CLA | 6 | 502 | X | - | - | - |
| 14 | CLA | 6 | 503 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | 6 | 504 | X | - | - | - |
| 14 | CLA | 6 | 505 | X | - | - | - |
| 14 | CLA | 6 | 506 | X | - | - | - |
| 14 | CLA | 6 | 507 | X | - | - | - |
| 14 | CLA | 6 | 508 | X | - | - | - |
| 14 | CLA | 6 | 509 | X | - | - | - |
| 14 | CLA | 6 | 510 | X | - | - | - |
| 14 | CLA | 6 | 511 | X | - | - | - |
| 14 | CLA | 6 | 512 | X | - | - | - |
| 14 | CLA | 6 | 513 | X | - | - | - |
| 14 | CLA | 6 | 516 | X | - | - | - |
| 14 | CLA | 6 | 517 | X | - | - | - |
| 14 | CLA | 6 | 518 | X | - | - | - |
| 14 | CLA | 6 | 519 | X | - | - | - |
| 14 | CLA | A | 1011 | X | - | - | - |
| 14 | CLA | A | 1013 | X | - | - | - |
| 14 | CLA | A | 1022 | X | - | - | - |
| 14 | CLA | A | 1101 | X | - | - | - |
| 14 | CLA | A | 1102 | X | - | - | - |
| 14 | CLA | A | 1103 | X | - | - | - |
| 14 | CLA | A | 1104 | X | - | - | - |
| 14 | CLA | A | 1105 | X | - | - | - |
| 14 | CLA | A | 1106 | X | - | - | - |
| 14 | CLA | A | 1107 | X | - | - | - |
| 14 | CLA | A | 1108 | X | - | - | - |
| 14 | CLA | A | 1109 | X | - | - | - |
| 14 | CLA | A | 1110 | X | - | - | - |
| 14 | CLA | A | 1111 | X | - | - | - |
| 14 | CLA | A | 1112 | X | - | - | - |
| 14 | CLA | A | 1113 | X | - | - | - |
| 14 | CLA | A | 1114 | X | - | - | - |
| 14 | CLA | A | 1115 | X | - | - | - |
| 14 | CLA | A | 1116 | X | - | - | - |
| 14 | CLA | A | 1117 | X | - | - | - |
| 14 | CLA | A | 1118 | X | - | - | - |
| 14 | CLA | A | 1119 | X | - | - | - |
| 14 | CLA | A | 1120 | X | - | - | - |
| 14 | CLA | A | 1121 | X | - | - | - |
| 14 | CLA | A | 1122 | X | - | - | - |
| 14 | CLA | A | 1123 | X | - | - | - |
| 14 | CLA | A | 1124 | X | - | - | - |
| 14 | CLA | A | 1125 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | A | 1126 | X | - | - | - |
| 14 | CLA | A | 1127 | X | - | - | - |
| 14 | CLA | A | 1128 | X | - | - | - |
| 14 | CLA | A | 1129 | X | - | - | - |
| 14 | CLA | A | 1130 | X | - | - | - |
| 14 | CLA | A | 1131 | X | - | - | - |
| 14 | CLA | A | 1132 | X | - | - | - |
| 14 | CLA | A | 1133 | X | - | - | - |
| 14 | CLA | A | 1134 | X | - | - | - |
| 14 | CLA | A | 1135 | X | - | - | - |
| 14 | CLA | A | 1136 | X | - | - | - |
| 14 | CLA | A | 1137 | X | - | - | - |
| 14 | CLA | A | 1138 | X | - | - | - |
| 14 | CLA | A | 1139 | X | - | - | - |
| 14 | CLA | A | 1140 | X | - | - | - |
| 14 | CLA | A | 1237 | X | - | - | - |
| 14 | CLA | A | 1801 | X | - | - | - |
| 14 | CLA | B | 1012 | X | - | - | - |
| 14 | CLA | B | 1021 | X | - | - | - |
| 14 | CLA | B | 1023 | X | - | - | - |
| 14 | CLA | B | 1201 | X | - | - | - |
| 14 | CLA | B | 1202 | X | - | - | - |
| 14 | CLA | B | 1203 | X | - | - | - |
| 14 | CLA | B | 1204 | X | - | - | - |
| 14 | CLA | B | 1205 | X | - | - | - |
| 14 | CLA | B | 1206 | X | - | - | - |
| 14 | CLA | B | 1207 | X | - | - | - |
| 14 | CLA | B | 1208 | X | - | - | - |
| 14 | CLA | B | 1209 | X | - | - | - |
| 14 | CLA | B | 1210 | X | - | - | - |
| 14 | CLA | B | 1211 | X | - | - | - |
| 14 | CLA | B | 1212 | X | - | - | - |
| 14 | CLA | B | 1213 | X | - | - | - |
| 14 | CLA | B | 1214 | X | - | - | - |
| 14 | CLA | B | 1215 | X | - | - | - |
| 14 | CLA | B | 1216 | X | - | - | - |
| 14 | CLA | B | 1217 | X | - | - | - |
| 14 | CLA | B | 1218 | X | - | - | - |
| 14 | CLA | B | 1219 | X | - | - | - |
| 14 | CLA | B | 1220 | X | - | - | - |
| 14 | CLA | B | 1221 | X | - | - | - |
| 14 | CLA | B | 1222 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | B | 1223 | X | - | - | - |
| 14 | CLA | B | 1224 | X | - | - | - |
| 14 | CLA | B | 1225 | X | - | - | - |
| 14 | CLA | B | 1226 | X | - | - | - |
| 14 | CLA | B | 1227 | X | - | - | - |
| 14 | CLA | B | 1228 | X | - | - | - |
| 14 | CLA | B | 1229 | X | - | - | - |
| 14 | CLA | B | 1230 | X | - | - | - |
| 14 | CLA | B | 1231 | X | - | - | - |
| 14 | CLA | B | 1232 | X | - | - | - |
| 14 | CLA | B | 1234 | X | - | - | - |
| 14 | CLA | B | 1235 | X | - | - | - |
| 14 | CLA | B | 1236 | X | - | - | - |
| 14 | CLA | B | 1238 | X | - | - | - |
| 14 | CLA | B | 1239 | X | - | - | - |
| 14 | CLA | B | 1240 | X | - | - | - |
| 14 | CLA | F | 1301 | X | - | - | - |
| 14 | CLA | F | 1302 | X | - | - | - |
| 14 | CLA | G | 1011 | X | - | - | - |
| 14 | CLA | G | 1013 | X | - | - | - |
| 14 | CLA | G | 1022 | X | - | - | - |
| 14 | CLA | G | 1101 | X | - | - | - |
| 14 | CLA | G | 1102 | X | - | - | - |
| 14 | CLA | G | 1103 | X | - | - | - |
| 14 | CLA | G | 1104 | X | - | - | - |
| 14 | CLA | G | 1105 | X | - | - | - |
| 14 | CLA | G | 1106 | X | - | - | - |
| 14 | CLA | G | 1107 | X | - | - | - |
| 14 | CLA | G | 1108 | X | - | - | - |
| 14 | CLA | G | 1109 | X | - | - | - |
| 14 | CLA | G | 1110 | X | - | - | - |
| 14 | CLA | G | 1111 | X | - | - | - |
| 14 | CLA | G | 1112 | X | - | - | - |
| 14 | CLA | G | 1113 | X | - | - | - |
| 14 | CLA | G | 1114 | X | - | - | - |
| 14 | CLA | G | 1115 | X | - | - | - |
| 14 | CLA | G | 1116 | X | - | - | - |
| 14 | CLA | G | 1117 | X | - | - | - |
| 14 | CLA | G | 1118 | X | - | - | - |
| 14 | CLA | G | 1119 | X | - | - | - |
| 14 | CLA | G | 1120 | X | - | - | - |
| 14 | CLA | G | 1121 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | G | 1122 | X | - | - | - |
| 14 | CLA | G | 1123 | X | - | - | - |
| 14 | CLA | G | 1124 | X | - | - | - |
| 14 | CLA | G | 1125 | X | - | - | - |
| 14 | CLA | G | 1126 | X | - | - | - |
| 14 | CLA | G | 1127 | X | - | - | - |
| 14 | CLA | G | 1128 | X | - | - | - |
| 14 | CLA | G | 1129 | X | - | - | - |
| 14 | CLA | G | 1130 | X | - | - | - |
| 14 | CLA | G | 1131 | X | - | - | - |
| 14 | CLA | G | 1132 | X | - | - | - |
| 14 | CLA | G | 1133 | X | - | - | - |
| 14 | CLA | G | 1134 | X | - | - | - |
| 14 | CLA | G | 1135 | X | - | - | - |
| 14 | CLA | G | 1136 | X | - | - | - |
| 14 | CLA | G | 1137 | X | - | - | - |
| 14 | CLA | G | 1138 | X | - | - | - |
| 14 | CLA | G | 1139 | X | - | - | - |
| 14 | CLA | G | 1140 | X | - | - | - |
| 14 | CLA | G | 1237 | X | - | - | - |
| 14 | CLA | G | 1801 | X | - | - | - |
| 14 | CLA | H | 1012 | X | - | - | - |
| 14 | CLA | H | 1021 | X | - | - | - |
| 14 | CLA | H | 1023 | X | - | - | - |
| 14 | CLA | H | 1201 | X | - | - | - |
| 14 | CLA | H | 1202 | X | - | - | - |
| 14 | CLA | H | 1203 | X | - | - | - |
| 14 | CLA | H | 1204 | X | - | - | - |
| 14 | CLA | H | 1205 | X | - | - | - |
| 14 | CLA | H | 1206 | X | - | - | - |
| 14 | CLA | H | 1207 | X | - | - | - |
| 14 | CLA | H | 1208 | X | - | - | - |
| 14 | CLA | H | 1209 | X | - | - | - |
| 14 | CLA | H | 1210 | X | - | - | - |
| 14 | CLA | H | 1211 | X | - | - | - |
| 14 | CLA | H | 1212 | X | - | - | - |
| 14 | CLA | H | 1213 | X | - | - | - |
| 14 | CLA | H | 1214 | X | - | - | - |
| 14 | CLA | H | 1215 | X | - | - | - |
| 14 | CLA | H | 1216 | X | - | - | - |
| 14 | CLA | H | 1217 | X | - | - | - |
| 14 | CLA | H | 1218 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | H | 1219 | X | - | - | - |
| 14 | CLA | H | 1220 | X | - | - | - |
| 14 | CLA | H | 1221 | X | - | - | - |
| 14 | CLA | H | 1222 | X | - | - | - |
| 14 | CLA | H | 1223 | X | - | - | - |
| 14 | CLA | H | 1224 | X | - | - | - |
| 14 | CLA | H | 1225 | X | - | - | - |
| 14 | CLA | H | 1226 | X | - | - | - |
| 14 | CLA | H | 1227 | X | - | - | - |
| 14 | CLA | H | 1228 | X | - | - | - |
| 14 | CLA | H | 1229 | X | - | - | - |
| 14 | CLA | H | 1230 | X | - | - | - |
| 14 | CLA | H | 1231 | X | - | - | - |
| 14 | CLA | H | 1232 | X | - | - | - |
| 14 | CLA | H | 1234 | X | - | - | - |
| 14 | CLA | H | 1235 | X | - | - | - |
| 14 | CLA | H | 1236 | X | - | - | - |
| 14 | CLA | H | 1238 | X | - | - | - |
| 14 | CLA | H | 1239 | X | - | - | - |
| 14 | CLA | H | 1240 | X | - | - | - |
| 14 | CLA | J | 1302 | X | - | - | - |
| 14 | CLA | J | 1303 | X | - | - | - |
| 14 | CLA | K | 1103 | X | - | - | - |
| 14 | CLA | K | 1105 | X | - | - | - |
| 14 | CLA | K | 1401 | X | - | - | - |
| 14 | CLA | L | 1501 | X | - | - | - |
| 14 | CLA | L | 1502 | X | - | - | - |
| 14 | CLA | L | 1503 | X | - | - | - |
| 14 | CLA | R | 1301 | X | - | - | - |
| 14 | CLA | R | 1302 | X | - | - | - |
| 14 | CLA | T | 1302 | X | - | - | - |
| 14 | CLA | T | 1303 | X | - | - | - |
| 14 | CLA | U | 1103 | X | - | - | - |
| 14 | CLA | U | 1105 | X | - | - | - |
| 14 | CLA | U | 1401 | X | - | - | - |
| 14 | CLA | V | 1501 | X | - | - | - |
| 14 | CLA | V | 1502 | X | - | - | - |
| 14 | CLA | V | 1503 | X | - | - | - |
| 14 | CLA | Y | 501 | X | - | - | - |
| 14 | CLA | Y | 502 | X | - | - | - |
| 14 | CLA | Y | 503 | X | - | - | - |
| 14 | CLA | Y | 504 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | Y | 505 | X | - | - | - |
| 14 | CLA | Y | 506 | X | - | - | - |
| 14 | CLA | Y | 507 | X | - | - | - |
| 14 | CLA | Y | 508 | X | - | - | - |
| 14 | CLA | Y | 509 | X | - | - | - |
| 14 | CLA | Y | 510 | X | - | - | - |
| 14 | CLA | Y | 511 | X | - | - | - |
| 14 | CLA | Y | 512 | X | - | - | - |
| 14 | CLA | Y | 513 | X | - | - | - |
| 14 | CLA | Y | 516 | X | - | - | - |
| 14 | CLA | Y | 517 | X | - | - | - |
| 14 | CLA | Y | 518 | X | - | - | - |
| 14 | CLA | Y | 519 | X | - | - | - |
| 14 | CLA | Z | 501 | X | - | - | - |
| 14 | CLA | Z | 502 | X | - | - | - |
| 14 | CLA | Z | 503 | X | - | - | - |
| 14 | CLA | Z | 504 | X | - | - | - |
| 14 | CLA | Z | 505 | X | - | - | - |
| 14 | CLA | Z | 506 | X | - | - | - |
| 14 | CLA | Z | 507 | X | - | - | - |
| 14 | CLA | Z | 508 | X | - | - | - |
| 14 | CLA | Z | 509 | X | - | - | - |
| 14 | CLA | Z | 510 | X | - | - | - |
| 14 | CLA | Z | 511 | X | - | - | - |
| 14 | CLA | Z | 512 | X | - | - | - |
| 14 | CLA | Z | 513 | X | - | - | - |
| 14 | CLA | Z | 518 | X | - | - | - |
| 14 | CLA | Z | 519 | X | - | - | - |
| 14 | CLA | a | 501 | X | - | - | - |
| 14 | CLA | a | 502 | X | - | - | - |
| 14 | CLA | a | 503 | X | - | - | - |
| 14 | CLA | a | 504 | X | - | - | - |
| 14 | CLA | a | 505 | X | - | - | - |
| 14 | CLA | a | 506 | X | - | - | - |
| 14 | CLA | a | 507 | X | - | - | - |
| 14 | CLA | a | 508 | X | - | - | - |
| 14 | CLA | a | 509 | X | - | - | - |
| 14 | CLA | a | 510 | X | - | - | - |
| 14 | CLA | a | 511 | X | - | - | - |
| 14 | CLA | a | 512 | X | - | - | - |
| 14 | CLA | a | 513 | X | - | - | - |
| 14 | CLA | a | 516 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | a | 517 | X | - | - | - |
| 14 | CLA | a | 518 | X | - | - | - |
| 14 | CLA | a | 519 | X | - | - | - |
| 14 | CLA | b | 501 | X | - | - | - |
| 14 | CLA | b | 502 | X | - | - | - |
| 14 | CLA | b | 503 | X | - | - | - |
| 14 | CLA | b | 504 | X | - | - | - |
| 14 | CLA | b | 505 | X | - | - | - |
| 14 | CLA | b | 506 | X | - | - | - |
| 14 | CLA | b | 507 | X | - | - | - |
| 14 | CLA | b | 508 | X | - | - | - |
| 14 | CLA | b | 509 | X | - | - | - |
| 14 | CLA | b | 510 | X | - | - | - |
| 14 | CLA | b | 511 | X | - | - | - |
| 14 | CLA | b | 512 | X | - | - | - |
| 14 | CLA | b | 513 | X | - | - | - |
| 14 | CLA | b | 516 | X | - | - | - |
| 14 | CLA | b | 517 | X | - | - | - |
| 14 | CLA | b | 518 | X | - | - | - |
| 14 | CLA | b | 519 | X | - | - | - |
| 14 | CLA | c | 501 | X | - | - | - |
| 14 | CLA | c | 502 | X | - | - | - |
| 14 | CLA | c | 503 | X | - | - | - |
| 14 | CLA | c | 504 | X | - | - | - |
| 14 | CLA | c | 505 | X | - | - | - |
| 14 | CLA | c | 506 | X | - | - | - |
| 14 | CLA | c | 507 | X | - | - | - |
| 14 | CLA | c | 508 | X | - | - | - |
| 14 | CLA | c | 509 | X | - | - | - |
| 14 | CLA | c | 510 | X | - | - | - |
| 14 | CLA | c | 511 | X | - | - | - |
| 14 | CLA | c | 512 | X | - | - | - |
| 14 | CLA | c | 513 | X | - | - | - |
| 14 | CLA | c | 516 | X | - | - | - |
| 14 | CLA | c | 517 | X | - | - | - |
| 14 | CLA | c | 518 | X | - | - | - |
| 14 | CLA | c | 519 | X | - | - | - |
| 14 | CLA | d | 501 | X | - | - | - |
| 14 | CLA | d | 502 | X | - | - | - |
| 14 | CLA | d | 503 | X | - | - | - |
| 14 | CLA | d | 504 | X | - | - | - |
| 14 | CLA | d | 505 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | d | 506 | X | - | - | - |
| 14 | CLA | d | 507 | X | - | - | - |
| 14 | CLA | d | 508 | X | - | - | - |
| 14 | CLA | d | 509 | X | - | - | - |
| 14 | CLA | d | 510 | X | - | - | - |
| 14 | CLA | d | 511 | X | - | - | - |
| 14 | CLA | d | 512 | X | - | - | - |
| 14 | CLA | d | 513 | X | - | - | - |
| 14 | CLA | d | 516 | X | - | - | - |
| 14 | CLA | d | 517 | X | - | - | - |
| 14 | CLA | d | 518 | X | - | - | - |
| 14 | CLA | d | 519 | X | - | - | - |
| 14 | CLA | e | 1011 | X | - | - | - |
| 14 | CLA | e | 1013 | X | - | - | - |
| 14 | CLA | e | 1022 | X | - | - | - |
| 14 | CLA | e | 1101 | X | - | - | - |
| 14 | CLA | e | 1102 | X | - | - | - |
| 14 | CLA | e | 1103 | X | - | - | - |
| 14 | CLA | e | 1104 | X | - | - | - |
| 14 | CLA | e | 1105 | X | - | - | - |
| 14 | CLA | e | 1106 | X | - | - | - |
| 14 | CLA | e | 1107 | X | - | - | - |
| 14 | CLA | e | 1108 | X | - | - | - |
| 14 | CLA | e | 1109 | X | - | - | - |
| 14 | CLA | e | 1110 | X | - | - | - |
| 14 | CLA | e | 1111 | X | - | - | - |
| 14 | CLA | e | 1112 | X | - | - | - |
| 14 | CLA | e | 1113 | X | - | - | - |
| 14 | CLA | e | 1114 | X | - | - | - |
| 14 | CLA | e | 1115 | X | - | - | - |
| 14 | CLA | e | 1116 | X | - | - | - |
| 14 | CLA | e | 1117 | X | - | - | - |
| 14 | CLA | e | 1118 | X | - | - | - |
| 14 | CLA | e | 1119 | X | - | - | - |
| 14 | CLA | e | 1120 | X | - | - | - |
| 14 | CLA | e | 1121 | X | - | - | - |
| 14 | CLA | e | 1122 | X | - | - | - |
| 14 | CLA | e | 1123 | X | - | - | - |
| 14 | CLA | e | 1124 | X | - | - | - |
| 14 | CLA | e | 1125 | X | - | - | - |
| 14 | CLA | e | 1126 | X | - | - | - |
| 14 | CLA | e | 1127 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | e | 1128 | X | - | - | - |
| 14 | CLA | e | 1129 | X | - | - | - |
| 14 | CLA | e | 1130 | X | - | - | - |
| 14 | CLA | e | 1131 | X | - | - | - |
| 14 | CLA | e | 1132 | X | - | - | - |
| 14 | CLA | e | 1133 | X | - | - | - |
| 14 | CLA | e | 1134 | X | - | - | - |
| 14 | CLA | e | 1135 | X | - | - | - |
| 14 | CLA | e | 1136 | X | - | - | - |
| 14 | CLA | e | 1137 | X | - | - | - |
| 14 | CLA | e | 1138 | X | - | - | - |
| 14 | CLA | e | 1139 | X | - | - | - |
| 14 | CLA | e | 1140 | X | - | - | - |
| 14 | CLA | e | 1237 | X | - | - | - |
| 14 | CLA | e | 1801 | X | - | - | - |
| 14 | CLA | f | 1012 | X | - | - | - |
| 14 | CLA | f | 1021 | X | - | - | - |
| 14 | CLA | f | 1023 | X | - | - | - |
| 14 | CLA | f | 1201 | X | - | - | - |
| 14 | CLA | f | 1202 | X | - | - | - |
| 14 | CLA | f | 1203 | X | - | - | - |
| 14 | CLA | f | 1204 | X | - | - | - |
| 14 | CLA | f | 1205 | X | - | - | - |
| 14 | CLA | f | 1206 | X | - | - | - |
| 14 | CLA | f | 1207 | X | - | - | - |
| 14 | CLA | f | 1208 | X | - | - | - |
| 14 | CLA | f | 1209 | X | - | - | - |
| 14 | CLA | f | 1210 | X | - | - | - |
| 14 | CLA | f | 1211 | X | - | - | - |
| 14 | CLA | f | 1212 | X | - | - | - |
| 14 | CLA | f | 1213 | X | - | - | - |
| 14 | CLA | f | 1214 | X | - | - | - |
| 14 | CLA | f | 1215 | X | - | - | - |
| 14 | CLA | f | 1216 | X | - | - | - |
| 14 | CLA | f | 1217 | X | - | - | - |
| 14 | CLA | f | 1218 | X | - | - | - |
| 14 | CLA | f | 1219 | X | - | - | - |
| 14 | CLA | f | 1220 | X | - | - | - |
| 14 | CLA | f | 1221 | X | - | - | - |
| 14 | CLA | f | 1222 | X | - | - | - |
| 14 | CLA | f | 1223 | X | - | - | - |
| 14 | CLA | f | 1224 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | CLA | f | 1225 | X | - | - | - |
| 14 | CLA | f | 1226 | X | - | - | - |
| 14 | CLA | f | 1227 | X | - | - | - |
| 14 | CLA | f | 1228 | X | - | - | - |
| 14 | CLA | f | 1229 | X | - | - | - |
| 14 | CLA | f | 1230 | X | - | - | - |
| 14 | CLA | f | 1231 | X | - | - | - |
| 14 | CLA | f | 1232 | X | - | - | - |
| 14 | CLA | f | 1234 | X | - | - | - |
| 14 | CLA | f | 1235 | X | - | - | - |
| 14 | CLA | f | 1236 | X | - | - | - |
| 14 | CLA | f | 1238 | X | - | - | - |
| 14 | CLA | f | 1239 | X | - | - | - |
| 14 | CLA | f | 1240 | X | - | - | - |
| 14 | CLA | j | 1301 | X | - | - | - |
| 14 | CLA | j | 1302 | X | - | - | - |
| 14 | CLA | l | 1302 | X | - | - | - |
| 14 | CLA | l | 1303 | X | - | - | - |
| 14 | CLA | m | 1103 | X | - | - | - |
| 14 | CLA | m | 1105 | X | - | - | - |
| 14 | CLA | m | 1401 | X | - | - | - |
| 14 | CLA | n | 1501 | X | - | - | - |
| 14 | CLA | n | 1502 | X | - | - | - |
| 14 | CLA | n | 1503 | X | - | - | - |
| 14 | CLA | q | 501 | X | - | - | - |
| 14 | CLA | q | 502 | X | - | - | - |
| 14 | CLA | q | 503 | X | - | - | - |
| 14 | CLA | q | 504 | X | - | - | - |
| 14 | CLA | q | 505 | X | - | - | - |
| 14 | CLA | q | 506 | X | - | - | - |
| 14 | CLA | q | 507 | X | - | - | - |
| 14 | CLA | q | 508 | X | - | - | - |
| 14 | CLA | q | 509 | X | - | - | - |
| 14 | CLA | q | 510 | X | - | - | - |
| 14 | CLA | q | 511 | X | - | - | - |
| 14 | CLA | q | 512 | X | - | - | - |
| 14 | CLA | q | 513 | X | - | - | - |
| 14 | CLA | q | 516 | X | - | - | - |
| 14 | CLA | q | 517 | X | - | - | - |
| 14 | CLA | q | 518 | X | - | - | - |
| 14 | CLA | q | 519 | X | - | - | - |
| 14 | CLA | r | 501 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | r | 502 | X | - | - | - |
| 14 | CLA | r | 503 | X | - | - | - |
| 14 | CLA | r | 504 | X | - | - | - |
| 14 | CLA | r | 505 | X | - | - | - |
| 14 | CLA | r | 506 | X | - | - | - |
| 14 | CLA | r | 507 | X | - | - | - |
| 14 | CLA | r | 508 | X | - | - | - |
| 14 | CLA | r | 509 | X | - | - | - |
| 14 | CLA | r | 510 | X | - | - | - |
| 14 | CLA | r | 511 | X | - | - | - |
| 14 | CLA | r | 512 | X | - | - | - |
| 14 | CLA | r | 513 | X | - | - | - |
| 14 | CLA | r | 518 | X | - | - | - |
| 14 | CLA | r | 519 | X | - | - | - |
| 14 | CLA | s | 501 | X | - | - | - |
| 14 | CLA | s | 502 | X | - | - | - |
| 14 | CLA | s | 503 | X | - | - | - |
| 14 | CLA | s | 504 | X | - | - | - |
| 14 | CLA | s | 505 | X | - | - | - |
| 14 | CLA | s | 506 | X | - | - | - |
| 14 | CLA | s | 507 | X | - | - | - |
| 14 | CLA | s | 508 | X | - | - | - |
| 14 | CLA | s | 509 | X | - | - | - |
| 14 | CLA | s | 510 | X | - | - | - |
| 14 | CLA | s | 511 | X | - | - | - |
| 14 | CLA | s | 512 | X | - | - | - |
| 14 | CLA | s | 513 | X | - | - | - |
| 14 | CLA | s | 516 | X | - | - | - |
| 14 | CLA | s | 517 | X | - | - | - |
| 14 | CLA | s | 518 | X | - | - | - |
| 14 | CLA | s | 519 | X | - | - | - |
| 14 | CLA | t | 501 | X | - | - | - |
| 14 | CLA | t | 502 | X | - | - | - |
| 14 | CLA | t | 503 | X | - | - | - |
| 14 | CLA | t | 504 | X | - | - | - |
| 14 | CLA | t | 505 | X | - | - | - |
| 14 | CLA | t | 506 | X | - | - | - |
| 14 | CLA | t | 507 | X | - | - | - |
| 14 | CLA | t | 508 | X | - | - | - |
| 14 | CLA | t | 509 | X | - | - | - |
| 14 | CLA | t | 510 | X | - | - | - |
| 14 | CLA | t | 511 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14 | CLA | t | 512 | X | - | - | - |
| 14 | CLA | t | 513 | X | - | - | - |
| 14 | CLA | t | 516 | X | - | - | - |
| 14 | CLA | t | 517 | X | - | - | - |
| 14 | CLA | t | 518 | X | - | - | - |
| 14 | CLA | t | 519 | X | - | - | - |
| 14 | CLA | u | 501 | X | - | - | - |
| 14 | CLA | u | 502 | X | - | - | - |
| 14 | CLA | u | 503 | X | - | - | - |
| 14 | CLA | u | 504 | X | - | - | - |
| 14 | CLA | u | 505 | X | - | - | - |
| 14 | CLA | u | 506 | X | - | - | - |
| 14 | CLA | u | 507 | X | - | - | - |
| 14 | CLA | u | 508 | X | - | - | - |
| 14 | CLA | u | 509 | X | - | - | - |
| 14 | CLA | u | 510 | X | - | - | - |
| 14 | CLA | u | 511 | X | - | - | - |
| 14 | CLA | u | 512 | X | - | - | - |
| 14 | CLA | u | 513 | X | - | - | - |
| 14 | CLA | u | 516 | X | - | - | - |
| 14 | CLA | u | 517 | X | - | - | - |
| 14 | CLA | u | 518 | X | - | - | - |
| 14 | CLA | u | 519 | X | - | - | - |
| 14 | CLA | v | 501 | X | - | - | - |
| 14 | CLA | v | 502 | X | - | - | - |
| 14 | CLA | v | 503 | X | - | - | - |
| 14 | CLA | v | 504 | X | - | - | - |
| 14 | CLA | v | 505 | X | - | - | - |
| 14 | CLA | v | 506 | X | - | - | - |
| 14 | CLA | v | 507 | X | - | - | - |
| 14 | CLA | v | 508 | X | - | - | - |
| 14 | CLA | v | 509 | X | - | - | - |
| 14 | CLA | v | 510 | X | - | - | - |
| 14 | CLA | v | 511 | X | - | - | - |
| 14 | CLA | v | 512 | X | - | - | - |
| 14 | CLA | v | 513 | X | - | - | - |
| 14 | CLA | v | 516 | X | - | - | - |
| 14 | CLA | v | 517 | X | - | - | - |
| 14 | CLA | v | 518 | X | - | - | - |
| 14 | CLA | v | 519 | X | - | - | - |

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 144312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|----|---------|-------|
| 1 | A | 751 | Total | C | N | O | S | 0 | 0 |
| | | | 5865 | 3847 | 1002 | 999 | 17 | | |
| 1 | G | 751 | Total | C | N | O | S | 0 | 0 |
| | | | 5865 | 3847 | 1002 | 999 | 17 | | |
| 1 | e | 751 | Total | C | N | O | S | 0 | 0 |
| | | | 5865 | 3847 | 1002 | 999 | 17 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | B | 733 | Total | C | N | O | S | 0 | 0 |
| | | | 5789 | 3811 | 970 | 994 | 14 | | |
| 2 | H | 733 | Total | C | N | O | S | 0 | 0 |
| | | | 5789 | 3811 | 970 | 994 | 14 | | |
| 2 | f | 733 | Total | C | N | O | S | 0 | 0 |
| | | | 5789 | 3811 | 970 | 994 | 14 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3 | C | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 598 | 368 | 103 | 116 | 11 | | |
| 3 | N | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 598 | 368 | 103 | 116 | 11 | | |
| 3 | g | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 598 | 368 | 103 | 116 | 11 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | D | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 702 | 187 | 208 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | O | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 702 | 187 | 208 | 1 | | |
| 4 | h | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 702 | 187 | 208 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|--|---------|-------|
| 5 | E | 71 | Total | C | N | O | | 0 | 0 |
| | | | 543 | 343 | 95 | 105 | | | |
| 5 | Q | 71 | Total | C | N | O | | 0 | 0 |
| | | | 543 | 343 | 95 | 105 | | | |
| 5 | i | 71 | Total | C | N | O | | 0 | 0 |
| | | | 543 | 343 | 95 | 105 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | F | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1036 | 670 | 174 | 190 | 2 | | |
| 6 | R | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1036 | 670 | 174 | 190 | 2 | | |
| 6 | j | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1036 | 670 | 174 | 190 | 2 | | |

- Molecule 7 is a protein called Photosystem I PsaI protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | I | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 282 | 191 | 38 | 51 | 2 | | |
| 7 | S | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 282 | 191 | 38 | 51 | 2 | | |
| 7 | k | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 282 | 191 | 38 | 51 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8 | J | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 335 | 228 | 52 | 54 | 1 | | |
| 8 | T | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 335 | 228 | 52 | 54 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8 | l | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 335 | 228 | 52 | 54 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9 | K | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 364 | 91 | 93 | 1 | | |
| 9 | U | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 364 | 91 | 93 | 1 | | |
| 9 | m | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 364 | 91 | 93 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | L | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 782 | 201 | 225 | 2 | | |
| 10 | V | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 782 | 201 | 225 | 2 | | |
| 10 | n | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 782 | 201 | 225 | 2 | | |

- Molecule 11 is a protein called Psam.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11 | M | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 228 | 151 | 36 | 40 | 1 | | |
| 11 | W | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 228 | 151 | 36 | 40 | 1 | | |
| 11 | o | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 228 | 151 | 36 | 40 | 1 | | |

- Molecule 12 is a protein called Flavodoxin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | P | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1318 | 831 | 210 | 275 | 2 | | |
| 12 | X | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1318 | 831 | 210 | 275 | 2 | | |
| 12 | p | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1318 | 831 | 210 | 275 | 2 | | |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| P | -2 | GLY | - | expression tag | UNP P10340 |
| P | -1 | SER | - | expression tag | UNP P10340 |
| P | 0 | HIS | - | expression tag | UNP P10340 |
| X | -2 | GLY | - | expression tag | UNP P10340 |
| X | -1 | SER | - | expression tag | UNP P10340 |
| X | 0 | HIS | - | expression tag | UNP P10340 |
| p | -2 | GLY | - | expression tag | UNP P10340 |
| p | -1 | SER | - | expression tag | UNP P10340 |
| p | 0 | HIS | - | expression tag | UNP P10340 |

- Molecule 13 is a protein called Iron stress-induced chlorophyll-binding protein.

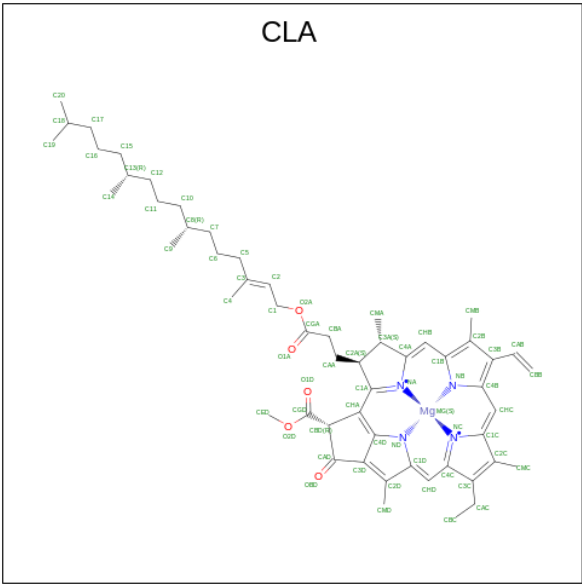
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | 1 | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | 2 | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | 3 | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | 4 | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | 5 | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | 6 | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | Y | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | Z | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | a | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | b | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | c | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | d | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | q | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | r | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | s | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | t | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | u | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |
| 13 | v | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2605 | 1722 | 428 | 448 | 7 | | |

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 14 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 63 | 53 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | B | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | B | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | F | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | F | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | J | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | J | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | K | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 38 | 1 | 4 | 5 | |
| 14 | K | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | L | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 4 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | 5 | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | G | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 50 | C 40 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 53 | C 43 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 14 | G | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 53 | C 43 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 51 | C 41 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 61 | C 51 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 63 | 53 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | H | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | H | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | R | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | R | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | T | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | T | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | U | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | U | 1 | Total 48 | C 38 | Mg 1 | N 4 | O 5 | 0 |
| 14 | U | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | V | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | V | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | V | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Y | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | Z | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 44 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | e | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 55 | C 45 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 56 | C 46 | Mg 1 | N 4 | O 5 | 0 |
| 14 | e | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 60 | C 50 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | f | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 63 | 53 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | f | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | j | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | j | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | l | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | l | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | m | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | m | 1 | Total | C | Mg | N | O | 0 |
| | | | 48 | 38 | 1 | 4 | 5 | |
| 14 | m | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | n | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | n | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | n | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | q | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 60 | 50 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | r | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 55 | 45 | 1 | 4 | 5 | |
| 14 | s | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | t | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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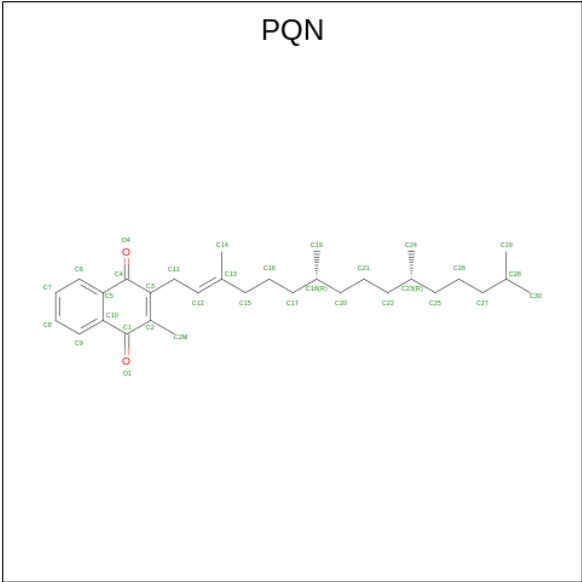
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | t | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |
| 14 | u | 1 | Total 45 | C 35 | Mg 1 | N 4 | O 5 | 0 |

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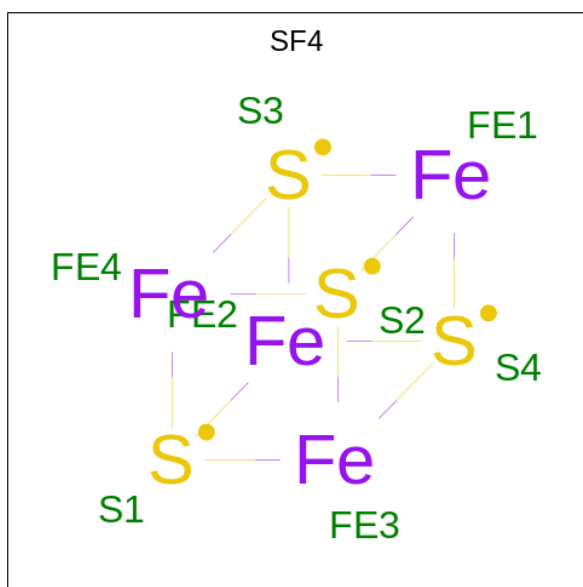
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14 | u | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | u | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | u | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 14 | v | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



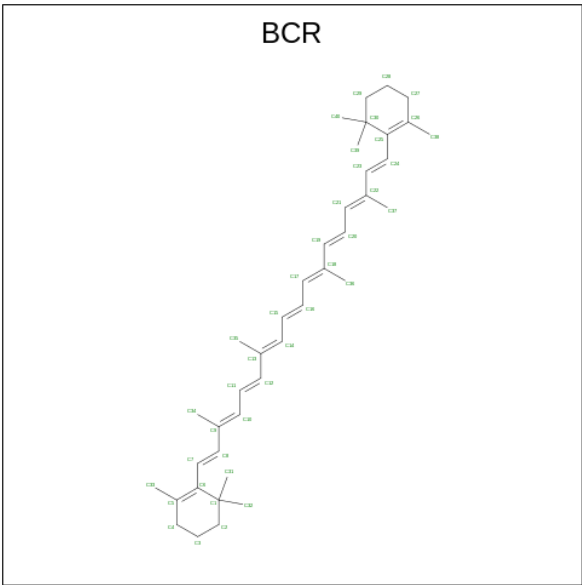
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15 | A | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 15 | B | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 15 | G | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 15 | H | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 15 | e | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 15 | f | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16 | A | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | C | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | C | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | G | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | N | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | N | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | e | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | g | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 16 | g | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | A | 1 | Total C 40 40 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 |
| 17 | A | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | B | 1 | Total C 40 40 | 0 |
| 17 | F | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | I | 1 | Total C 40 40 | 0 |
| 17 | J | 1 | Total C 40 40 | 0 |
| 17 | J | 1 | Total C 40 40 | 0 |
| 17 | J | 1 | Total C 40 40 | 0 |
| 17 | K | 1 | Total C 40 40 | 0 |
| 17 | L | 1 | Total C 40 40 | 0 |
| 17 | L | 1 | Total C 40 40 | 0 |
| 17 | L | 1 | Total C 40 40 | 0 |
| 17 | L | 1 | Total C 40 40 | 0 |
| 17 | M | 1 | Total C 40 40 | 0 |
| 17 | 1 | 1 | Total C 40 40 | 0 |
| 17 | 1 | 1 | Total C 40 40 | 0 |
| 17 | 1 | 1 | Total C 40 40 | 0 |
| 17 | 1 | 1 | Total C 40 40 | 0 |
| 17 | 2 | 1 | Total C 40 40 | 0 |
| 17 | 2 | 1 | Total C 40 40 | 0 |
| 17 | 2 | 1 | Total C 40 40 | 0 |
| 17 | 2 | 1 | Total C 40 40 | 0 |
| 17 | 3 | 1 | Total C 40 40 | 0 |
| 17 | 3 | 1 | Total C 40 40 | 0 |
| 17 | 3 | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | 3 | 1 | Total C 40 40 | 0 |
| 17 | 4 | 1 | Total C 40 40 | 0 |
| 17 | 4 | 1 | Total C 40 40 | 0 |
| 17 | 4 | 1 | Total C 40 40 | 0 |
| 17 | 4 | 1 | Total C 40 40 | 0 |
| 17 | 5 | 1 | Total C 40 40 | 0 |
| 17 | 5 | 1 | Total C 40 40 | 0 |
| 17 | 5 | 1 | Total C 40 40 | 0 |
| 17 | 5 | 1 | Total C 40 40 | 0 |
| 17 | 6 | 1 | Total C 40 40 | 0 |
| 17 | 6 | 1 | Total C 40 40 | 0 |
| 17 | 6 | 1 | Total C 40 40 | 0 |
| 17 | 6 | 1 | Total C 40 40 | 0 |
| 17 | G | 1 | Total C 40 40 | 0 |
| 17 | G | 1 | Total C 40 40 | 0 |
| 17 | G | 1 | Total C 40 40 | 0 |
| 17 | G | 1 | Total C 40 40 | 0 |
| 17 | G | 1 | Total C 40 40 | 0 |
| 17 | G | 1 | Total C 40 40 | 0 |
| 17 | H | 1 | Total C 40 40 | 0 |
| 17 | H | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | H | 1 | Total C 40 40 | 0 |
| 17 | H | 1 | Total C 40 40 | 0 |
| 17 | H | 1 | Total C 40 40 | 0 |
| 17 | H | 1 | Total C 40 40 | 0 |
| 17 | H | 1 | Total C 40 40 | 0 |
| 17 | R | 1 | Total C 40 40 | 0 |
| 17 | S | 1 | Total C 40 40 | 0 |
| 17 | T | 1 | Total C 40 40 | 0 |
| 17 | T | 1 | Total C 40 40 | 0 |
| 17 | T | 1 | Total C 40 40 | 0 |
| 17 | U | 1 | Total C 40 40 | 0 |
| 17 | V | 1 | Total C 40 40 | 0 |
| 17 | V | 1 | Total C 40 40 | 0 |
| 17 | V | 1 | Total C 40 40 | 0 |
| 17 | V | 1 | Total C 40 40 | 0 |
| 17 | V | 1 | Total C 40 40 | 0 |
| 17 | W | 1 | Total C 40 40 | 0 |
| 17 | Y | 1 | Total C 40 40 | 0 |
| 17 | Y | 1 | Total C 40 40 | 0 |
| 17 | Y | 1 | Total C 40 40 | 0 |
| 17 | Y | 1 | Total C 40 40 | 0 |
| 17 | Z | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | Z | 1 | Total C 40 40 | 0 |
| 17 | Z | 1 | Total C 40 40 | 0 |
| 17 | Z | 1 | Total C 40 40 | 0 |
| 17 | a | 1 | Total C 40 40 | 0 |
| 17 | a | 1 | Total C 40 40 | 0 |
| 17 | a | 1 | Total C 40 40 | 0 |
| 17 | a | 1 | Total C 40 40 | 0 |
| 17 | b | 1 | Total C 40 40 | 0 |
| 17 | b | 1 | Total C 40 40 | 0 |
| 17 | b | 1 | Total C 40 40 | 0 |
| 17 | b | 1 | Total C 40 40 | 0 |
| 17 | c | 1 | Total C 40 40 | 0 |
| 17 | c | 1 | Total C 40 40 | 0 |
| 17 | c | 1 | Total C 40 40 | 0 |
| 17 | c | 1 | Total C 40 40 | 0 |
| 17 | d | 1 | Total C 40 40 | 0 |
| 17 | d | 1 | Total C 40 40 | 0 |
| 17 | d | 1 | Total C 40 40 | 0 |
| 17 | d | 1 | Total C 40 40 | 0 |
| 17 | e | 1 | Total C 40 40 | 0 |
| 17 | e | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | e | 1 | Total C 40 40 | 0 |
| 17 | e | 1 | Total C 40 40 | 0 |
| 17 | e | 1 | Total C 40 40 | 0 |
| 17 | e | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | f | 1 | Total C 40 40 | 0 |
| 17 | j | 1 | Total C 40 40 | 0 |
| 17 | k | 1 | Total C 40 40 | 0 |
| 17 | l | 1 | Total C 40 40 | 0 |
| 17 | l | 1 | Total C 40 40 | 0 |
| 17 | l | 1 | Total C 40 40 | 0 |
| 17 | m | 1 | Total C 40 40 | 0 |
| 17 | n | 1 | Total C 40 40 | 0 |
| 17 | n | 1 | Total C 40 40 | 0 |
| 17 | n | 1 | Total C 40 40 | 0 |
| 17 | n | 1 | Total C 40 40 | 0 |

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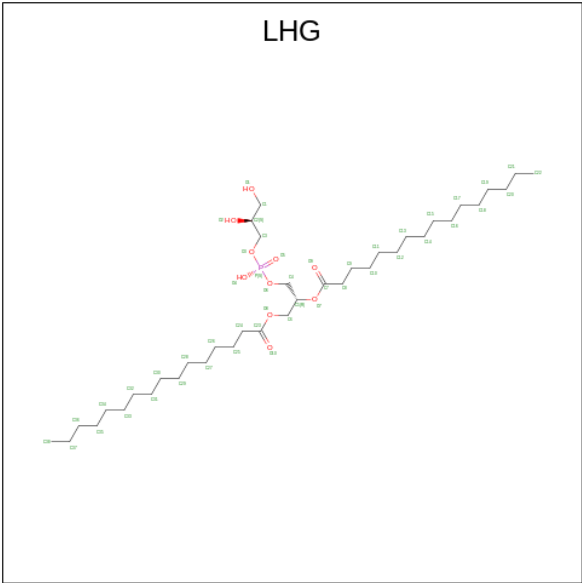
| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 17 | o | 1 | Total C 40 40 | 0 |
| 17 | q | 1 | Total C 40 40 | 0 |
| 17 | q | 1 | Total C 40 40 | 0 |
| 17 | q | 1 | Total C 40 40 | 0 |
| 17 | q | 1 | Total C 40 40 | 0 |
| 17 | r | 1 | Total C 40 40 | 0 |
| 17 | r | 1 | Total C 40 40 | 0 |
| 17 | r | 1 | Total C 40 40 | 0 |
| 17 | r | 1 | Total C 40 40 | 0 |
| 17 | s | 1 | Total C 40 40 | 0 |
| 17 | s | 1 | Total C 40 40 | 0 |
| 17 | s | 1 | Total C 40 40 | 0 |
| 17 | s | 1 | Total C 40 40 | 0 |
| 17 | t | 1 | Total C 40 40 | 0 |
| 17 | t | 1 | Total C 40 40 | 0 |
| 17 | t | 1 | Total C 40 40 | 0 |
| 17 | t | 1 | Total C 40 40 | 0 |
| 17 | u | 1 | Total C 40 40 | 0 |
| 17 | u | 1 | Total C 40 40 | 0 |
| 17 | u | 1 | Total C 40 40 | 0 |
| 17 | u | 1 | Total C 40 40 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 17 | v | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 17 | v | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 17 | v | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 17 | v | 1 | Total | C | 0 |
| | | | 40 | 40 | |

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 47 | 36 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 42 | 31 | 10 | 1 | |

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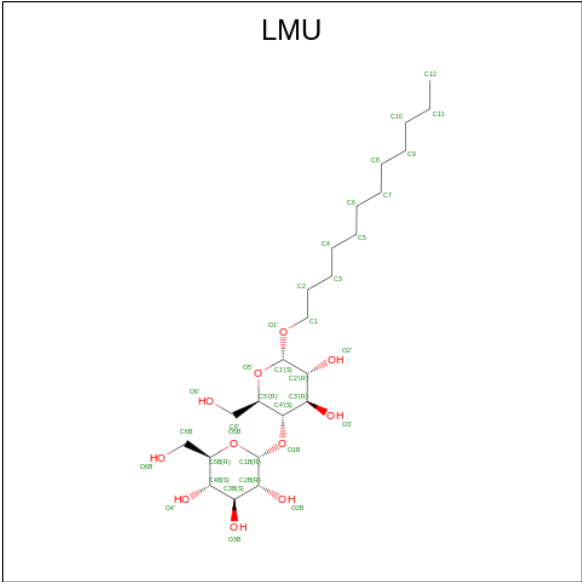
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 18 | A | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 18 | B | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 18 | B | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 18 | I | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | |
| 18 | L | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 18 | L | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 18 | L | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 47 | 36 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 42 | 31 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 18 | G | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 18 | H | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 18 | H | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 18 | S | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | |
| 18 | V | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |

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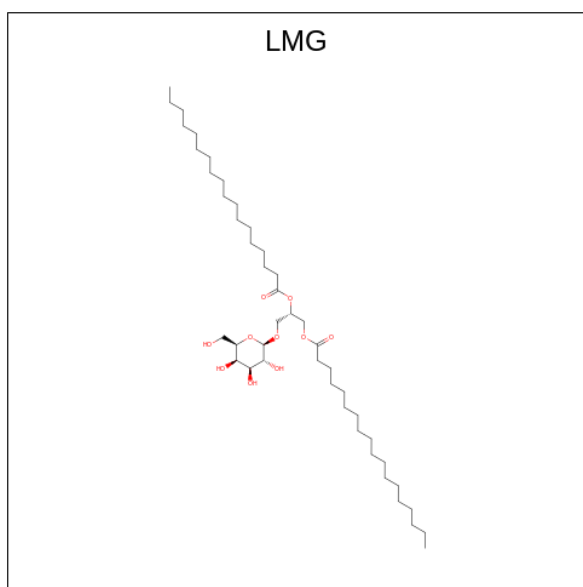
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 18 | V | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 18 | V | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 43 | 32 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 47 | 36 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 35 | 24 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 42 | 31 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 18 | e | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 18 | f | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 18 | f | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 18 | k | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | |
| 18 | n | 1 | Total | C | O | P | 0 |
| | | | 37 | 26 | 10 | 1 | |
| 18 | n | 1 | Total | C | O | P | 0 |
| | | | 41 | 30 | 10 | 1 | |
| 18 | n | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |

- Molecule 19 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



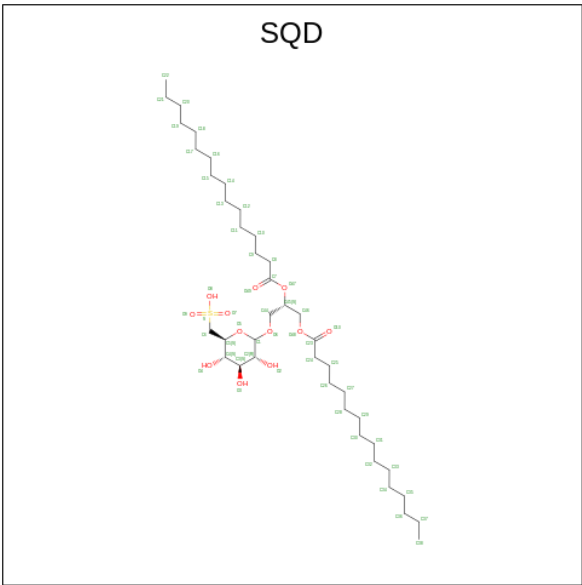
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 19 | A | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | A | 1 | Total | C | O | 0 |
| | | | 23 | 17 | 6 | |
| 19 | B | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | J | 1 | Total | C | O | 0 |
| | | | 22 | 16 | 6 | |
| 19 | G | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | G | 1 | Total | C | O | 0 |
| | | | 23 | 17 | 6 | |
| 19 | H | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | T | 1 | Total | C | O | 0 |
| | | | 22 | 16 | 6 | |
| 19 | e | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | e | 1 | Total | C | O | 0 |
| | | | 23 | 17 | 6 | |
| 19 | f | 1 | Total | C | O | 0 |
| | | | 35 | 24 | 11 | |
| 19 | l | 1 | Total | C | O | 0 |
| | | | 22 | 16 | 6 | |

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 20 | B | 1 | Total | C | O | 0 |
| | | | 53 | 43 | 10 | |
| 20 | J | 1 | Total | C | O | 0 |
| | | | 32 | 22 | 10 | |
| 20 | H | 1 | Total | C | O | 0 |
| | | | 53 | 43 | 10 | |
| 20 | T | 1 | Total | C | O | 0 |
| | | | 32 | 22 | 10 | |
| 20 | f | 1 | Total | C | O | 0 |
| | | | 53 | 43 | 10 | |
| 20 | l | 1 | Total | C | O | 0 |
| | | | 32 | 22 | 10 | |

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



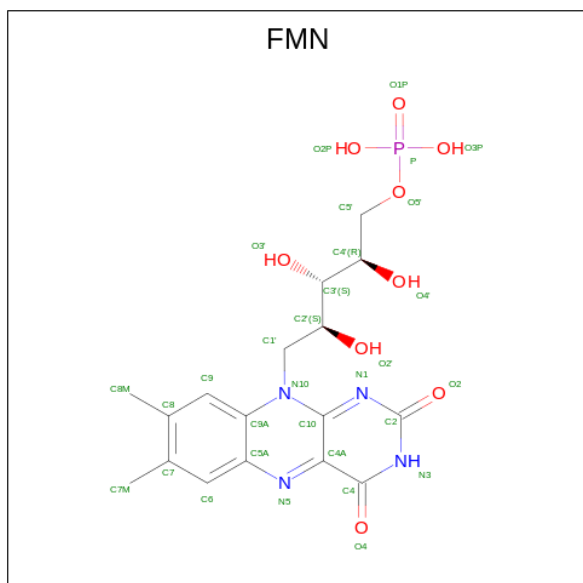
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 21 | B | 1 | Total | C | O | S | 0 |
| | | | 40 | 27 | 12 | 1 | |
| 21 | L | 1 | Total | C | O | S | 0 |
| | | | 46 | 33 | 12 | 1 | |
| 21 | 1 | 1 | Total | C | O | S | 0 |
| | | | 32 | 19 | 12 | 1 | |
| 21 | 2 | 1 | Total | C | O | S | 0 |
| | | | 28 | 15 | 12 | 1 | |
| 21 | 3 | 1 | Total | C | O | S | 0 |
| | | | 28 | 15 | 12 | 1 | |
| 21 | 4 | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | 5 | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | 6 | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | H | 1 | Total | C | O | S | 0 |
| | | | 40 | 27 | 12 | 1 | |
| 21 | V | 1 | Total | C | O | S | 0 |
| | | | 46 | 33 | 12 | 1 | |
| 21 | Y | 1 | Total | C | O | S | 0 |
| | | | 32 | 19 | 12 | 1 | |
| 21 | Z | 1 | Total | C | O | S | 0 |
| | | | 28 | 15 | 12 | 1 | |
| 21 | a | 1 | Total | C | O | S | 0 |
| | | | 28 | 15 | 12 | 1 | |
| 21 | b | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 21 | c | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | d | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | f | 1 | Total | C | O | S | 0 |
| | | | 40 | 27 | 12 | 1 | |
| 21 | n | 1 | Total | C | O | S | 0 |
| | | | 46 | 33 | 12 | 1 | |
| 21 | q | 1 | Total | C | O | S | 0 |
| | | | 32 | 19 | 12 | 1 | |
| 21 | r | 1 | Total | C | O | S | 0 |
| | | | 28 | 15 | 12 | 1 | |
| 21 | s | 1 | Total | C | O | S | 0 |
| | | | 28 | 15 | 12 | 1 | |
| 21 | t | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | u | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |
| 21 | v | 1 | Total | C | O | S | 0 |
| | | | 26 | 13 | 12 | 1 | |

- Molecule 22 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 22 | P | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 22 | X | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |
| 22 | p | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

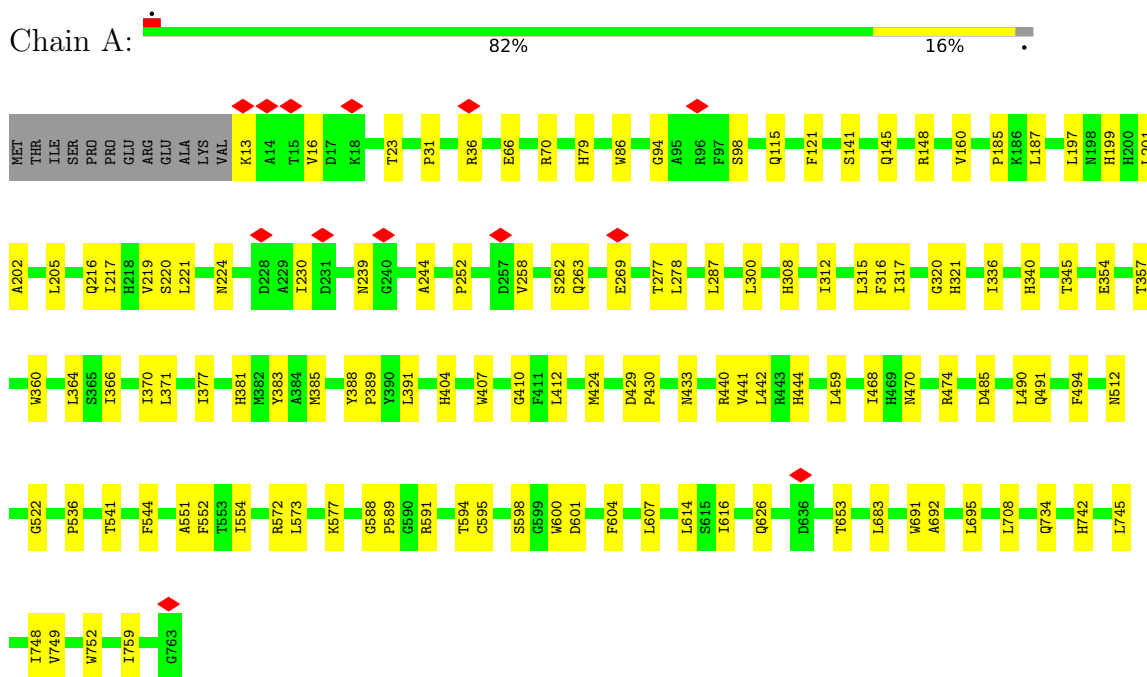
- Molecule 23 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|---|---------|
| 23 | A | 9 | Total | O | 0 |
| | | | 9 | 9 | |
| 23 | B | 7 | Total | O | 0 |
| | | | 7 | 7 | |
| 23 | F | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 23 | L | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 23 | G | 9 | Total | O | 0 |
| | | | 9 | 9 | |
| 23 | H | 7 | Total | O | 0 |
| | | | 7 | 7 | |
| 23 | R | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 23 | V | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 23 | e | 9 | Total | O | 0 |
| | | | 9 | 9 | |
| 23 | f | 7 | Total | O | 0 |
| | | | 7 | 7 | |
| 23 | j | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 23 | n | 1 | Total | O | 0 |
| | | | 1 | 1 | |

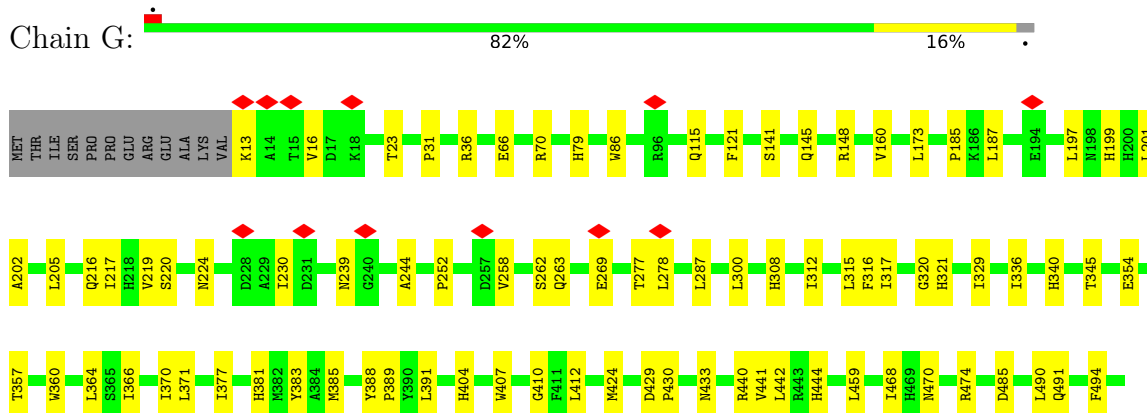
3 Residue-property plots

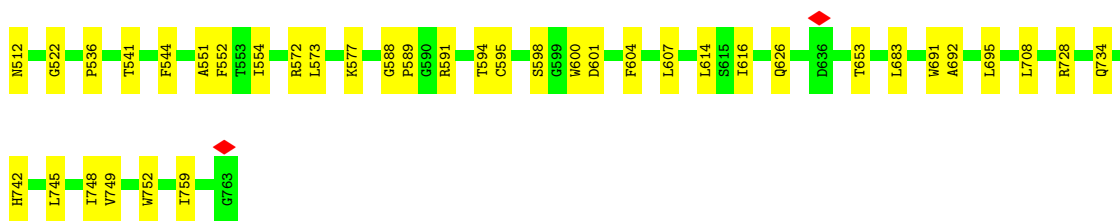
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



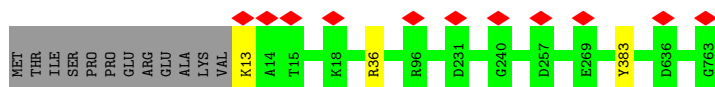
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





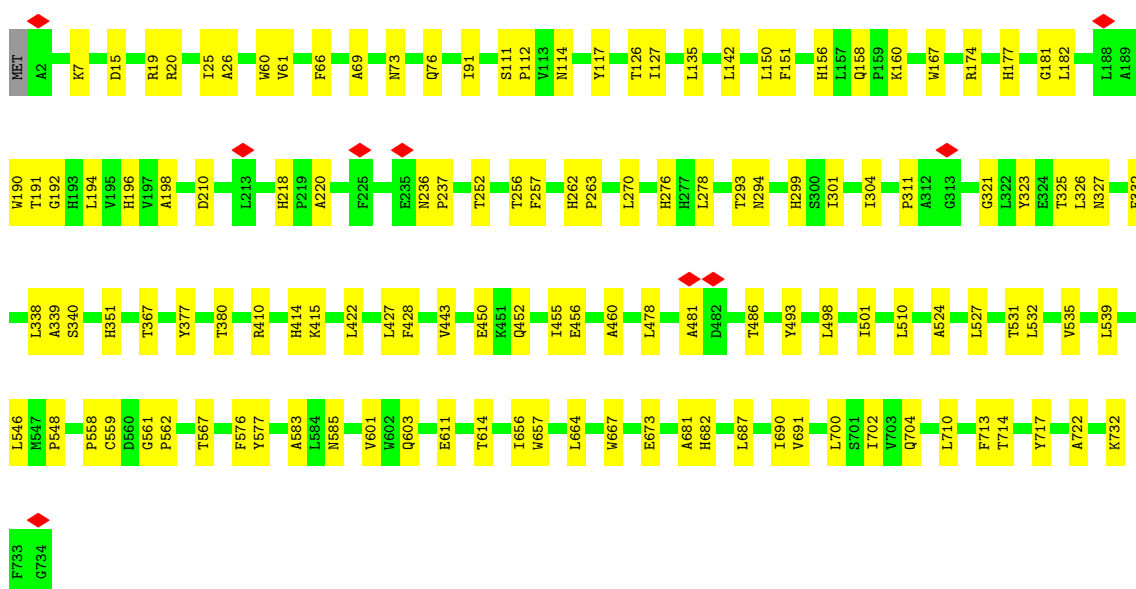
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e: 98%



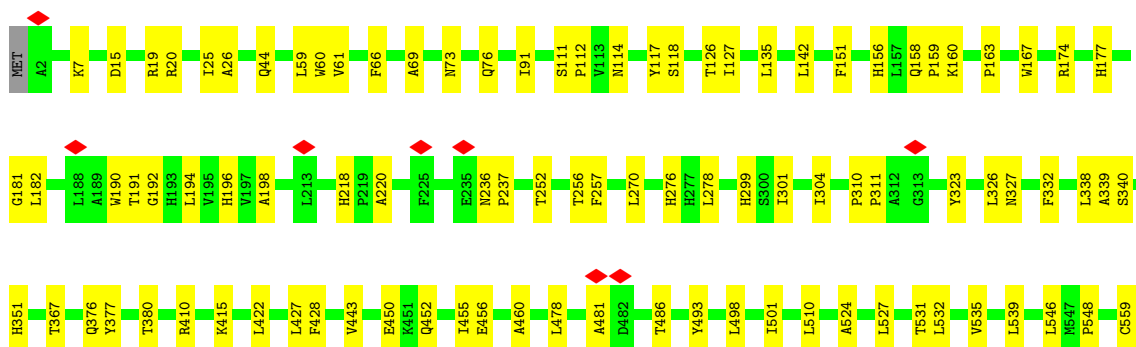
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 82% 17%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

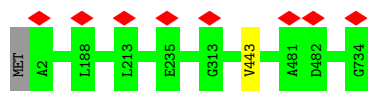
Chain H: 83% 17%





- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f: 100%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 80% 19%



- Molecule 3: Photosystem I iron-sulfur center

Chain N: 79% 20%



- Molecule 3: Photosystem I iron-sulfur center

Chain g: 99%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 81% 19%



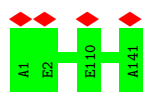
- Molecule 4: Photosystem I reaction center subunit II

Chain O: 81% 19%




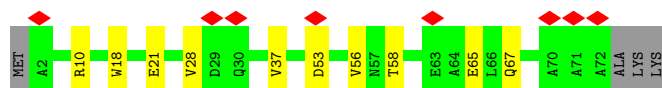
- Molecule 4: Photosystem I reaction center subunit II

Chain h:  100%




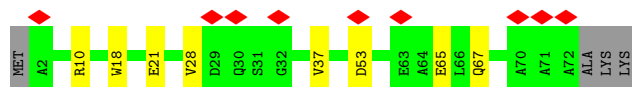
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  11% 81% 13% 5%



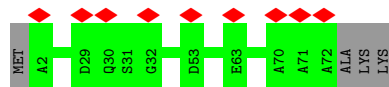
- Molecule 5: Photosystem I reaction center subunit IV

Chain Q:  12% 84% 11% 5%




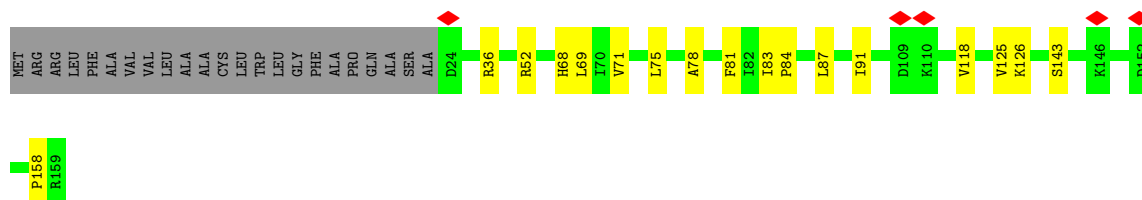
- Molecule 5: Photosystem I reaction center subunit IV

Chain i:  12% 95% 5%




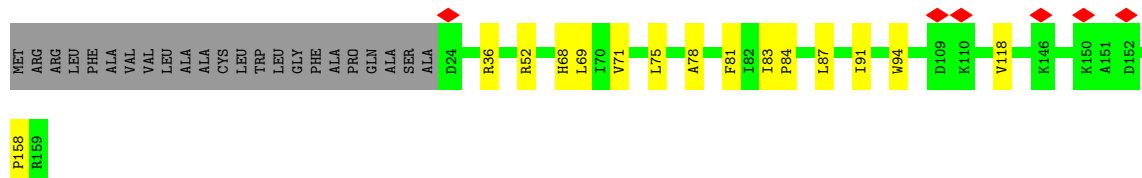
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  75% 11% 14%




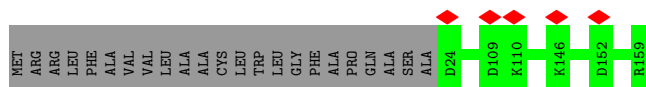
- Molecule 6: Photosystem I reaction center subunit III

Chain R:  76% 9% 14%




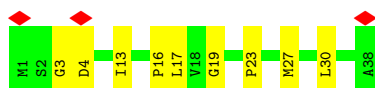
- Molecule 6: Photosystem I reaction center subunit III

Chain j:  86% 14%




- Molecule 7: Photosystem I PsaI protein

Chain I:  8% 76% 24%



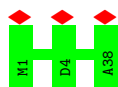
- Molecule 7: Photosystem I PsaI protein

Chain S:  5% 84% 16%




- Molecule 7: Photosystem I PsaI protein

Chain k:  8% 100%




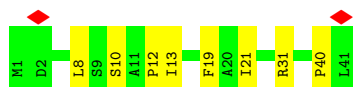
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  5% 80% 20%



- Molecule 8: Photosystem I reaction center subunit IX

Chain T:  5% 80% 20%

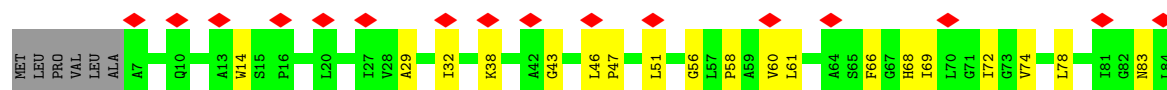


- Molecule 8: Photosystem I reaction center subunit IX

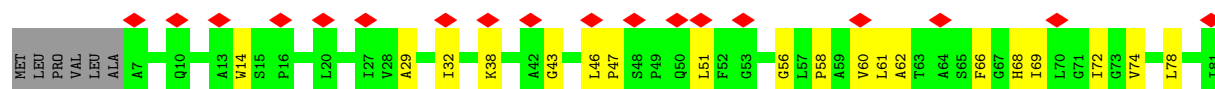
Chain l:  5% 100%



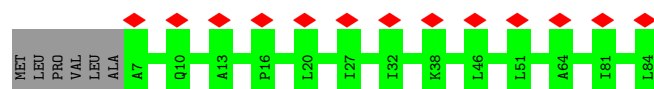
- Molecule 9: Photosystem I reaction center subunit PsaK



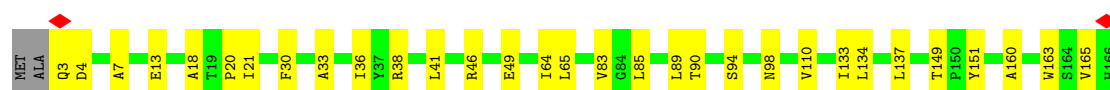
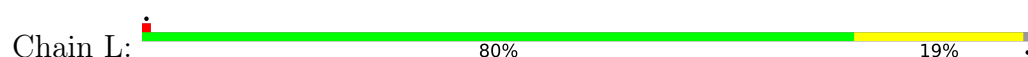
- Molecule 9: Photosystem I reaction center subunit PsaK



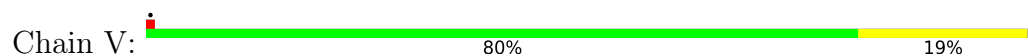
- Molecule 9: Photosystem I reaction center subunit PsaK



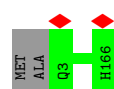
- Molecule 10: Photosystem I reaction center subunit XI




- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XI




- Molecule 11: PsaM

Chain M:  79% 21%



• Molecule 11: PsaM

Chain W:  86% 14%




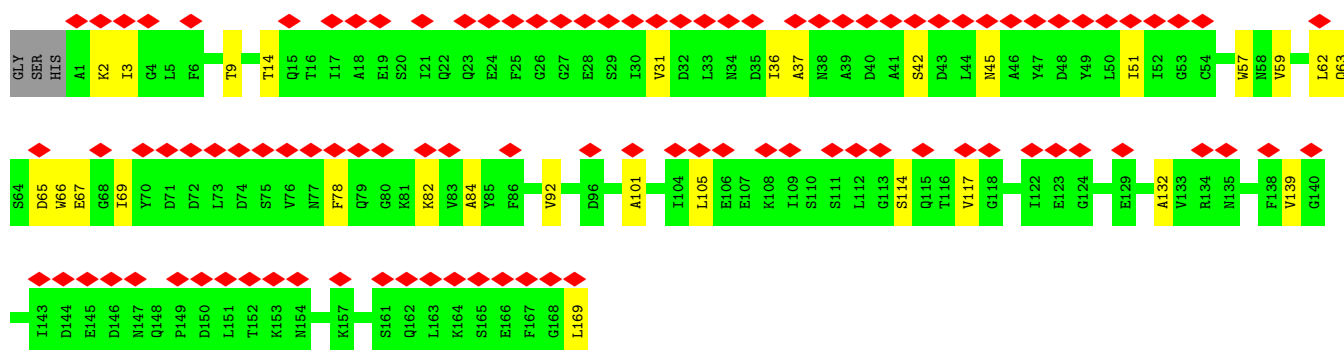
• Molecule 11: PsaM

Chain o:  100%


There are no outlier residues recorded for this chain.

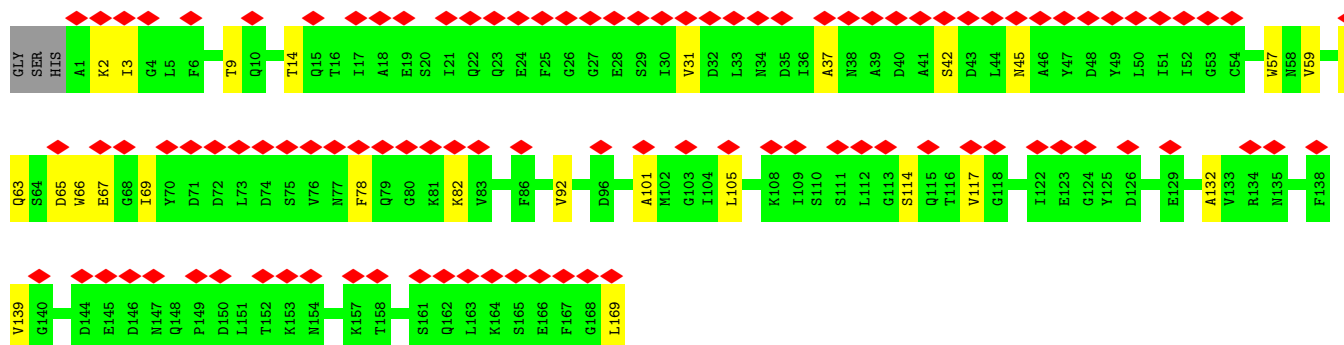
• Molecule 12: Flavodoxin

Chain P:  58% 81% 17%



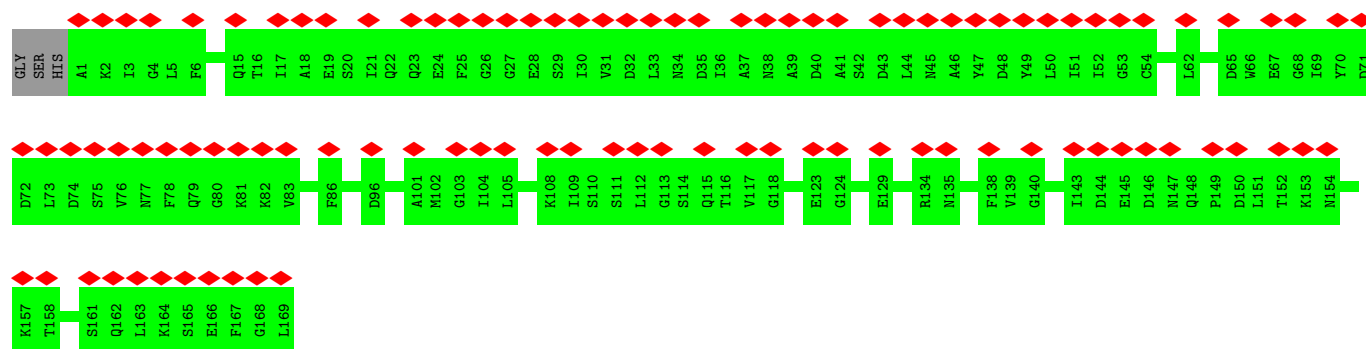
• Molecule 12: Flavodoxin

Chain X:  60% 83% 15%



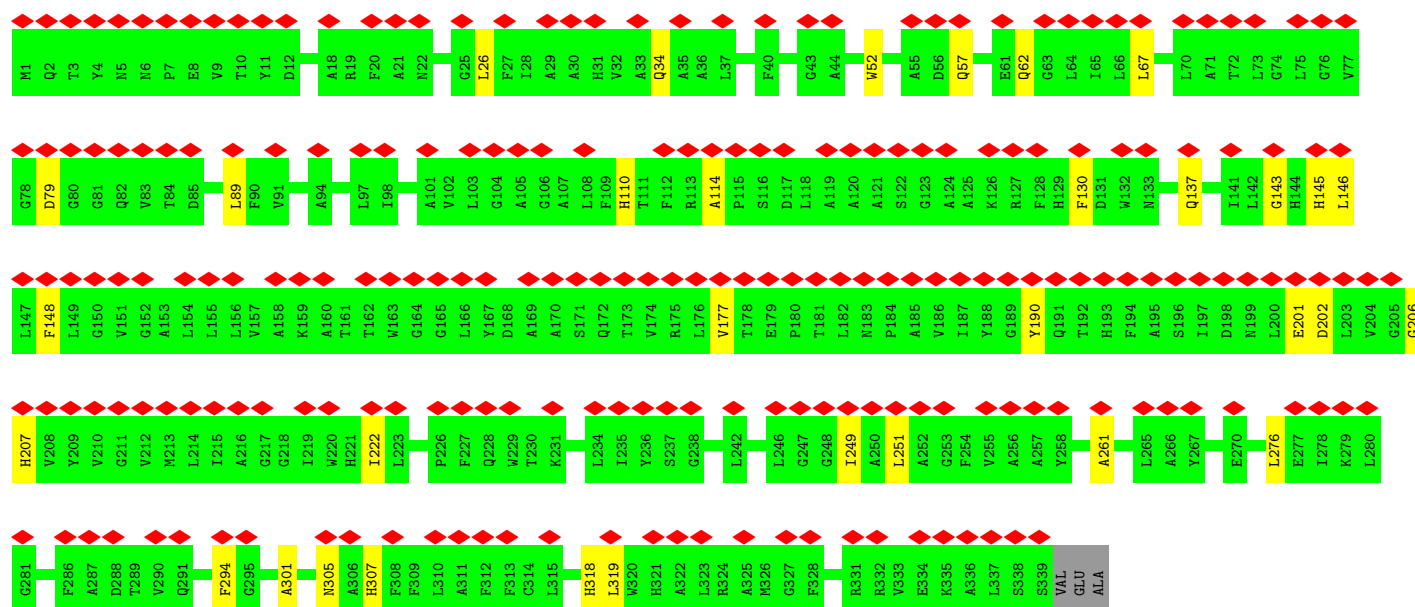
• Molecule 12: Flavodoxin

Chain p:  58% 98%



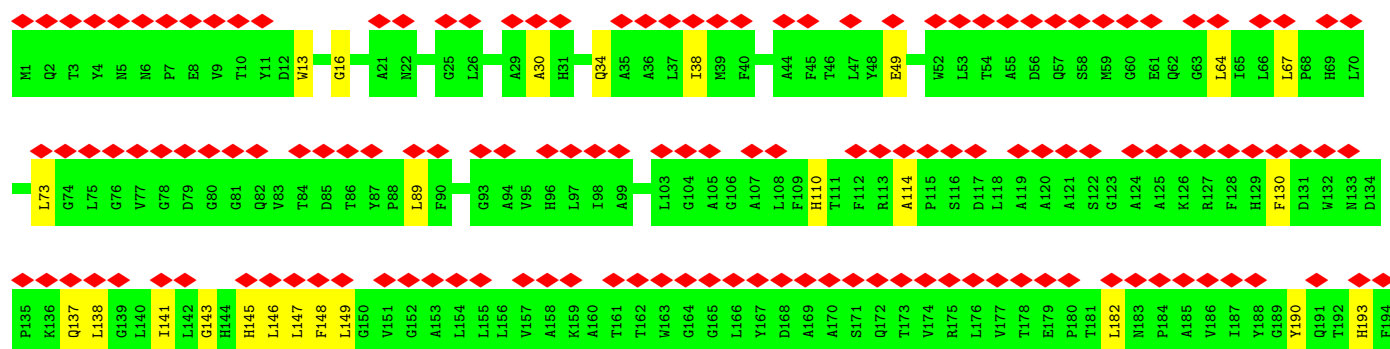
• Molecule 13: Iron stress-induced chlorophyll-binding protein

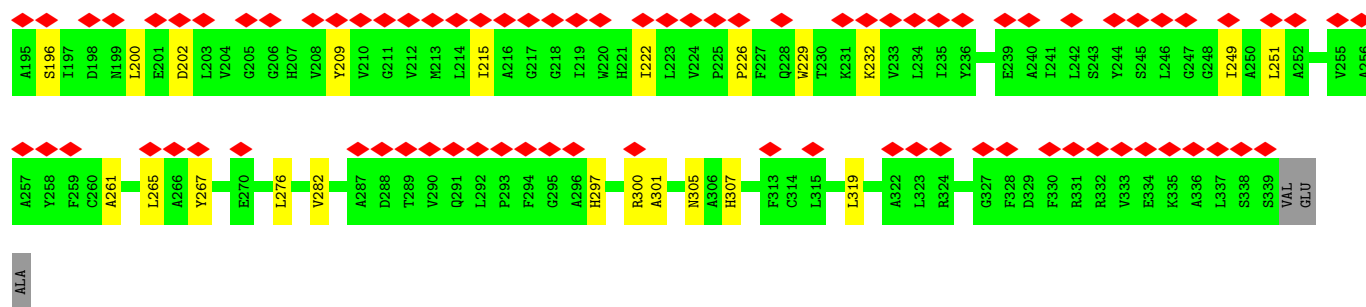
Chain 1: 64% 89% 10% .



• Molecule 13: Iron stress-induced chlorophyll-binding protein

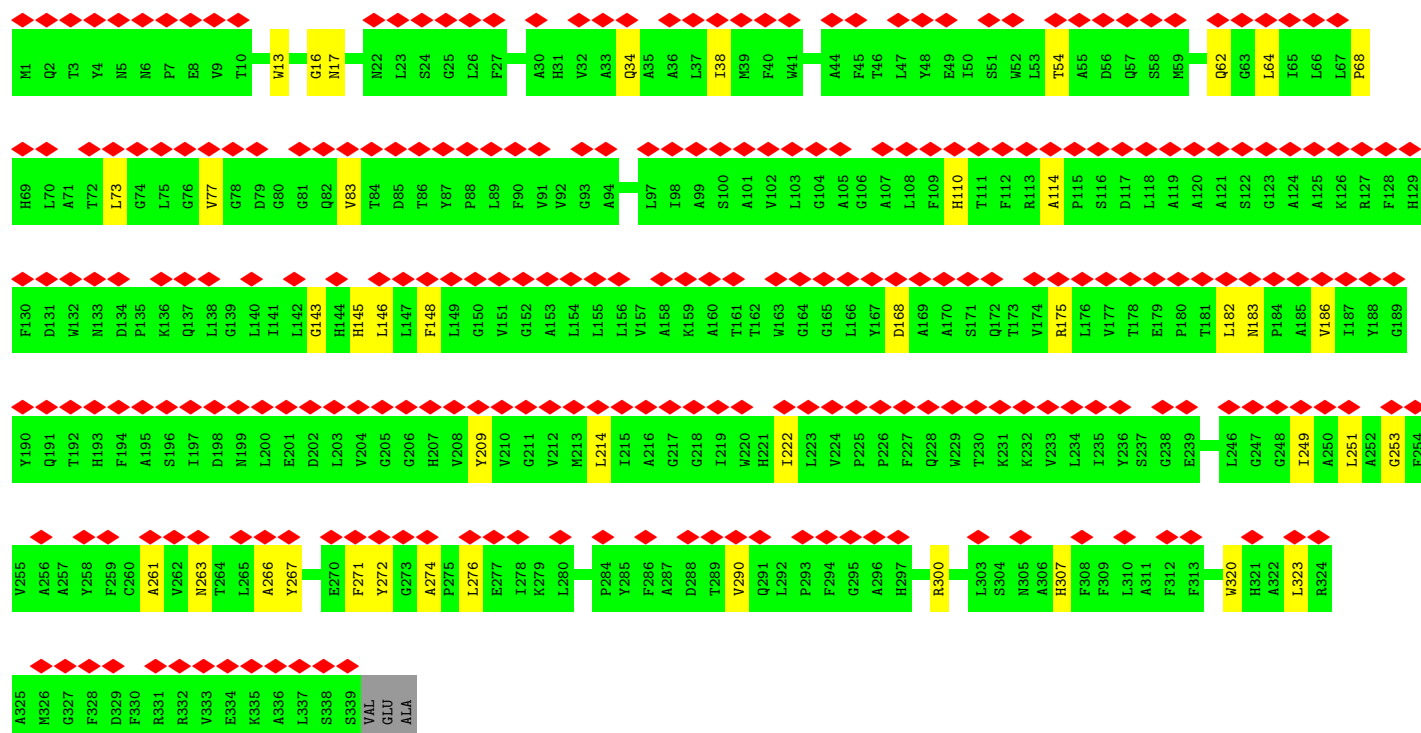
Chain 2: 65% 85% 14% .





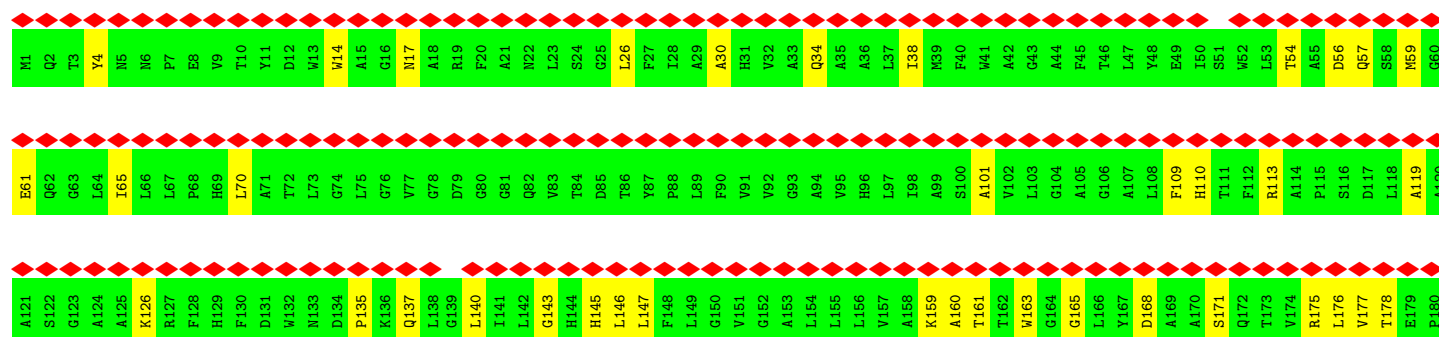
• Molecule 13: Iron stress-induced chlorophyll-binding protein

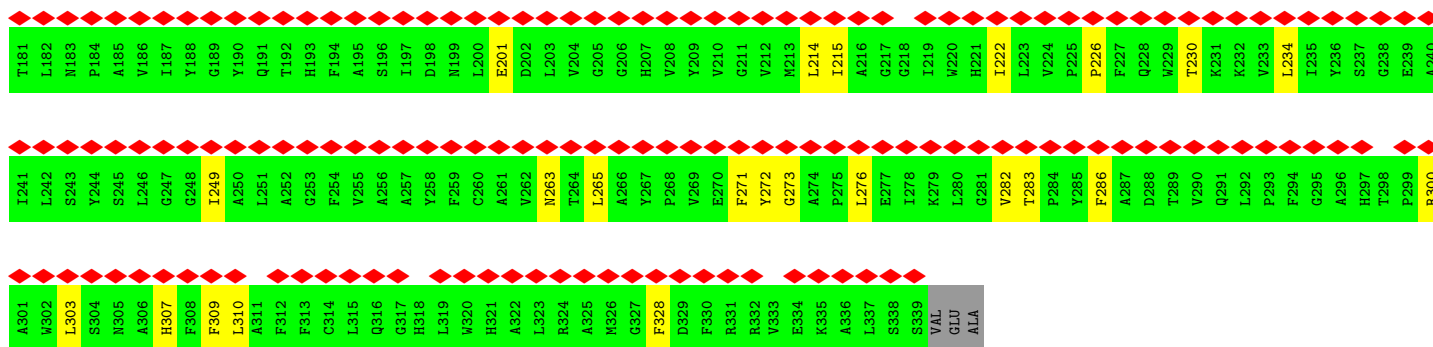
Chain 3: 76% 87% 12%



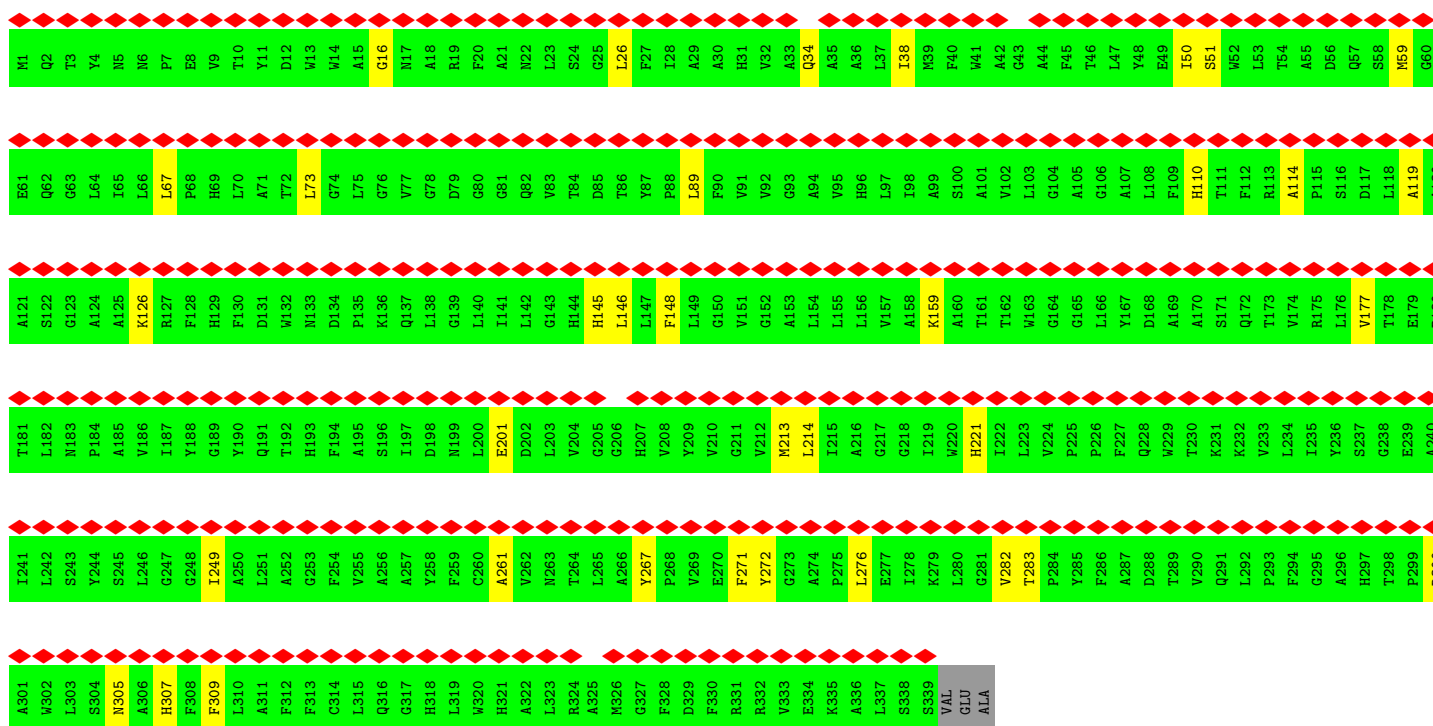
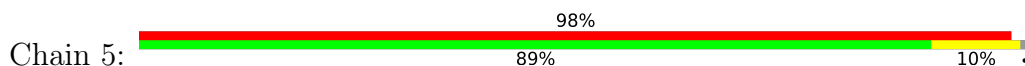
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain 4: 97% 81% 18%

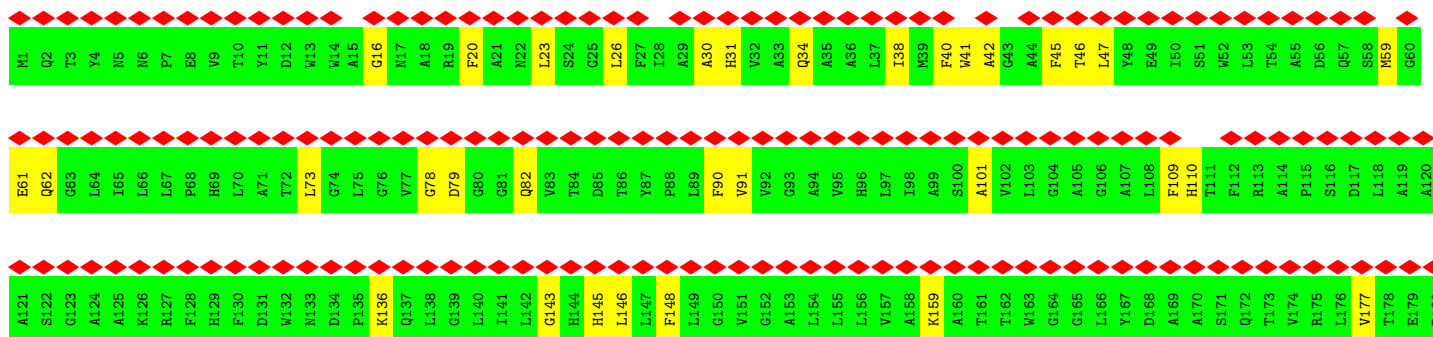
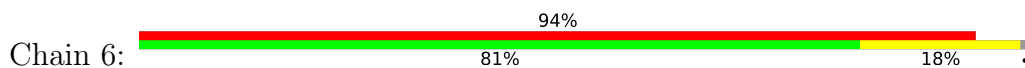


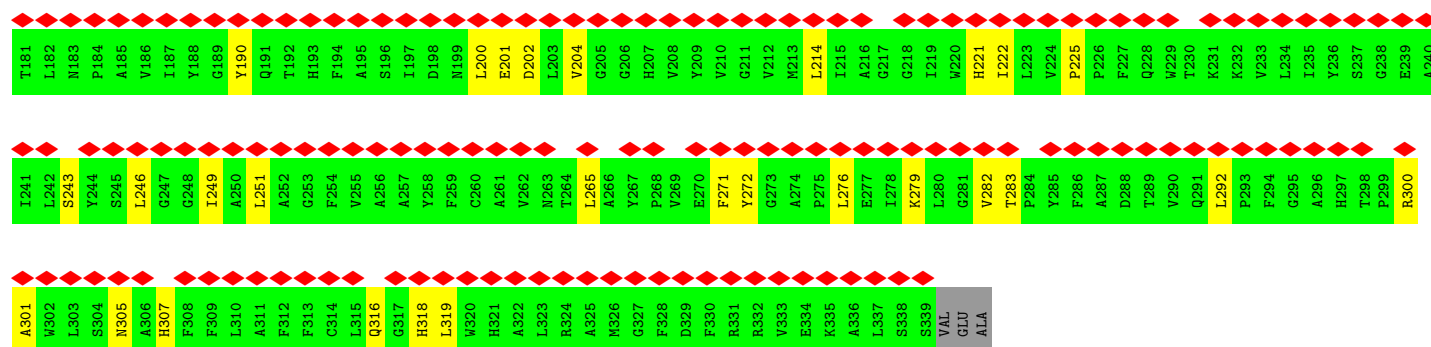


• Molecule 13: Iron stress-induced chlorophyll-binding protein



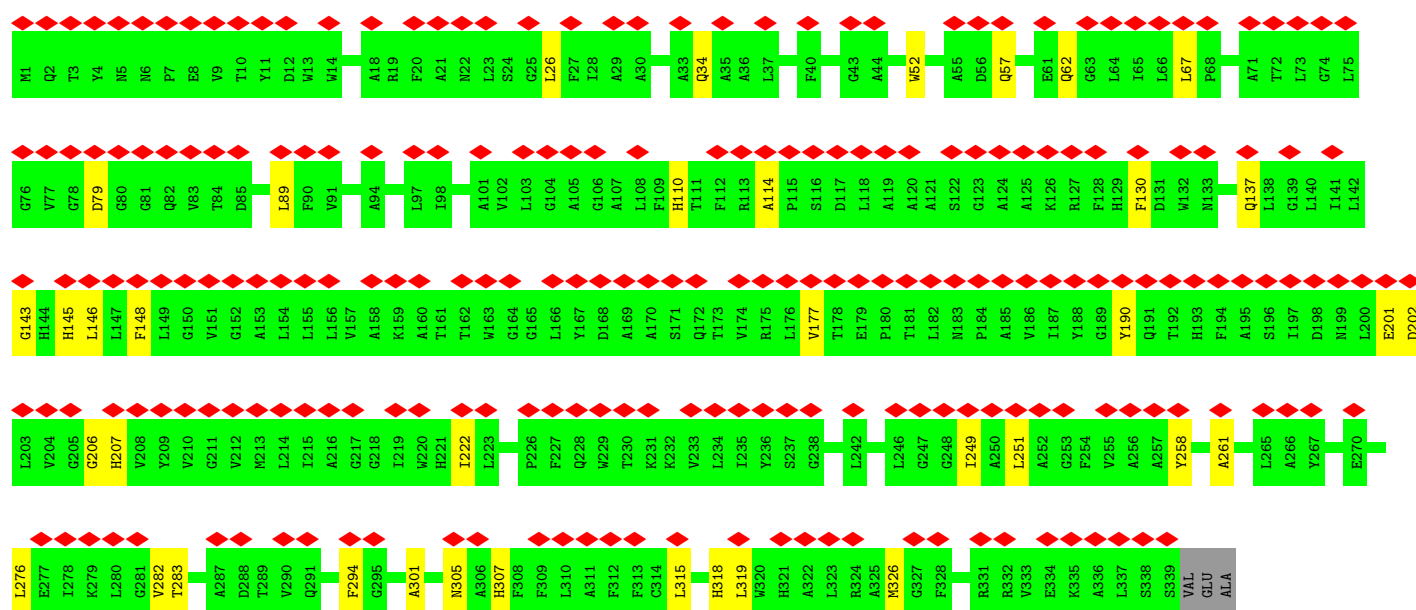
• Molecule 13: Iron stress-induced chlorophyll-binding protein





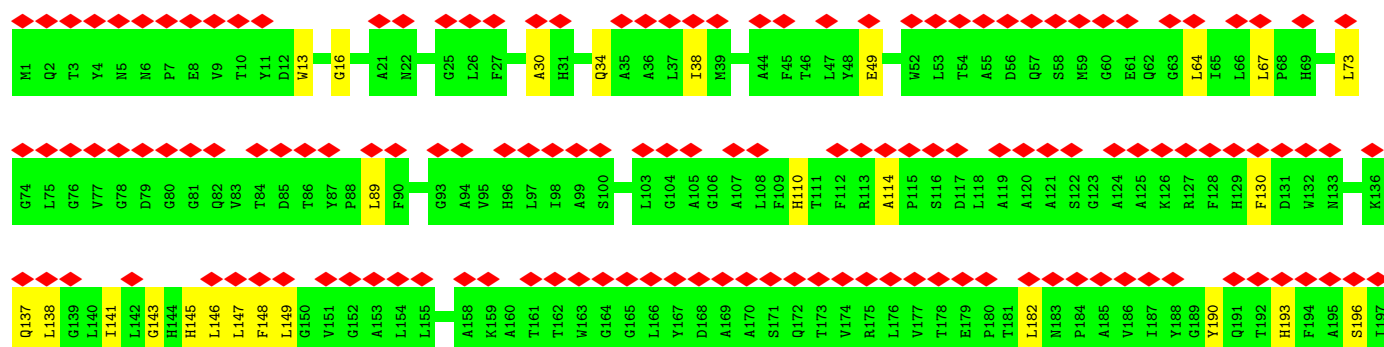
• Molecule 13: Iron stress-induced chlorophyll-binding protein

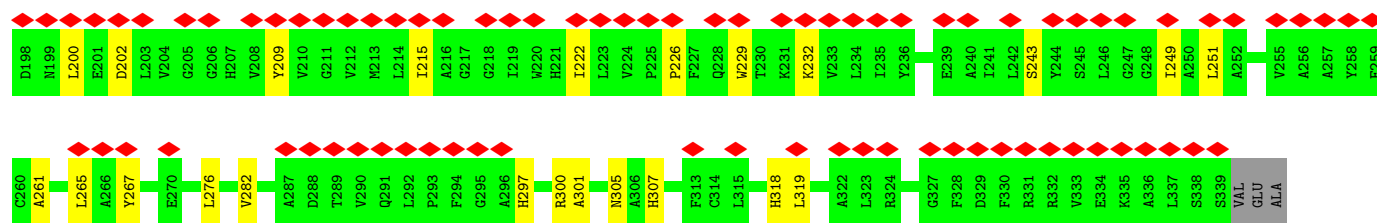
Chain Y: 65% 88% 11%



• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain Z: 65% 85% 14%





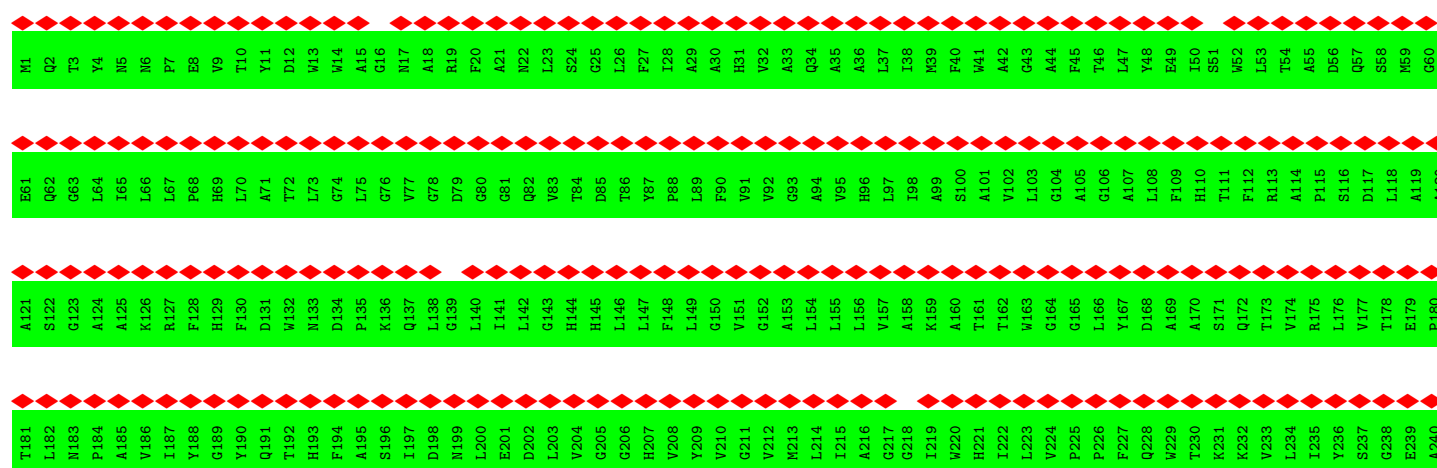
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain a: 78% 99%



• Molecule 13: Iron stress-induced chlorophyll-binding protein

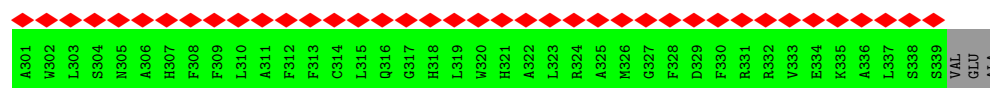
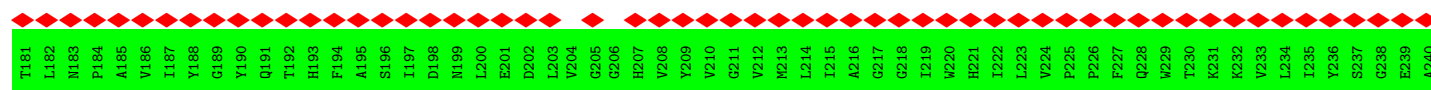
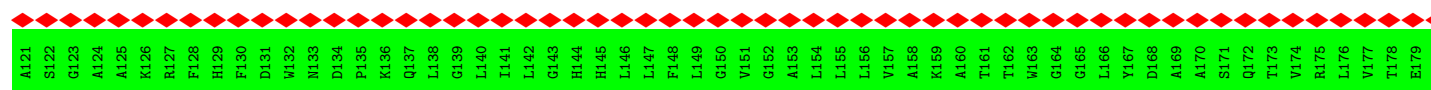
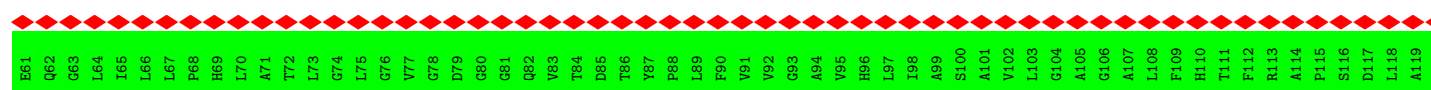
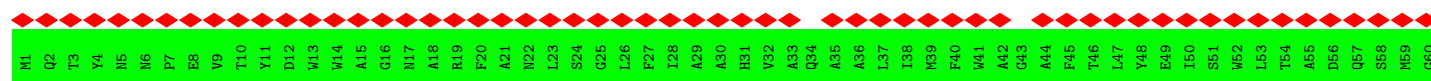
Chain b: 97% 99%





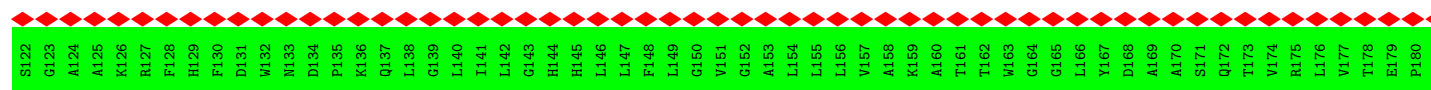
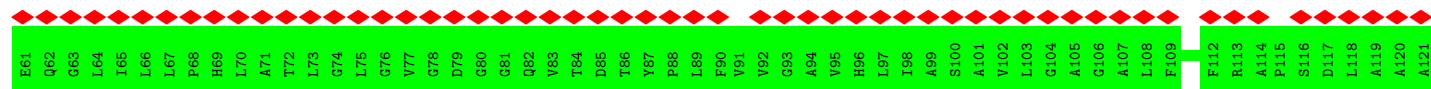
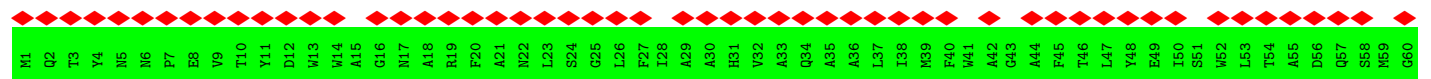
• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain c: 98%
99%

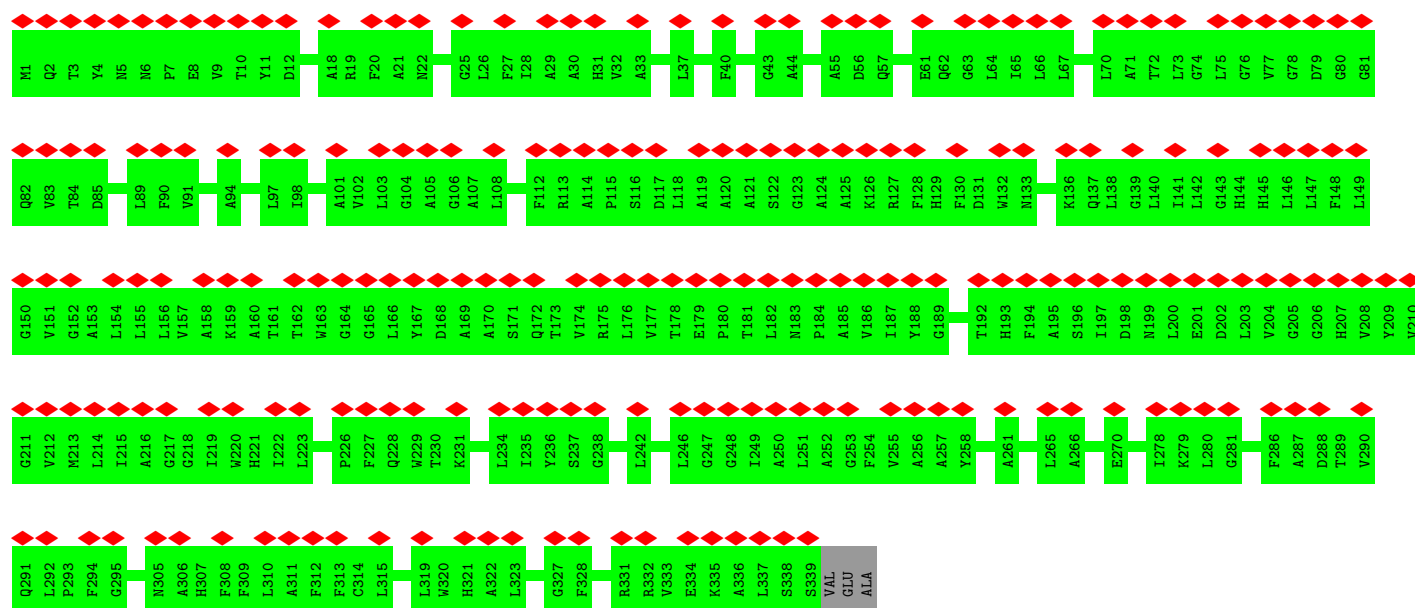


• Molecule 13: Iron stress-induced chlorophyll-binding protein

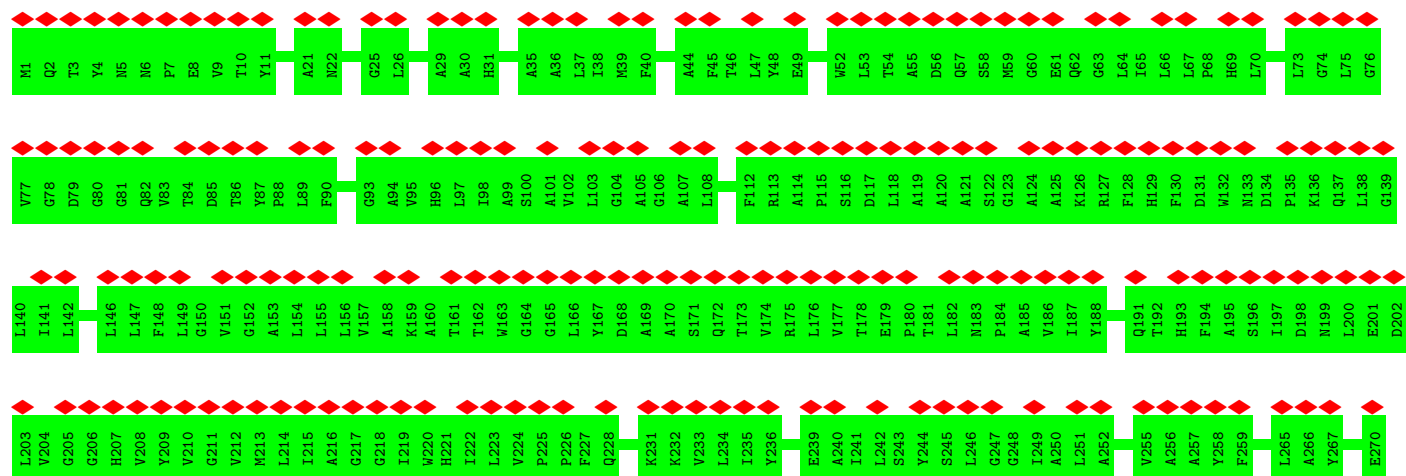
Chain d: 93%
99%

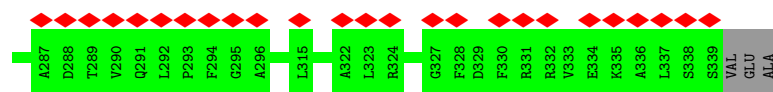


- Molecule 13: Iron stress-induced chlorophyll-binding protein

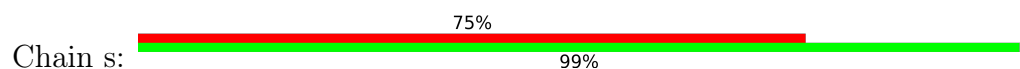


- Molecule 13: Iron stress-induced chlorophyll-binding protein

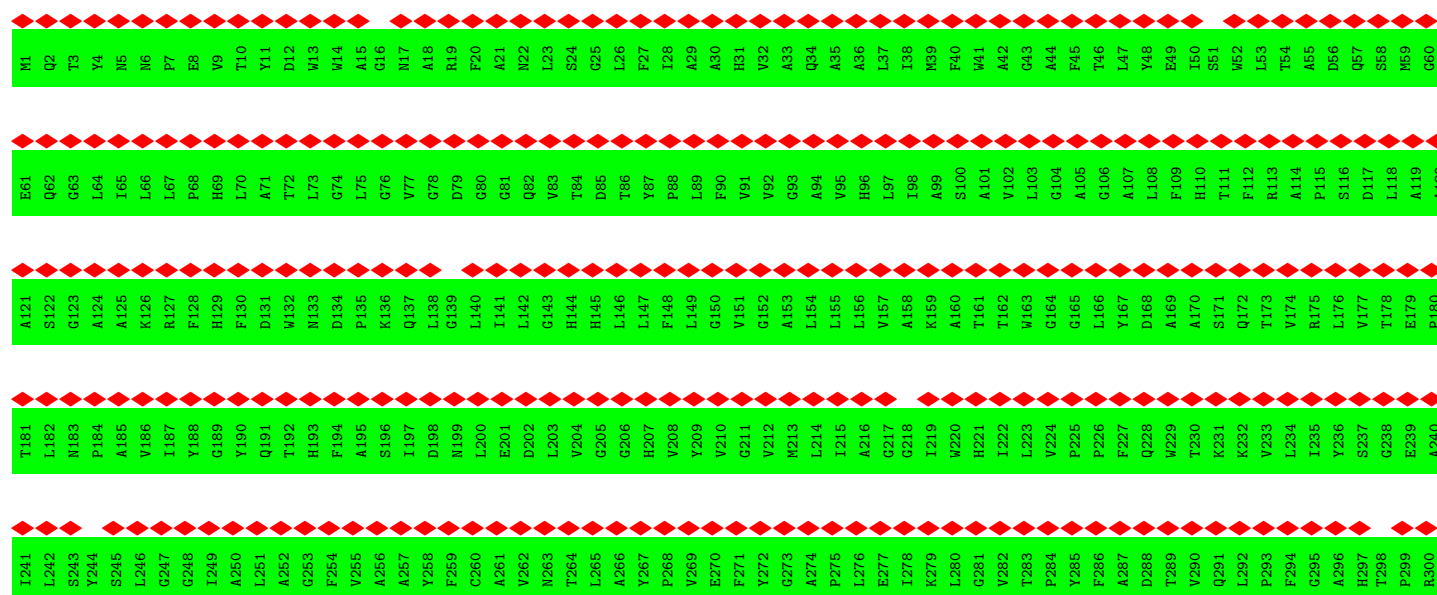


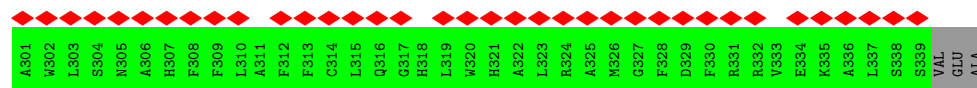


- Molecule 13: Iron stress-induced chlorophyll-binding protein



- Molecule 13: Iron stress-induced chlorophyll-binding protein





• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain u:

• Molecule 13: Iron stress-induced chlorophyll-binding protein

Chain v:

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|
| W302 | L303 | S304 | N305 | A306 | H307 | F308 | F309 | L310 | A311 | F312 | F313 | C314 | L315 | Q316 | G317 | H318 | L319 | W320 | H321 | A322 | L323 | R324 | A325 | M326 | G327 | F328 | D329 | F330 | R331 | R332 | V333 | E334 | K335 | A336 | L337 | S338 | S339 | VAL | GLU | ALA |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C3 | Depositor |
| Number of particles used | 29295 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.118 | Depositor |
| Minimum map value | -0.042 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.014 | Depositor |
| Map size (Å) | 480.0, 480.0, 480.0 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.0, 1.0, 1.0 | 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: LHG, LMU, PQN, SQD, LMG, BCR, SF4, CLA, FMN

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 | 0.54 | 0/6064 | 0.57 | 0/8274 |
| 1 | G | 0.54 | 0/6064 | 0.57 | 0/8274 |
| 1 | e | 0.54 | 0/6064 | 0.57 | 0/8274 |
| 2 | B | 0.46 | 0/5999 | 0.54 | 0/8199 |
| 2 | H | 0.46 | 0/5999 | 0.54 | 0/8199 |
| 2 | f | 0.46 | 0/5999 | 0.54 | 0/8199 |
| 3 | C | 0.44 | 0/608 | 0.56 | 0/823 |
| 3 | N | 0.44 | 0/608 | 0.56 | 0/823 |
| 3 | g | 0.44 | 0/608 | 0.56 | 0/823 |
| 4 | D | 0.48 | 0/1124 | 0.58 | 0/1516 |
| 4 | O | 0.48 | 0/1124 | 0.58 | 0/1516 |
| 4 | h | 0.48 | 0/1124 | 0.58 | 0/1516 |
| 5 | E | 0.44 | 0/553 | 0.53 | 0/750 |
| 5 | Q | 0.44 | 0/553 | 0.53 | 0/750 |
| 5 | i | 0.44 | 0/553 | 0.53 | 0/750 |
| 6 | F | 0.43 | 0/1062 | 0.54 | 0/1442 |
| 6 | R | 0.43 | 0/1062 | 0.54 | 0/1442 |
| 6 | j | 0.43 | 0/1062 | 0.54 | 0/1442 |
| 7 | I | 0.49 | 0/289 | 0.71 | 0/393 |
| 7 | S | 0.49 | 0/289 | 0.71 | 0/393 |
| 7 | k | 0.49 | 0/289 | 0.71 | 0/393 |
| 8 | J | 0.37 | 0/346 | 0.55 | 0/469 |
| 8 | T | 0.37 | 0/346 | 0.55 | 0/469 |
| 8 | l | 0.38 | 0/346 | 0.55 | 0/469 |
| 9 | K | 0.33 | 0/560 | 0.58 | 0/765 |
| 9 | U | 0.34 | 0/560 | 0.58 | 0/765 |
| 9 | m | 0.34 | 0/560 | 0.58 | 0/765 |
| 10 | L | 0.42 | 0/1242 | 0.55 | 0/1696 |
| 10 | V | 0.42 | 0/1242 | 0.55 | 0/1696 |
| 10 | n | 0.42 | 0/1242 | 0.55 | 0/1696 |
| 11 | M | 0.42 | 0/231 | 0.60 | 0/314 |
| 11 | W | 0.42 | 0/231 | 0.60 | 0/314 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|----------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 11 | o | 0.42 | 0/231 | 0.60 | 0/314 |
| 12 | P | 0.31 | 0/1344 | 0.50 | 0/1822 |
| 12 | X | 0.31 | 0/1344 | 0.50 | 0/1822 |
| 12 | p | 0.31 | 0/1344 | 0.50 | 0/1822 |
| 13 | 1 | 0.30 | 0/2689 | 0.48 | 0/3678 |
| 13 | 2 | 0.30 | 0/2689 | 0.48 | 0/3678 |
| 13 | 3 | 0.28 | 0/2689 | 0.47 | 0/3678 |
| 13 | 4 | 0.28 | 0/2689 | 0.49 | 0/3678 |
| 13 | 5 | 0.29 | 0/2689 | 0.48 | 0/3678 |
| 13 | 6 | 0.28 | 0/2689 | 0.47 | 0/3678 |
| 13 | Y | 0.30 | 0/2689 | 0.48 | 0/3678 |
| 13 | Z | 0.30 | 0/2689 | 0.48 | 0/3678 |
| 13 | a | 0.28 | 0/2689 | 0.47 | 0/3678 |
| 13 | b | 0.28 | 0/2689 | 0.49 | 0/3678 |
| 13 | c | 0.29 | 0/2689 | 0.48 | 0/3678 |
| 13 | d | 0.28 | 0/2689 | 0.48 | 0/3678 |
| 13 | q | 0.30 | 0/2689 | 0.48 | 0/3678 |
| 13 | r | 0.30 | 0/2689 | 0.49 | 0/3678 |
| 13 | s | 0.28 | 0/2689 | 0.47 | 0/3678 |
| 13 | t | 0.28 | 0/2689 | 0.49 | 0/3678 |
| 13 | u | 0.29 | 0/2689 | 0.48 | 0/3678 |
| 13 | v | 0.29 | 0/2689 | 0.48 | 0/3678 |
| All | All | 0.40 | 0/106668 | 0.52 | 0/145593 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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 | 5865 | 0 | 5744 | 102 | 0 |
| 1 | G | 5865 | 0 | 5744 | 103 | 0 |
| 1 | e | 5865 | 0 | 5744 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | B | 5789 | 0 | 5575 | 104 | 0 |
| 2 | H | 5789 | 0 | 5575 | 107 | 0 |
| 2 | f | 5789 | 0 | 5575 | 0 | 0 |
| 3 | C | 598 | 0 | 579 | 9 | 0 |
| 3 | N | 598 | 0 | 579 | 10 | 0 |
| 3 | g | 598 | 0 | 579 | 0 | 0 |
| 4 | D | 1098 | 0 | 1099 | 20 | 0 |
| 4 | O | 1098 | 0 | 1099 | 20 | 0 |
| 4 | h | 1098 | 0 | 1099 | 0 | 0 |
| 5 | E | 543 | 0 | 525 | 7 | 0 |
| 5 | Q | 543 | 0 | 525 | 6 | 0 |
| 5 | i | 543 | 0 | 525 | 0 | 0 |
| 6 | F | 1036 | 0 | 1031 | 17 | 0 |
| 6 | R | 1036 | 0 | 1031 | 13 | 0 |
| 6 | j | 1036 | 0 | 1031 | 0 | 0 |
| 7 | I | 282 | 0 | 291 | 8 | 0 |
| 7 | S | 282 | 0 | 291 | 5 | 0 |
| 7 | k | 282 | 0 | 291 | 0 | 0 |
| 8 | J | 335 | 0 | 344 | 8 | 0 |
| 8 | T | 335 | 0 | 344 | 8 | 0 |
| 8 | l | 335 | 0 | 344 | 0 | 0 |
| 9 | K | 549 | 0 | 597 | 15 | 0 |
| 9 | U | 549 | 0 | 597 | 16 | 0 |
| 9 | m | 549 | 0 | 597 | 0 | 0 |
| 10 | L | 1210 | 0 | 1206 | 34 | 0 |
| 10 | V | 1210 | 0 | 1206 | 31 | 0 |
| 10 | n | 1210 | 0 | 1206 | 0 | 0 |
| 11 | M | 228 | 0 | 246 | 6 | 0 |
| 11 | W | 228 | 0 | 246 | 4 | 0 |
| 11 | o | 228 | 0 | 246 | 0 | 0 |
| 12 | P | 1318 | 0 | 1233 | 19 | 0 |
| 12 | X | 1318 | 0 | 1233 | 17 | 0 |
| 12 | p | 1318 | 0 | 1233 | 0 | 0 |
| 13 | 1 | 2605 | 0 | 2564 | 36 | 0 |
| 13 | 2 | 2605 | 0 | 2564 | 42 | 0 |
| 13 | 3 | 2605 | 0 | 2564 | 37 | 0 |
| 13 | 4 | 2605 | 0 | 2564 | 44 | 0 |
| 13 | 5 | 2605 | 0 | 2564 | 31 | 0 |
| 13 | 6 | 2605 | 0 | 2564 | 46 | 0 |
| 13 | Y | 2605 | 0 | 2564 | 40 | 0 |
| 13 | Z | 2605 | 0 | 2564 | 44 | 0 |
| 13 | a | 2605 | 0 | 2564 | 0 | 0 |

Continued on next page...

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13 | b | 2605 | 0 | 2564 | 0 | 0 |
| 13 | c | 2605 | 0 | 2564 | 0 | 0 |
| 13 | d | 2605 | 0 | 2564 | 0 | 0 |
| 13 | q | 2605 | 0 | 2564 | 0 | 0 |
| 13 | r | 2605 | 0 | 2564 | 0 | 0 |
| 13 | s | 2605 | 0 | 2564 | 0 | 0 |
| 13 | t | 2605 | 0 | 2564 | 0 | 0 |
| 13 | u | 2605 | 0 | 2564 | 0 | 0 |
| 13 | v | 2605 | 0 | 2564 | 0 | 0 |
| 14 | 1 | 765 | 0 | 561 | 26 | 0 |
| 14 | 2 | 850 | 0 | 720 | 31 | 0 |
| 14 | 3 | 785 | 0 | 593 | 22 | 0 |
| 14 | 4 | 765 | 0 | 561 | 21 | 0 |
| 14 | 5 | 785 | 0 | 600 | 20 | 0 |
| 14 | 6 | 785 | 0 | 600 | 25 | 0 |
| 14 | A | 2712 | 0 | 2766 | 133 | 0 |
| 14 | B | 2515 | 0 | 2595 | 130 | 0 |
| 14 | F | 90 | 0 | 66 | 4 | 0 |
| 14 | G | 2712 | 0 | 2766 | 138 | 0 |
| 14 | H | 2515 | 0 | 2595 | 125 | 0 |
| 14 | J | 100 | 0 | 82 | 4 | 0 |
| 14 | K | 148 | 0 | 118 | 3 | 0 |
| 14 | L | 185 | 0 | 190 | 9 | 0 |
| 14 | R | 90 | 0 | 66 | 4 | 0 |
| 14 | T | 100 | 0 | 82 | 4 | 0 |
| 14 | U | 148 | 0 | 118 | 3 | 0 |
| 14 | V | 185 | 0 | 190 | 13 | 0 |
| 14 | Y | 765 | 0 | 561 | 29 | 0 |
| 14 | Z | 850 | 0 | 720 | 32 | 0 |
| 14 | a | 785 | 0 | 593 | 0 | 0 |
| 14 | b | 765 | 0 | 561 | 0 | 0 |
| 14 | c | 785 | 0 | 600 | 0 | 0 |
| 14 | d | 785 | 0 | 600 | 0 | 0 |
| 14 | e | 2712 | 0 | 2766 | 0 | 0 |
| 14 | f | 2515 | 0 | 2595 | 0 | 0 |
| 14 | j | 90 | 0 | 66 | 0 | 0 |
| 14 | l | 100 | 0 | 82 | 0 | 0 |
| 14 | m | 148 | 0 | 118 | 0 | 0 |
| 14 | n | 185 | 0 | 190 | 0 | 0 |
| 14 | q | 765 | 0 | 561 | 0 | 0 |
| 14 | r | 850 | 0 | 720 | 0 | 0 |
| 14 | s | 785 | 0 | 593 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | t | 765 | 0 | 561 | 0 | 0 |
| 14 | u | 785 | 0 | 600 | 0 | 0 |
| 14 | v | 785 | 0 | 600 | 0 | 0 |
| 15 | A | 33 | 0 | 46 | 4 | 0 |
| 15 | B | 33 | 0 | 46 | 4 | 0 |
| 15 | G | 33 | 0 | 46 | 3 | 0 |
| 15 | H | 33 | 0 | 46 | 5 | 0 |
| 15 | e | 33 | 0 | 46 | 0 | 0 |
| 15 | f | 33 | 0 | 46 | 0 | 0 |
| 16 | A | 8 | 0 | 0 | 0 | 0 |
| 16 | C | 16 | 0 | 0 | 0 | 0 |
| 16 | G | 8 | 0 | 0 | 0 | 0 |
| 16 | N | 16 | 0 | 0 | 0 | 0 |
| 16 | e | 8 | 0 | 0 | 0 | 0 |
| 16 | g | 16 | 0 | 0 | 0 | 0 |
| 17 | 1 | 160 | 0 | 224 | 16 | 0 |
| 17 | 2 | 160 | 0 | 224 | 16 | 0 |
| 17 | 3 | 160 | 0 | 224 | 5 | 0 |
| 17 | 4 | 160 | 0 | 224 | 7 | 0 |
| 17 | 5 | 160 | 0 | 224 | 7 | 0 |
| 17 | 6 | 160 | 0 | 224 | 12 | 0 |
| 17 | A | 240 | 0 | 336 | 22 | 0 |
| 17 | B | 280 | 0 | 392 | 31 | 0 |
| 17 | F | 40 | 0 | 56 | 6 | 0 |
| 17 | G | 240 | 0 | 336 | 20 | 0 |
| 17 | H | 280 | 0 | 392 | 29 | 0 |
| 17 | I | 40 | 0 | 56 | 4 | 0 |
| 17 | J | 120 | 0 | 168 | 15 | 0 |
| 17 | K | 40 | 0 | 56 | 3 | 0 |
| 17 | L | 160 | 0 | 224 | 18 | 0 |
| 17 | M | 40 | 0 | 56 | 2 | 0 |
| 17 | R | 40 | 0 | 56 | 6 | 0 |
| 17 | S | 40 | 0 | 56 | 3 | 0 |
| 17 | T | 120 | 0 | 168 | 14 | 0 |
| 17 | U | 40 | 0 | 56 | 3 | 0 |
| 17 | V | 160 | 0 | 224 | 22 | 0 |
| 17 | W | 40 | 0 | 56 | 3 | 0 |
| 17 | Y | 160 | 0 | 224 | 13 | 0 |
| 17 | Z | 160 | 0 | 224 | 16 | 0 |
| 17 | a | 160 | 0 | 224 | 0 | 0 |
| 17 | b | 160 | 0 | 224 | 0 | 0 |
| 17 | c | 160 | 0 | 224 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17 | d | 160 | 0 | 224 | 0 | 0 |
| 17 | e | 240 | 0 | 336 | 0 | 0 |
| 17 | f | 280 | 0 | 392 | 0 | 0 |
| 17 | j | 40 | 0 | 56 | 0 | 0 |
| 17 | k | 40 | 0 | 56 | 0 | 0 |
| 17 | l | 120 | 0 | 168 | 0 | 0 |
| 17 | m | 40 | 0 | 56 | 0 | 0 |
| 17 | n | 160 | 0 | 224 | 0 | 0 |
| 17 | o | 40 | 0 | 56 | 0 | 0 |
| 17 | q | 160 | 0 | 224 | 0 | 0 |
| 17 | r | 160 | 0 | 224 | 0 | 0 |
| 17 | s | 160 | 0 | 224 | 0 | 0 |
| 17 | t | 160 | 0 | 224 | 0 | 0 |
| 17 | u | 160 | 0 | 224 | 0 | 0 |
| 17 | v | 160 | 0 | 224 | 0 | 0 |
| 18 | A | 374 | 0 | 493 | 32 | 0 |
| 18 | B | 78 | 0 | 96 | 6 | 0 |
| 18 | G | 374 | 0 | 493 | 32 | 0 |
| 18 | H | 78 | 0 | 96 | 6 | 0 |
| 18 | I | 48 | 0 | 69 | 2 | 0 |
| 18 | L | 127 | 0 | 170 | 7 | 0 |
| 18 | S | 48 | 0 | 69 | 0 | 0 |
| 18 | V | 127 | 0 | 170 | 14 | 0 |
| 18 | e | 374 | 0 | 493 | 0 | 0 |
| 18 | f | 78 | 0 | 96 | 0 | 0 |
| 18 | k | 48 | 0 | 69 | 0 | 0 |
| 18 | n | 127 | 0 | 170 | 0 | 0 |
| 19 | A | 58 | 0 | 76 | 3 | 0 |
| 19 | B | 35 | 0 | 46 | 1 | 0 |
| 19 | G | 58 | 0 | 76 | 3 | 0 |
| 19 | H | 35 | 0 | 46 | 1 | 0 |
| 19 | J | 22 | 0 | 28 | 0 | 0 |
| 19 | T | 22 | 0 | 28 | 0 | 0 |
| 19 | e | 58 | 0 | 76 | 0 | 0 |
| 19 | f | 35 | 0 | 46 | 0 | 0 |
| 19 | l | 22 | 0 | 28 | 0 | 0 |
| 20 | B | 53 | 0 | 76 | 5 | 0 |
| 20 | H | 53 | 0 | 76 | 6 | 0 |
| 20 | J | 32 | 0 | 34 | 0 | 0 |
| 20 | T | 32 | 0 | 34 | 1 | 0 |
| 20 | f | 53 | 0 | 76 | 0 | 0 |
| 20 | l | 32 | 0 | 34 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 21 | 1 | 32 | 0 | 28 | 1 | 0 |
| 21 | 2 | 28 | 0 | 20 | 0 | 0 |
| 21 | 3 | 28 | 0 | 20 | 2 | 0 |
| 21 | 4 | 26 | 0 | 16 | 0 | 0 |
| 21 | 5 | 26 | 0 | 16 | 0 | 0 |
| 21 | 6 | 26 | 0 | 16 | 0 | 0 |
| 21 | B | 40 | 0 | 42 | 8 | 0 |
| 21 | H | 40 | 0 | 42 | 9 | 0 |
| 21 | L | 46 | 0 | 58 | 4 | 0 |
| 21 | V | 46 | 0 | 58 | 6 | 0 |
| 21 | Y | 32 | 0 | 28 | 1 | 0 |
| 21 | Z | 28 | 0 | 20 | 0 | 0 |
| 21 | a | 28 | 0 | 20 | 0 | 0 |
| 21 | b | 26 | 0 | 16 | 0 | 0 |
| 21 | c | 26 | 0 | 16 | 0 | 0 |
| 21 | d | 26 | 0 | 16 | 0 | 0 |
| 21 | f | 40 | 0 | 42 | 0 | 0 |
| 21 | n | 46 | 0 | 58 | 0 | 0 |
| 21 | q | 32 | 0 | 28 | 0 | 0 |
| 21 | r | 28 | 0 | 20 | 0 | 0 |
| 21 | s | 28 | 0 | 20 | 0 | 0 |
| 21 | t | 26 | 0 | 16 | 0 | 0 |
| 21 | u | 26 | 0 | 16 | 0 | 0 |
| 21 | v | 26 | 0 | 16 | 0 | 0 |
| 22 | P | 31 | 0 | 19 | 1 | 0 |
| 22 | X | 31 | 0 | 19 | 1 | 0 |
| 22 | p | 31 | 0 | 19 | 0 | 0 |
| 23 | A | 9 | 0 | 0 | 1 | 0 |
| 23 | B | 7 | 0 | 0 | 0 | 0 |
| 23 | F | 1 | 0 | 0 | 0 | 0 |
| 23 | G | 9 | 0 | 0 | 1 | 0 |
| 23 | H | 7 | 0 | 0 | 0 | 0 |
| 23 | L | 1 | 0 | 0 | 0 | 0 |
| 23 | R | 1 | 0 | 0 | 0 | 0 |
| 23 | V | 1 | 0 | 0 | 0 | 0 |
| 23 | e | 9 | 0 | 0 | 0 | 0 |
| 23 | f | 7 | 0 | 0 | 0 | 0 |
| 23 | j | 1 | 0 | 0 | 0 | 0 |
| 23 | n | 1 | 0 | 0 | 0 | 0 |
| All | All | 144312 | 0 | 142227 | 1516 | 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 9.

All (1516) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L:3:GLN:HG2 | 10:L:4:ASP:H | 0.93 | 1.06 |
| 10:V:3:GLN:HG2 | 10:V:4:ASP:H | 0.93 | 1.05 |
| 10:L:3:GLN:HG2 | 10:L:4:ASP:N | 1.75 | 1.00 |
| 10:V:3:GLN:HG2 | 10:V:4:ASP:N | 1.75 | 0.98 |
| 10:L:94:SER:HB2 | 14:V:1501:CLA:HMD1 | 1.54 | 0.87 |
| 10:V:3:GLN:CG | 10:V:4:ASP:H | 1.82 | 0.87 |
| 18:A:5009:LHG:H131 | 17:1:521:BCR:H322 | 1.57 | 0.86 |
| 10:L:137:LEU:HD13 | 17:V:4022:BCR:C24 | 2.06 | 0.85 |
| 10:L:3:GLN:CG | 10:L:4:ASP:H | 1.82 | 0.85 |
| 18:G:5009:LHG:H131 | 17:Y:521:BCR:H322 | 1.57 | 0.85 |
| 14:B:1207:CLA:H42 | 18:V:5221:LHG:H252 | 1.59 | 0.82 |
| 14:G:1013:CLA:H111 | 17:G:4011:BCR:H23C | 1.67 | 0.76 |
| 13:4:145:HIS:NE2 | 14:4:512:CLA:NA | 2.32 | 0.76 |
| 4:O:41:GLU:H | 4:O:71:GLN:HE22 | 1.35 | 0.75 |
| 14:A:1013:CLA:H111 | 17:A:4011:BCR:H23C | 1.67 | 0.74 |
| 13:Y:148:PHE:CZ | 14:Y:516:CLA:HBC2 | 2.22 | 0.74 |
| 13:1:148:PHE:CZ | 14:1:516:CLA:HBC2 | 2.22 | 0.74 |
| 14:A:1130:CLA:H2 | 14:L:1502:CLA:H43 | 1.68 | 0.74 |
| 14:G:1130:CLA:H2 | 14:V:1502:CLA:H43 | 1.68 | 0.74 |
| 4:D:41:GLU:H | 4:D:71:GLN:HE22 | 1.35 | 0.73 |
| 9:K:60:VAL:HG22 | 14:K:1105:CLA:HAC2 | 1.71 | 0.72 |
| 10:L:137:LEU:HD13 | 17:V:4022:BCR:H24C | 1.71 | 0.71 |
| 13:1:52:TRP:CE3 | 14:1:504:CLA:HED3 | 2.25 | 0.71 |
| 1:G:410:GLY:HA3 | 1:G:614:LEU:HD11 | 1.73 | 0.71 |
| 1:A:410:GLY:HA3 | 1:A:614:LEU:HD11 | 1.73 | 0.71 |
| 9:U:60:VAL:HG22 | 14:U:1105:CLA:HAC2 | 1.71 | 0.71 |
| 13:Y:148:PHE:HZ | 14:Y:516:CLA:HBC2 | 1.54 | 0.71 |
| 14:6:505:CLA:H43 | 17:6:524:BCR:HC7 | 1.72 | 0.71 |
| 13:Y:52:TRP:CE3 | 14:Y:504:CLA:HED3 | 2.25 | 0.71 |
| 14:B:1216:CLA:H2 | 14:B:1221:CLA:H102 | 1.71 | 0.71 |
| 14:H:1216:CLA:H2 | 14:H:1221:CLA:H102 | 1.71 | 0.71 |
| 14:H:1222:CLA:HMA1 | 17:H:4010:BCR:H14C | 1.74 | 0.70 |
| 13:1:148:PHE:HZ | 14:1:516:CLA:HBC2 | 1.54 | 0.70 |
| 14:A:1104:CLA:H42 | 14:A:1128:CLA:H2 | 1.74 | 0.69 |
| 11:M:21:TYR:OH | 10:V:26:PHE:HB2 | 1.92 | 0.69 |
| 13:5:146:LEU:HD21 | 14:5:506:CLA:HAB | 1.75 | 0.69 |
| 14:F:1302:CLA:HMB2 | 17:F:4016:BCR:H24C | 1.74 | 0.69 |
| 13:3:110:HIS:NE2 | 14:3:513:CLA:NB | 2.40 | 0.69 |
| 14:H:1234:CLA:H71 | 14:H:1235:CLA:H12 | 1.75 | 0.69 |
| 14:R:1302:CLA:HMB2 | 17:R:4016:BCR:H24C | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:Y:222:ILE:HG23 | 14:Y:516:CLA:HMA1 | 1.75 | 0.69 |
| 14:B:1234:CLA:H71 | 14:B:1235:CLA:H12 | 1.75 | 0.69 |
| 14:G:1104:CLA:H42 | 14:G:1128:CLA:H2 | 1.74 | 0.69 |
| 13:Y:318:HIS:NE2 | 14:Y:505:CLA:NB | 2.42 | 0.68 |
| 14:B:1222:CLA:HMA1 | 17:B:4010:BCR:H14C | 1.74 | 0.67 |
| 13:1:222:ILE:HG23 | 14:1:516:CLA:HMA1 | 1.75 | 0.67 |
| 13:2:146:LEU:HD21 | 14:2:506:CLA:HAB | 1.75 | 0.67 |
| 13:Z:146:LEU:HD21 | 14:Z:506:CLA:HAB | 1.75 | 0.67 |
| 18:H:1855:LHG:HC82 | 18:H:1855:LHG:H252 | 1.77 | 0.67 |
| 18:B:1855:LHG:HC82 | 18:B:1855:LHG:H252 | 1.77 | 0.66 |
| 5:E:10:ARG:HB3 | 5:E:67:GLN:HG2 | 1.78 | 0.66 |
| 5:Q:10:ARG:HB3 | 5:Q:67:GLN:HG2 | 1.77 | 0.66 |
| 13:1:318:HIS:NE2 | 14:1:505:CLA:NB | 2.42 | 0.65 |
| 6:R:91:ILE:HG23 | 14:R:1301:CLA:HAA1 | 1.78 | 0.65 |
| 10:L:134:LEU:HD13 | 10:V:134:LEU:HD13 | 1.78 | 0.65 |
| 10:L:133:ILE:CG2 | 10:V:48:LEU:HD21 | 2.26 | 0.64 |
| 13:3:272:TYR:HB3 | 13:3:300:ARG:HB2 | 1.80 | 0.64 |
| 14:A:1126:CLA:H201 | 17:J:4012:BCR:H12C | 1.80 | 0.64 |
| 14:B:1207:CLA:H42 | 18:V:5221:LHG:C25 | 2.27 | 0.64 |
| 6:F:91:ILE:HG23 | 14:F:1301:CLA:HAA1 | 1.78 | 0.64 |
| 14:H:1239:CLA:HBA2 | 15:H:2002:PQN:H251 | 1.80 | 0.64 |
| 14:H:1203:CLA:H152 | 14:H:1225:CLA:HBB2 | 1.79 | 0.64 |
| 14:G:1136:CLA:HBC1 | 18:V:5220:LHG:H282 | 1.80 | 0.63 |
| 18:A:5005:LHG:HC61 | 17:2:521:BCR:HC22 | 1.81 | 0.63 |
| 14:B:1203:CLA:H152 | 14:B:1225:CLA:HBB2 | 1.79 | 0.63 |
| 17:A:4011:BCR:H362 | 14:B:1012:CLA:H2 | 1.80 | 0.63 |
| 17:J:4013:BCR:H362 | 17:J:4012:BCR:H17C | 1.81 | 0.63 |
| 18:G:5005:LHG:HC61 | 17:Z:521:BCR:HC22 | 1.81 | 0.63 |
| 14:B:1214:CLA:HBA2 | 14:B:1223:CLA:HBB2 | 1.80 | 0.63 |
| 14:B:1239:CLA:HBA2 | 15:B:2002:PQN:H251 | 1.80 | 0.63 |
| 17:V:4022:BCR:H333 | 21:V:5216:SQD:C14 | 2.29 | 0.63 |
| 17:L:4022:BCR:H333 | 21:L:5216:SQD:C14 | 2.29 | 0.62 |
| 17:T:4013:BCR:H362 | 17:T:4012:BCR:H17C | 1.81 | 0.62 |
| 14:G:1013:CLA:HBA2 | 2:H:427:LEU:HD12 | 1.82 | 0.62 |
| 14:H:1214:CLA:HBA2 | 14:H:1223:CLA:HBB2 | 1.80 | 0.62 |
| 4:O:73:ARG:NH1 | 4:O:106:GLU:OE2 | 2.31 | 0.62 |
| 4:D:73:ARG:NH1 | 4:D:106:GLU:OE2 | 2.31 | 0.62 |
| 6:F:143:SER:HB2 | 13:4:14:TRP:CZ3 | 2.34 | 0.62 |
| 13:6:249:ILE:HG12 | 14:6:502:CLA:HAC1 | 1.82 | 0.62 |
| 14:G:1126:CLA:H201 | 17:T:4012:BCR:H12C | 1.80 | 0.62 |
| 14:G:1101:CLA:H112 | 17:T:4013:BCR:H19C | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:A:1136:CLA:HBC1 | 18:L:5220:LHG:H282 | 1.80 | 0.62 |
| 13:6:272:TYR:HB3 | 13:6:300:ARG:HB2 | 1.81 | 0.62 |
| 14:A:1101:CLA:H112 | 17:J:4013:BCR:H19C | 1.82 | 0.62 |
| 17:G:4011:BCR:H362 | 14:H:1012:CLA:H2 | 1.80 | 0.61 |
| 14:B:1209:CLA:H71 | 14:B:1209:CLA:HBB1 | 1.83 | 0.61 |
| 13:2:34:GLN:OE1 | 14:2:510:CLA:NC | 2.34 | 0.61 |
| 14:B:1217:CLA:HBB1 | 17:B:4004:BCR:H14C | 1.82 | 0.61 |
| 14:B:1226:CLA:H42 | 20:B:5002:LMG:H302 | 1.82 | 0.61 |
| 13:3:249:ILE:HG12 | 14:3:502:CLA:HAC1 | 1.81 | 0.61 |
| 14:H:1217:CLA:HBB1 | 17:H:4004:BCR:H14C | 1.82 | 0.61 |
| 17:G:4011:BCR:H24C | 14:H:1230:CLA:HMC2 | 1.82 | 0.61 |
| 1:A:752:TRP:NE1 | 14:A:1126:CLA:O1A | 2.29 | 0.61 |
| 13:Z:34:GLN:OE1 | 14:Z:510:CLA:NC | 2.34 | 0.61 |
| 14:A:1011:CLA:HAA1 | 14:B:1021:CLA:HMB1 | 1.83 | 0.61 |
| 14:A:1013:CLA:HBA2 | 2:B:427:LEU:HD12 | 1.82 | 0.61 |
| 14:H:1202:CLA:H8 | 14:H:1221:CLA:HBA2 | 1.83 | 0.61 |
| 1:A:86:TRP:HA | 14:A:1105:CLA:HBB2 | 1.83 | 0.60 |
| 13:6:251:LEU:HD13 | 14:6:505:CLA:H122 | 1.82 | 0.60 |
| 1:G:86:TRP:HA | 14:G:1105:CLA:HBB2 | 1.83 | 0.60 |
| 13:6:61:GLU:HG3 | 13:6:292:LEU:HD13 | 1.82 | 0.60 |
| 14:G:1011:CLA:HAA1 | 14:H:1021:CLA:HMB1 | 1.83 | 0.60 |
| 14:H:1226:CLA:H42 | 20:H:5002:LMG:H302 | 1.82 | 0.60 |
| 14:B:1202:CLA:H8 | 14:B:1221:CLA:HBA2 | 1.83 | 0.60 |
| 17:A:4011:BCR:H24C | 14:B:1230:CLA:HMC2 | 1.82 | 0.60 |
| 1:G:494:PHE:HB3 | 14:G:1135:CLA:H11 | 1.84 | 0.60 |
| 4:D:32:TRP:NE1 | 4:D:50:MET:SD | 2.72 | 0.60 |
| 2:B:151:PHE:HE2 | 21:B:1852:SQD:H102 | 1.66 | 0.60 |
| 2:H:15:ASP:HB3 | 2:H:20:ARG:HB2 | 1.84 | 0.60 |
| 14:A:1102:CLA:H43 | 14:A:1109:CLA:HMC2 | 1.84 | 0.60 |
| 1:A:490:LEU:HD22 | 17:L:4219:BCR:H331 | 1.84 | 0.60 |
| 14:B:1225:CLA:H12 | 17:B:4005:BCR:H393 | 1.84 | 0.60 |
| 13:6:34:GLN:OE1 | 14:6:510:CLA:NC | 2.34 | 0.59 |
| 1:G:407:TRP:HB3 | 14:G:1126:CLA:HMC3 | 1.84 | 0.59 |
| 2:H:151:PHE:HE2 | 21:H:1852:SQD:H102 | 1.66 | 0.59 |
| 1:A:494:PHE:HB3 | 14:A:1135:CLA:H11 | 1.84 | 0.59 |
| 13:5:34:GLN:OE1 | 14:5:510:CLA:NC | 2.35 | 0.59 |
| 1:G:490:LEU:HD22 | 17:V:4219:BCR:H331 | 1.84 | 0.59 |
| 14:A:1237:CLA:H141 | 10:L:85:LEU:HD11 | 1.85 | 0.59 |
| 13:6:316:GLN:NE2 | 14:6:518:CLA:O1A | 2.34 | 0.59 |
| 2:H:456:GLU:OE1 | 6:R:68:HIS:ND1 | 2.35 | 0.59 |
| 14:B:1207:CLA:H42 | 18:V:5221:LHG:C24 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:607:LEU:HD21 | 14:G:1128:CLA:HBC1 | 1.83 | 0.59 |
| 14:G:1237:CLA:H141 | 10:V:85:LEU:HD11 | 1.85 | 0.59 |
| 14:B:1223:CLA:H122 | 17:B:4010:BCR:H17C | 1.85 | 0.59 |
| 13:Z:267:TYR:O | 13:Z:300:ARG:NH2 | 2.36 | 0.59 |
| 1:A:607:LEU:HD21 | 14:A:1128:CLA:HBC1 | 1.83 | 0.59 |
| 1:G:370:ILE:HD11 | 14:G:1119:CLA:H71 | 1.85 | 0.59 |
| 14:H:1225:CLA:H12 | 17:H:4005:BCR:H393 | 1.84 | 0.59 |
| 1:A:407:TRP:HB3 | 14:A:1126:CLA:HMC3 | 1.84 | 0.59 |
| 14:A:1103:CLA:H142 | 17:A:4003:BCR:H372 | 1.85 | 0.59 |
| 14:H:1209:CLA:H71 | 14:H:1209:CLA:HBB1 | 1.83 | 0.59 |
| 2:B:15:ASP:HB3 | 2:B:20:ARG:HB2 | 1.84 | 0.59 |
| 14:V:1501:CLA:H121 | 17:V:4022:BCR:HC8 | 1.85 | 0.59 |
| 14:B:1229:CLA:H192 | 17:F:4016:BCR:H17C | 1.85 | 0.59 |
| 14:H:1229:CLA:H192 | 17:R:4016:BCR:H17C | 1.85 | 0.59 |
| 1:A:551:ALA:HB1 | 14:A:1136:CLA:HMB3 | 1.85 | 0.58 |
| 15:G:2001:PQN:H162 | 17:H:4014:BCR:H382 | 1.85 | 0.58 |
| 15:A:2001:PQN:H162 | 17:B:4014:BCR:H382 | 1.85 | 0.58 |
| 10:L:160:ALA:HB1 | 10:L:165:VAL:HB | 1.86 | 0.58 |
| 13:2:267:TYR:O | 13:2:300:ARG:NH2 | 2.36 | 0.58 |
| 13:Y:145:HIS:NE2 | 14:Y:512:CLA:NA | 2.51 | 0.58 |
| 9:U:51:LEU:O | 14:U:1105:CLA:ND | 2.37 | 0.58 |
| 13:3:34:GLN:OE1 | 14:3:510:CLA:NC | 2.37 | 0.58 |
| 14:H:1225:CLA:H203 | 17:H:4006:BCR:H15C | 1.86 | 0.58 |
| 14:L:1501:CLA:H121 | 17:L:4022:BCR:HC8 | 1.85 | 0.58 |
| 13:6:307:HIS:NE2 | 14:6:502:CLA:ND | 2.52 | 0.58 |
| 1:G:551:ALA:HB2 | 14:G:1136:CLA:HMA1 | 1.86 | 0.58 |
| 14:G:1102:CLA:H43 | 14:G:1109:CLA:HMC2 | 1.84 | 0.58 |
| 14:H:1223:CLA:H122 | 17:H:4010:BCR:H17C | 1.85 | 0.58 |
| 13:1:145:HIS:NE2 | 14:1:512:CLA:NA | 2.51 | 0.58 |
| 12:X:2:LYS:HE2 | 12:X:169:LEU:HD12 | 1.86 | 0.58 |
| 13:Y:249:ILE:HG12 | 14:Y:502:CLA:HAC1 | 1.85 | 0.58 |
| 9:K:51:LEU:O | 14:K:1105:CLA:ND | 2.37 | 0.58 |
| 13:5:272:TYR:HB3 | 13:5:300:ARG:HB2 | 1.85 | 0.58 |
| 1:A:551:ALA:HB2 | 14:A:1136:CLA:HMA1 | 1.86 | 0.57 |
| 14:A:1132:CLA:H162 | 14:L:1502:CLA:HMB2 | 1.85 | 0.57 |
| 14:B:1240:CLA:HMA1 | 18:B:1842:LHG:H272 | 1.86 | 0.57 |
| 14:H:1235:CLA:H172 | 17:R:4016:BCR:H272 | 1.85 | 0.57 |
| 14:B:1204:CLA:H111 | 17:I:4018:BCR:HC21 | 1.85 | 0.57 |
| 14:G:1103:CLA:H142 | 17:G:4003:BCR:H372 | 1.85 | 0.57 |
| 14:G:1132:CLA:H162 | 14:V:1502:CLA:HMB2 | 1.85 | 0.57 |
| 4:O:32:TRP:NE1 | 4:O:50:MET:SD | 2.72 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:P:2:LYS:HE2 | 12:P:169:LEU:HD12 | 1.86 | 0.57 |
| 1:G:277:THR:HB | 9:U:14:TRP:HB2 | 1.86 | 0.57 |
| 1:G:551:ALA:HB1 | 14:G:1136:CLA:HMB3 | 1.85 | 0.57 |
| 13:4:175:ARG:NH2 | 13:4:176:LEU:O | 2.37 | 0.57 |
| 1:G:412:LEU:HD21 | 14:G:1104:CLA:H142 | 1.87 | 0.57 |
| 14:H:1204:CLA:H111 | 17:S:4018:BCR:HC21 | 1.85 | 0.57 |
| 14:H:1216:CLA:HMB2 | 14:H:1221:CLA:HMA3 | 1.87 | 0.57 |
| 14:H:1229:CLA:HBB2 | 17:H:4014:BCR:HC41 | 1.86 | 0.57 |
| 14:H:1240:CLA:HMA1 | 18:H:1842:LHG:H272 | 1.86 | 0.57 |
| 1:A:370:ILE:HD11 | 14:A:1119:CLA:H71 | 1.85 | 0.57 |
| 14:B:1235:CLA:H172 | 17:F:4016:BCR:H272 | 1.85 | 0.57 |
| 18:G:5007:LHG:HC82 | 13:Z:297:HIS:NE2 | 2.19 | 0.57 |
| 14:B:1225:CLA:H203 | 17:B:4006:BCR:H15C | 1.86 | 0.57 |
| 14:B:1210:CLA:H112 | 14:B:1210:CLA:H51 | 1.87 | 0.57 |
| 13:2:249:ILE:HG12 | 14:2:502:CLA:HAC1 | 1.87 | 0.57 |
| 1:A:278:LEU:HD21 | 9:K:72:ILE:HD12 | 1.87 | 0.57 |
| 14:B:1229:CLA:HBB2 | 17:B:4014:BCR:HC41 | 1.86 | 0.57 |
| 7:I:13:ILE:HD11 | 10:V:155:LEU:HD22 | 1.87 | 0.57 |
| 13:1:249:ILE:HG12 | 14:1:502:CLA:HAC1 | 1.85 | 0.57 |
| 2:H:603:GLN:HE21 | 2:H:732:LYS:HD3 | 1.70 | 0.57 |
| 1:A:160:VAL:HG22 | 18:A:5007:LHG:H281 | 1.87 | 0.56 |
| 13:4:34:GLN:OE1 | 14:4:510:CLA:NC | 2.38 | 0.56 |
| 1:G:752:TRP:NE1 | 14:G:1126:CLA:O1A | 2.29 | 0.56 |
| 14:A:1103:CLA:H121 | 17:A:4002:BCR:HC41 | 1.87 | 0.56 |
| 14:B:1216:CLA:HMB2 | 14:B:1221:CLA:HMA3 | 1.87 | 0.56 |
| 13:6:148:PHE:HD2 | 14:6:512:CLA:H3A | 1.71 | 0.56 |
| 1:G:269:GLU:HG3 | 13:Y:294:PHE:HD1 | 1.71 | 0.56 |
| 1:A:216:GLN:HA | 1:A:220:SER:HB2 | 1.87 | 0.56 |
| 1:A:277:THR:HB | 9:K:14:TRP:HB2 | 1.86 | 0.56 |
| 18:A:5007:LHG:HC82 | 13:2:297:HIS:NE2 | 2.19 | 0.56 |
| 14:H:1218:CLA:H143 | 14:H:1218:CLA:HMC2 | 1.87 | 0.56 |
| 10:V:160:ALA:HB1 | 10:V:165:VAL:HB | 1.86 | 0.56 |
| 14:2:517:CLA:HBB1 | 17:2:524:BCR:H352 | 1.88 | 0.56 |
| 14:5:507:CLA:HED2 | 14:5:507:CLA:H2A | 1.88 | 0.56 |
| 1:A:412:LEU:HD21 | 14:A:1104:CLA:H142 | 1.87 | 0.56 |
| 14:G:1122:CLA:HBB2 | 18:G:5003:LHG:HC82 | 1.88 | 0.56 |
| 4:O:9:PRO:HD2 | 4:O:57:LEU:HD13 | 1.88 | 0.56 |
| 1:A:748:ILE:HG21 | 14:A:1126:CLA:HMC2 | 1.88 | 0.56 |
| 2:B:26:ALA:HA | 14:B:1226:CLA:H43 | 1.88 | 0.56 |
| 4:D:9:PRO:HD2 | 4:D:57:LEU:HD13 | 1.88 | 0.56 |
| 17:V:4219:BCR:H382 | 18:V:5221:LHG:H332 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:23:THR:HG21 | 18:A:5008:LHG:HC91 | 1.87 | 0.56 |
| 2:B:25:ILE:HA | 14:B:1201:CLA:HMD3 | 1.88 | 0.56 |
| 2:B:603:GLN:HE21 | 2:B:732:LYS:HD3 | 1.70 | 0.56 |
| 13:3:320:TRP:HH2 | 21:3:822:SQD:H462 | 1.69 | 0.56 |
| 14:G:1103:CLA:H121 | 17:G:4002:BCR:HC41 | 1.87 | 0.56 |
| 3:N:63:LEU:HD12 | 3:N:66:ARG:HH21 | 1.70 | 0.56 |
| 1:G:23:THR:HG21 | 18:G:5008:LHG:HC91 | 1.87 | 0.56 |
| 1:G:216:GLN:HA | 1:G:220:SER:HB2 | 1.87 | 0.56 |
| 1:G:748:ILE:HG21 | 14:G:1126:CLA:HMC2 | 1.87 | 0.56 |
| 14:H:1210:CLA:H112 | 14:H:1210:CLA:H51 | 1.87 | 0.56 |
| 2:B:548:PRO:HB3 | 6:F:158:PRO:HG2 | 1.88 | 0.56 |
| 10:L:38:ARG:O | 10:L:46:ARG:NH2 | 2.39 | 0.56 |
| 17:L:4219:BCR:H382 | 18:L:5221:LHG:H332 | 1.88 | 0.56 |
| 2:H:25:ILE:HA | 14:H:1201:CLA:HMD3 | 1.88 | 0.56 |
| 1:G:160:VAL:HG22 | 18:G:5007:LHG:H281 | 1.87 | 0.55 |
| 10:V:38:ARG:O | 10:V:46:ARG:NH2 | 2.39 | 0.55 |
| 1:A:589:PRO:HD3 | 2:B:561:GLY:HA2 | 1.89 | 0.55 |
| 13:1:34:GLN:OE1 | 14:1:510:CLA:NC | 2.39 | 0.55 |
| 4:O:61:ARG:NH1 | 4:O:63:GLU:OE1 | 2.39 | 0.55 |
| 3:C:63:LEU:HD12 | 3:C:66:ARG:HH21 | 1.70 | 0.55 |
| 4:D:85:ILE:HB | 4:D:98:HIS:HB3 | 1.88 | 0.55 |
| 4:O:85:ILE:HB | 4:O:98:HIS:HB3 | 1.88 | 0.55 |
| 13:Z:249:ILE:HG12 | 14:Z:502:CLA:HAC1 | 1.87 | 0.55 |
| 2:B:61:VAL:HG21 | 14:B:1225:CLA:H42 | 1.88 | 0.55 |
| 14:B:1207:CLA:H42 | 18:V:5221:LHG:H241 | 1.89 | 0.55 |
| 4:D:31:THR:HA | 4:D:55:ASN:O | 2.06 | 0.55 |
| 14:4:508:CLA:HBB2 | 14:4:509:CLA:HED1 | 1.89 | 0.55 |
| 2:B:456:GLU:OE1 | 6:F:68:HIS:ND1 | 2.35 | 0.55 |
| 2:H:160:LYS:HB3 | 21:H:1852:SQD:S | 2.47 | 0.55 |
| 14:H:1023:CLA:H122 | 17:S:4018:BCR:H281 | 1.89 | 0.55 |
| 4:O:31:THR:HA | 4:O:55:ASN:O | 2.06 | 0.55 |
| 14:Z:517:CLA:HBB1 | 17:Z:524:BCR:H352 | 1.87 | 0.55 |
| 14:L:1501:CLA:H102 | 14:L:1503:CLA:H122 | 1.89 | 0.55 |
| 12:P:42:SER:O | 12:P:45:ASN:ND2 | 2.38 | 0.55 |
| 13:1:301:ALA:O | 13:1:305:ASN:ND2 | 2.39 | 0.55 |
| 1:G:459:LEU:HB3 | 1:G:552:PHE:HB2 | 1.89 | 0.55 |
| 13:Y:301:ALA:O | 13:Y:305:ASN:ND2 | 2.39 | 0.55 |
| 14:B:1239:CLA:HBB1 | 17:B:4017:BCR:H363 | 1.89 | 0.55 |
| 10:L:83:VAL:HG11 | 10:V:142:PHE:CE1 | 2.42 | 0.55 |
| 2:H:351:HIS:ND1 | 14:H:1214:CLA:OBD | 2.40 | 0.55 |
| 2:H:548:PRO:HB3 | 6:R:158:PRO:HG2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:269:GLU:HG3 | 13:1:294:PHE:HD1 | 1.70 | 0.55 |
| 14:B:1207:CLA:H193 | 18:V:5221:LHG:H222 | 1.88 | 0.55 |
| 3:C:15:THR:HG22 | 3:C:28:MET:HG3 | 1.89 | 0.55 |
| 4:D:117:LYS:NZ | 4:D:119:ASP:OD1 | 2.40 | 0.55 |
| 2:B:160:LYS:HB3 | 21:B:1852:SQD:S | 2.47 | 0.55 |
| 13:6:110:HIS:NE2 | 14:6:513:CLA:NB | 2.55 | 0.55 |
| 14:G:1119:CLA:HMB2 | 14:G:1123:CLA:HMA3 | 1.89 | 0.55 |
| 3:N:15:THR:HG22 | 3:N:28:MET:HG3 | 1.89 | 0.55 |
| 14:V:1501:CLA:H102 | 14:V:1503:CLA:H122 | 1.89 | 0.55 |
| 14:A:1122:CLA:HBB2 | 18:A:5003:LHG:HC82 | 1.88 | 0.55 |
| 14:B:1218:CLA:H143 | 14:B:1218:CLA:HMC2 | 1.87 | 0.55 |
| 14:B:1231:CLA:H71 | 17:B:4010:BCR:H313 | 1.89 | 0.55 |
| 1:G:278:LEU:HD21 | 9:U:72:ILE:HD12 | 1.87 | 0.55 |
| 2:H:26:ALA:HA | 14:H:1226:CLA:H43 | 1.88 | 0.55 |
| 13:Y:34:GLN:OE1 | 14:Y:510:CLA:NC | 2.39 | 0.55 |
| 1:A:459:LEU:HB3 | 1:A:552:PHE:HB2 | 1.89 | 0.54 |
| 2:B:351:HIS:ND1 | 14:B:1214:CLA:OBD | 2.40 | 0.54 |
| 4:D:61:ARG:NH1 | 4:D:63:GLU:OE1 | 2.39 | 0.54 |
| 1:G:683:LEU:HD21 | 14:G:1126:CLA:H142 | 1.88 | 0.54 |
| 18:G:5004:LHG:H102 | 13:Z:282:VAL:HG13 | 1.89 | 0.54 |
| 10:V:33:ALA:HB1 | 14:V:1501:CLA:HAC1 | 1.89 | 0.54 |
| 2:B:66:PHE:HZ | 11:M:6:VAL:HG13 | 1.72 | 0.54 |
| 10:L:33:ALA:HB1 | 14:L:1501:CLA:HAC1 | 1.89 | 0.54 |
| 10:L:94:SER:CB | 14:V:1501:CLA:HMD1 | 2.34 | 0.54 |
| 13:4:109:PHE:HE1 | 13:4:113:ARG:HH21 | 1.55 | 0.54 |
| 13:6:319:LEU:HD21 | 14:6:505:CLA:HMB3 | 1.90 | 0.54 |
| 14:A:1119:CLA:HMB2 | 14:A:1123:CLA:HMA3 | 1.89 | 0.54 |
| 13:5:148:PHE:HD2 | 14:5:512:CLA:H3A | 1.73 | 0.54 |
| 14:G:1011:CLA:HMB1 | 14:H:1021:CLA:HAA1 | 1.88 | 0.54 |
| 2:H:61:VAL:HG21 | 14:H:1225:CLA:H42 | 1.88 | 0.54 |
| 4:O:58:TYR:H | 10:V:13:GLU:HG2 | 1.72 | 0.54 |
| 13:6:200:LEU:HG | 13:6:265:LEU:HD11 | 1.90 | 0.54 |
| 4:D:58:TYR:H | 10:L:13:GLU:HG2 | 1.72 | 0.54 |
| 13:2:307:HIS:NE2 | 14:2:502:CLA:NA | 2.56 | 0.54 |
| 1:G:589:PRO:HD3 | 2:H:561:GLY:HA2 | 1.88 | 0.54 |
| 13:Y:110:HIS:NE2 | 14:Y:513:CLA:NB | 2.56 | 0.54 |
| 1:A:683:LEU:HD21 | 14:A:1126:CLA:H142 | 1.88 | 0.54 |
| 14:B:1023:CLA:H122 | 17:I:4018:BCR:H281 | 1.89 | 0.54 |
| 13:1:110:HIS:NE2 | 14:1:513:CLA:NB | 2.56 | 0.54 |
| 13:4:140:LEU:HA | 13:4:222:ILE:HG22 | 1.90 | 0.54 |
| 13:6:145:HIS:NE2 | 14:6:512:CLA:NA | 2.56 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:524:ALA:HB2 | 14:H:1235:CLA:HMA1 | 1.90 | 0.54 |
| 13:Z:307:HIS:NE2 | 14:Z:502:CLA:NA | 2.56 | 0.54 |
| 4:O:39:VAL:HG22 | 4:O:49:VAL:HG22 | 1.90 | 0.54 |
| 2:B:524:ALA:HB2 | 14:B:1235:CLA:HMA1 | 1.90 | 0.54 |
| 12:P:9:THR:HB | 12:P:14:THR:HB | 1.89 | 0.54 |
| 13:3:145:HIS:NE2 | 14:3:512:CLA:NA | 2.55 | 0.54 |
| 12:P:62:LEU:HD21 | 12:P:105:LEU:HG | 1.90 | 0.54 |
| 18:V:5220:LHG:H311 | 18:V:5220:LHG:H171 | 1.90 | 0.54 |
| 2:B:117:TYR:HA | 2:B:367:THR:HG22 | 1.89 | 0.54 |
| 13:5:177:VAL:HG13 | 13:5:201:GLU:HG2 | 1.90 | 0.54 |
| 14:6:505:CLA:H12 | 17:6:524:BCR:H312 | 1.89 | 0.54 |
| 2:H:117:TYR:HA | 2:H:367:THR:HG22 | 1.89 | 0.54 |
| 12:X:9:THR:HB | 12:X:14:THR:HB | 1.89 | 0.54 |
| 14:A:1011:CLA:HMB1 | 14:B:1021:CLA:HAA1 | 1.88 | 0.53 |
| 12:X:42:SER:O | 12:X:45:ASN:ND2 | 2.38 | 0.53 |
| 13:Z:200:LEU:HG | 13:Z:265:LEU:HD11 | 1.90 | 0.53 |
| 14:B:1220:CLA:HAA1 | 17:B:4009:BCR:H16C | 1.91 | 0.53 |
| 13:2:200:LEU:HG | 13:2:265:LEU:HD11 | 1.90 | 0.53 |
| 13:2:226:PRO:HA | 14:2:506:CLA:HED3 | 1.91 | 0.53 |
| 13:5:119:ALA:O | 13:5:126:LYS:NZ | 2.41 | 0.53 |
| 14:H:1220:CLA:HAA1 | 17:H:4009:BCR:H16C | 1.91 | 0.53 |
| 14:H:1231:CLA:H71 | 17:H:4010:BCR:H313 | 1.89 | 0.53 |
| 13:Z:148:PHE:HD2 | 14:Z:512:CLA:H3A | 1.74 | 0.53 |
| 8:J:12:PRO:HB2 | 17:J:4013:BCR:H381 | 1.90 | 0.53 |
| 14:G:1119:CLA:H61 | 17:G:4007:BCR:H352 | 1.90 | 0.53 |
| 14:H:1229:CLA:HAB | 17:H:4014:BCR:H323 | 1.91 | 0.53 |
| 12:X:62:LEU:HD21 | 12:X:105:LEU:HG | 1.90 | 0.53 |
| 18:A:5004:LHG:H102 | 13:2:282:VAL:HG13 | 1.89 | 0.53 |
| 13:6:276:LEU:HD11 | 13:6:300:ARG:HG2 | 1.89 | 0.53 |
| 2:H:66:PHE:HZ | 11:W:6:VAL:HG13 | 1.72 | 0.53 |
| 14:H:1208:CLA:HMD3 | 21:H:1852:SQD:H101 | 1.91 | 0.53 |
| 1:A:16:VAL:HA | 1:A:185:PRO:HA | 1.91 | 0.53 |
| 13:4:310:LEU:HB3 | 14:4:502:CLA:HMC3 | 1.91 | 0.53 |
| 14:H:1239:CLA:HBB1 | 17:H:4017:BCR:H363 | 1.89 | 0.53 |
| 14:4:517:CLA:H2A | 14:4:517:CLA:HED2 | 1.91 | 0.53 |
| 13:6:73:LEU:O | 13:6:159:LYS:NZ | 2.42 | 0.53 |
| 14:Z:513:CLA:HBB1 | 17:Z:523:BCR:H24C | 1.90 | 0.53 |
| 1:G:16:VAL:HA | 1:G:185:PRO:HA | 1.91 | 0.53 |
| 14:B:1234:CLA:H52 | 14:F:1302:CLA:HBB2 | 1.91 | 0.53 |
| 8:T:12:PRO:HB2 | 17:T:4013:BCR:H381 | 1.90 | 0.53 |
| 4:D:39:VAL:HG22 | 4:D:49:VAL:HG22 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:2:148:PHE:HD2 | 14:2:512:CLA:H3A | 1.74 | 0.53 |
| 9:U:47:PRO:HG2 | 21:Y:822:SQD:H262 | 1.91 | 0.53 |
| 13:6:177:VAL:HG13 | 13:6:201:GLU:HG2 | 1.91 | 0.53 |
| 4:D:79:LYS:HZ3 | 12:P:92:VAL:HG13 | 1.73 | 0.52 |
| 14:2:513:CLA:HBB1 | 17:2:523:BCR:H24C | 1.90 | 0.52 |
| 13:4:146:LEU:HD22 | 13:4:214:LEU:HD22 | 1.91 | 0.52 |
| 1:G:598:SER:OG | 1:G:601:ASP:OD2 | 2.26 | 0.52 |
| 13:Z:226:PRO:HA | 14:Z:506:CLA:HED3 | 1.91 | 0.52 |
| 2:H:191:THR:HG21 | 2:H:278:LEU:HB2 | 1.91 | 0.52 |
| 1:A:598:SER:OG | 1:A:601:ASP:OD2 | 2.26 | 0.52 |
| 2:B:191:THR:HG21 | 2:B:278:LEU:HB2 | 1.91 | 0.52 |
| 1:G:79:HIS:HB2 | 14:G:1103:CLA:HMB2 | 1.92 | 0.52 |
| 14:G:1237:CLA:H152 | 17:V:4020:BCR:H16C | 1.91 | 0.52 |
| 2:H:158:GLN:HB3 | 21:H:1852:SQD:H5 | 1.92 | 0.52 |
| 2:H:181:GLY:HA3 | 14:H:1210:CLA:HBB1 | 1.91 | 0.52 |
| 2:H:656:ILE:HG12 | 14:H:1239:CLA:HMB3 | 1.91 | 0.52 |
| 13:Z:193:HIS:HB2 | 13:Z:196:SER:HB3 | 1.91 | 0.52 |
| 1:A:79:HIS:HB2 | 14:A:1103:CLA:HMB2 | 1.92 | 0.52 |
| 14:A:1124:CLA:HAB | 17:A:4008:BCR:H311 | 1.92 | 0.52 |
| 14:B:1235:CLA:H102 | 14:B:1235:CLA:HMC2 | 1.91 | 0.52 |
| 13:2:193:HIS:HB2 | 13:2:196:SER:HB3 | 1.91 | 0.52 |
| 12:X:66:TRP:HA | 12:X:69:ILE:HG22 | 1.91 | 0.52 |
| 1:A:708:LEU:HD21 | 14:A:1013:CLA:HED2 | 1.92 | 0.52 |
| 14:H:1204:CLA:HHB | 14:H:1205:CLA:HHB | 1.92 | 0.52 |
| 12:P:66:TRP:HA | 12:P:69:ILE:HG22 | 1.91 | 0.52 |
| 2:H:69:ALA:HB2 | 2:H:135:LEU:HB2 | 1.92 | 0.52 |
| 14:A:1118:CLA:H3A | 9:K:61:LEU:HD23 | 1.91 | 0.52 |
| 2:B:69:ALA:HB2 | 2:B:135:LEU:HB2 | 1.92 | 0.52 |
| 2:B:656:ILE:HG12 | 14:B:1239:CLA:HMB3 | 1.92 | 0.52 |
| 9:K:47:PRO:HG2 | 21:1:822:SQD:H262 | 1.91 | 0.52 |
| 1:A:315:LEU:HD13 | 14:A:1116:CLA:HMC1 | 1.91 | 0.52 |
| 18:L:5220:LHG:H311 | 18:L:5220:LHG:H171 | 1.90 | 0.52 |
| 13:1:148:PHE:HZ | 14:1:516:CLA:CBC | 2.22 | 0.52 |
| 14:G:1124:CLA:HAB | 17:G:4008:BCR:H311 | 1.92 | 0.52 |
| 2:H:151:PHE:CE2 | 21:H:1852:SQD:H102 | 2.45 | 0.52 |
| 2:H:422:LEU:HD13 | 2:H:532:LEU:HA | 1.92 | 0.52 |
| 14:H:1238:CLA:H2 | 14:H:1239:CLA:H122 | 1.92 | 0.52 |
| 15:H:2002:PQN:H242 | 17:H:4017:BCR:H17C | 1.92 | 0.52 |
| 2:B:338:LEU:HD21 | 14:B:1226:CLA:HAB | 1.92 | 0.52 |
| 14:B:1203:CLA:H191 | 20:B:5002:LMG:H252 | 1.92 | 0.52 |
| 10:L:98:ASN:ND2 | 10:V:39:ARG:O | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:L:4022:BCR:H333 | 21:L:5216:SQD:H142 | 1.92 | 0.52 |
| 14:3:513:CLA:HBB1 | 17:3:523:BCR:H402 | 1.92 | 0.52 |
| 13:6:301:ALA:O | 13:6:305:ASN:ND2 | 2.41 | 0.52 |
| 1:A:230:ILE:HG12 | 1:A:244:ALA:HA | 1.92 | 0.52 |
| 14:B:1227:CLA:HMC2 | 14:B:1240:CLA:H142 | 1.92 | 0.52 |
| 14:B:1229:CLA:HAB | 17:B:4014:BCR:H323 | 1.91 | 0.52 |
| 13:4:272:TYR:HB3 | 13:4:300:ARG:HB2 | 1.91 | 0.52 |
| 13:5:249:ILE:HG12 | 14:5:502:CLA:HAC1 | 1.92 | 0.52 |
| 14:H:1012:CLA:H201 | 17:T:4012:BCR:H362 | 1.91 | 0.52 |
| 4:O:79:LYS:HZ3 | 12:X:92:VAL:HG13 | 1.75 | 0.52 |
| 14:B:1204:CLA:HHB | 14:B:1205:CLA:HHB | 1.92 | 0.51 |
| 14:B:1208:CLA:HMD3 | 21:B:1852:SQD:H101 | 1.91 | 0.51 |
| 14:B:1238:CLA:H2 | 14:B:1239:CLA:H122 | 1.92 | 0.51 |
| 9:K:29:ALA:HA | 9:K:32:ILE:HG22 | 1.92 | 0.51 |
| 12:P:62:LEU:HD23 | 12:P:101:ALA:HB1 | 1.92 | 0.51 |
| 12:P:3:ILE:HB | 12:P:31:VAL:HG22 | 1.93 | 0.51 |
| 12:X:62:LEU:HD23 | 12:X:101:ALA:HB1 | 1.92 | 0.51 |
| 13:Y:34:GLN:HG2 | 14:Y:509:CLA:HHB | 1.93 | 0.51 |
| 14:G:1120:CLA:HMD2 | 17:G:4001:BCR:H24C | 1.93 | 0.51 |
| 14:H:1203:CLA:H191 | 20:H:5002:LMG:H252 | 1.92 | 0.51 |
| 3:N:22:PRO:HG2 | 3:N:23:LEU:HD12 | 1.92 | 0.51 |
| 14:A:1119:CLA:H61 | 17:A:4007:BCR:H352 | 1.90 | 0.51 |
| 14:A:1237:CLA:H152 | 17:L:4020:BCR:H16C | 1.91 | 0.51 |
| 12:P:37:ALA:HB2 | 12:P:65:ASP:OD2 | 2.11 | 0.51 |
| 1:A:573:LEU:O | 4:D:61:ARG:NH2 | 2.42 | 0.51 |
| 14:B:1229:CLA:H61 | 17:F:4016:BCR:HC32 | 1.93 | 0.51 |
| 13:3:168:ASP:OD2 | 13:3:175:ARG:NH2 | 2.42 | 0.51 |
| 1:G:315:LEU:HD13 | 14:G:1116:CLA:HMC1 | 1.91 | 0.51 |
| 13:Y:148:PHE:HZ | 14:Y:516:CLA:CBC | 2.22 | 0.51 |
| 13:Y:251:LEU:HB2 | 14:Y:505:CLA:HMC1 | 1.93 | 0.51 |
| 1:G:381:HIS:ND1 | 14:G:1116:CLA:OBD | 2.44 | 0.51 |
| 14:G:1118:CLA:H3A | 9:U:61:LEU:HD23 | 1.91 | 0.51 |
| 18:G:5004:LHG:H302 | 18:G:5006:LHG:H331 | 1.92 | 0.51 |
| 14:H:1235:CLA:HMC2 | 14:H:1235:CLA:H102 | 1.91 | 0.51 |
| 1:A:86:TRP:NE1 | 14:A:1126:CLA:OBD | 2.43 | 0.51 |
| 2:B:422:LEU:HD13 | 2:B:532:LEU:HA | 1.92 | 0.51 |
| 10:L:64:ILE:HD12 | 10:L:160:ALA:HB2 | 1.93 | 0.51 |
| 13:1:34:GLN:HG2 | 14:1:509:CLA:HHB | 1.93 | 0.51 |
| 14:A:1117:CLA:H203 | 14:A:1125:CLA:HAA1 | 1.93 | 0.51 |
| 2:B:181:GLY:HA3 | 14:B:1210:CLA:HBB1 | 1.91 | 0.51 |
| 3:C:22:PRO:HG2 | 3:C:23:LEU:HD12 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:742:HIS:CE1 | 14:G:1140:CLA:NA | 2.79 | 0.51 |
| 10:V:64:ILE:HD12 | 10:V:160:ALA:HB2 | 1.93 | 0.51 |
| 1:A:381:HIS:ND1 | 14:A:1116:CLA:OBD | 2.44 | 0.51 |
| 14:A:1129:CLA:HBB2 | 14:A:1137:CLA:HMC2 | 1.93 | 0.51 |
| 14:B:1012:CLA:H201 | 17:J:4012:BCR:H362 | 1.91 | 0.51 |
| 14:B:1208:CLA:HBB2 | 14:B:1210:CLA:HMA3 | 1.93 | 0.51 |
| 13:5:145:HIS:NE2 | 14:5:512:CLA:NA | 2.59 | 0.51 |
| 17:6:522:BCR:HC41 | 13:Y:258:TYR:HB2 | 1.93 | 0.51 |
| 1:G:230:ILE:HG12 | 1:G:244:ALA:HA | 1.92 | 0.51 |
| 2:H:60:TRP:NE1 | 14:H:1224:CLA:OBD | 2.44 | 0.51 |
| 2:H:611:GLU:OE2 | 6:R:36:ARG:NH1 | 2.43 | 0.51 |
| 2:H:687:LEU:HB2 | 17:V:4020:BCR:H282 | 1.92 | 0.51 |
| 9:U:74:VAL:HG23 | 14:U:1401:CLA:HMC3 | 1.93 | 0.51 |
| 1:A:424:MET:HE1 | 1:A:442:LEU:HD11 | 1.93 | 0.50 |
| 2:B:60:TRP:NE1 | 14:B:1224:CLA:OBD | 2.44 | 0.50 |
| 13:3:148:PHE:HD2 | 14:3:512:CLA:H3A | 1.76 | 0.50 |
| 13:6:177:VAL:HG21 | 13:6:204:VAL:HG21 | 1.91 | 0.50 |
| 13:6:190:TYR:HD2 | 17:6:524:BCR:H401 | 1.76 | 0.50 |
| 1:G:708:LEU:HD21 | 14:G:1013:CLA:HED2 | 1.92 | 0.50 |
| 18:G:5008:LHG:C7 | 13:Z:13:TRP:HE1 | 2.24 | 0.50 |
| 1:A:742:HIS:CE1 | 14:A:1140:CLA:NA | 2.79 | 0.50 |
| 14:A:1118:CLA:HBB1 | 17:K:4104:BCR:H342 | 1.94 | 0.50 |
| 13:6:146:LEU:HD21 | 14:6:506:CLA:HAB | 1.92 | 0.50 |
| 1:G:345:THR:HG21 | 18:G:5003:LHG:HC11 | 1.94 | 0.50 |
| 14:H:1234:CLA:H52 | 14:R:1302:CLA:HBB2 | 1.91 | 0.50 |
| 4:O:121:ARG:NH1 | 5:Q:65:GLU:OE2 | 2.44 | 0.50 |
| 14:B:1219:CLA:HBA2 | 14:B:1219:CLA:H43 | 1.93 | 0.50 |
| 13:1:251:LEU:HB2 | 14:1:505:CLA:HMC1 | 1.93 | 0.50 |
| 13:2:34:GLN:HG2 | 14:2:509:CLA:HHB | 1.93 | 0.50 |
| 13:4:70:LEU:HD21 | 14:4:503:CLA:HED2 | 1.93 | 0.50 |
| 13:4:135:PRO:HB2 | 13:4:226:PRO:HD2 | 1.94 | 0.50 |
| 18:A:5004:LHG:H302 | 18:A:5006:LHG:H331 | 1.92 | 0.50 |
| 2:B:158:GLN:HB3 | 21:B:1852:SQD:H5 | 1.92 | 0.50 |
| 15:B:2002:PQN:H242 | 17:B:4017:BCR:H17C | 1.92 | 0.50 |
| 4:D:31:THR:O | 4:D:83:TYR:HA | 2.12 | 0.50 |
| 4:D:121:ARG:NH1 | 5:E:65:GLU:OE2 | 2.44 | 0.50 |
| 9:K:74:VAL:HG23 | 14:K:1401:CLA:HMC3 | 1.93 | 0.50 |
| 10:L:41:LEU:O | 10:L:46:ARG:NH1 | 2.45 | 0.50 |
| 13:4:161:THR:HA | 13:4:177:VAL:HB | 1.93 | 0.50 |
| 13:6:136:LYS:HG3 | 13:6:225:PRO:HB3 | 1.92 | 0.50 |
| 18:G:5009:LHG:H131 | 17:Y:521:BCR:H313 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:G:1848:LMU:H5B | 17:T:4013:BCR:HC21 | 1.94 | 0.50 |
| 4:O:117:LYS:NZ | 4:O:119:ASP:OD1 | 2.40 | 0.50 |
| 17:V:4022:BCR:H333 | 21:V:5216:SQD:H142 | 1.92 | 0.50 |
| 12:X:3:ILE:HB | 12:X:31:VAL:HG22 | 1.93 | 0.50 |
| 12:X:37:ALA:HB2 | 12:X:65:ASP:OD2 | 2.11 | 0.50 |
| 1:A:441:VAL:HG11 | 14:A:1119:CLA:H192 | 1.94 | 0.50 |
| 19:A:1848:LMU:O6B | 8:J:31:ARG:NH1 | 2.44 | 0.50 |
| 14:H:1208:CLA:HBB2 | 14:H:1210:CLA:HMA3 | 1.93 | 0.50 |
| 14:H:1227:CLA:HMC2 | 14:H:1240:CLA:H142 | 1.92 | 0.50 |
| 9:U:29:ALA:HA | 9:U:32:ILE:HG22 | 1.92 | 0.50 |
| 18:A:5009:LHG:H131 | 17:1:521:BCR:H313 | 1.94 | 0.50 |
| 17:L:4022:BCR:H333 | 21:L:5216:SQD:H141 | 1.93 | 0.50 |
| 13:4:230:THR:HG23 | 13:4:234:LEU:HD12 | 1.92 | 0.50 |
| 13:6:146:LEU:HD22 | 13:6:214:LEU:HD22 | 1.91 | 0.50 |
| 1:G:692:ALA:HB3 | 14:G:1013:CLA:HBB2 | 1.94 | 0.50 |
| 2:H:338:LEU:HD21 | 14:H:1226:CLA:HAB | 1.92 | 0.50 |
| 14:H:1218:CLA:HMD2 | 17:H:4004:BCR:H23C | 1.93 | 0.50 |
| 2:B:127:ILE:HG12 | 2:B:190:TRP:HH2 | 1.77 | 0.50 |
| 2:B:710:LEU:HD23 | 20:B:5002:LMG:H362 | 1.94 | 0.50 |
| 13:2:110:HIS:NE2 | 14:2:513:CLA:NB | 2.60 | 0.50 |
| 14:G:1129:CLA:HBB2 | 14:G:1137:CLA:HMC2 | 1.93 | 0.50 |
| 2:H:452:GLN:NE2 | 2:H:614:THR:OG1 | 2.45 | 0.50 |
| 2:B:311:PRO:HD2 | 18:B:1842:LHG:HC31 | 1.94 | 0.50 |
| 2:B:452:GLN:NE2 | 2:B:614:THR:OG1 | 2.45 | 0.50 |
| 14:B:1206:CLA:H2A | 14:B:1206:CLA:HED3 | 1.93 | 0.50 |
| 13:4:263:ASN:HD21 | 13:4:265:LEU:HB3 | 1.77 | 0.50 |
| 14:H:1219:CLA:HBA2 | 14:H:1219:CLA:H43 | 1.93 | 0.50 |
| 14:H:1229:CLA:H61 | 17:R:4016:BCR:HC32 | 1.93 | 0.50 |
| 14:A:1119:CLA:H101 | 17:A:4008:BCR:H10C | 1.94 | 0.50 |
| 18:A:5008:LHG:C7 | 13:2:13:TRP:HE1 | 2.24 | 0.50 |
| 13:2:261:ALA:HA | 13:2:276:LEU:HD12 | 1.94 | 0.50 |
| 1:G:424:MET:HE1 | 1:G:442:LEU:HD11 | 1.94 | 0.50 |
| 14:G:1117:CLA:H203 | 14:G:1125:CLA:HAA1 | 1.93 | 0.50 |
| 19:G:1848:LMU:O6B | 8:T:31:ARG:NH1 | 2.44 | 0.50 |
| 17:V:4022:BCR:H333 | 21:V:5216:SQD:H141 | 1.94 | 0.50 |
| 2:H:311:PRO:HD2 | 18:H:1842:LHG:HC31 | 1.94 | 0.49 |
| 2:H:714:THR:HG21 | 20:H:5002:LMG:H402 | 1.94 | 0.49 |
| 18:H:1855:LHG:H192 | 14:R:1302:CLA:HBB1 | 1.94 | 0.49 |
| 13:Y:148:PHE:CE2 | 14:Y:512:CLA:HBB | 2.47 | 0.49 |
| 13:Z:261:ALA:HA | 13:Z:276:LEU:HD12 | 1.94 | 0.49 |
| 1:A:626:GLN:HE21 | 1:A:759:ILE:HD13 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:A:1120:CLA:HMD2 | 17:A:4001:BCR:H24C | 1.93 | 0.49 |
| 14:A:1237:CLA:HAB | 2:B:691:VAL:HG11 | 1.94 | 0.49 |
| 19:A:1848:LMU:H5B | 17:J:4013:BCR:HC21 | 1.94 | 0.49 |
| 13:6:59:MET:HB2 | 13:6:271:PHE:HA | 1.93 | 0.49 |
| 14:A:1106:CLA:HMB2 | 17:J:4012:BCR:H373 | 1.93 | 0.49 |
| 14:A:1134:CLA:HMB1 | 17:A:4008:BCR:H291 | 1.93 | 0.49 |
| 2:B:151:PHE:CE2 | 21:B:1852:SQD:H102 | 2.45 | 0.49 |
| 18:B:1855:LHG:H192 | 14:F:1302:CLA:HBB1 | 1.94 | 0.49 |
| 13:1:148:PHE:CE2 | 14:1:512:CLA:HHB | 2.47 | 0.49 |
| 14:4:513:CLA:HBB1 | 17:4:523:BCR:H402 | 1.94 | 0.49 |
| 14:G:1106:CLA:HMC3 | 14:G:1107:CLA:HMD2 | 1.94 | 0.49 |
| 14:G:1119:CLA:H101 | 17:G:4008:BCR:H10C | 1.94 | 0.49 |
| 12:P:78:PHE:HB3 | 12:P:114:SER:HB3 | 1.95 | 0.49 |
| 14:G:1106:CLA:HMB2 | 17:T:4012:BCR:H373 | 1.93 | 0.49 |
| 14:G:1134:CLA:HMB1 | 17:G:4008:BCR:H291 | 1.93 | 0.49 |
| 14:H:1206:CLA:H2A | 14:H:1206:CLA:HED3 | 1.93 | 0.49 |
| 14:H:1228:CLA:HBC1 | 14:H:1234:CLA:H18 | 1.94 | 0.49 |
| 4:O:31:THR:O | 4:O:83:TYR:HA | 2.12 | 0.49 |
| 10:V:41:LEU:O | 10:V:46:ARG:NH1 | 2.45 | 0.49 |
| 13:Z:110:HIS:NE2 | 14:Z:513:CLA:NB | 2.60 | 0.49 |
| 14:B:1202:CLA:HBD | 14:B:1202:CLA:H122 | 1.93 | 0.49 |
| 1:G:360:TRP:HB3 | 14:G:1103:CLA:HAC1 | 1.94 | 0.49 |
| 1:G:695:LEU:HB2 | 14:G:1013:CLA:HMC3 | 1.94 | 0.49 |
| 2:H:710:LEU:HD23 | 20:H:5002:LMG:H362 | 1.94 | 0.49 |
| 14:A:1117:CLA:H8 | 14:A:1117:CLA:HAB | 1.95 | 0.49 |
| 2:B:158:GLN:HG3 | 21:B:1852:SQD:H1 | 1.94 | 0.49 |
| 14:B:1218:CLA:HMD2 | 17:B:4004:BCR:H23C | 1.93 | 0.49 |
| 14:B:1228:CLA:HBC1 | 14:B:1234:CLA:H18 | 1.94 | 0.49 |
| 3:C:58:CYS:HB3 | 3:C:63:LEU:HD22 | 1.95 | 0.49 |
| 6:F:126:LYS:HB2 | 13:3:13:TRP:CE2 | 2.48 | 0.49 |
| 13:6:282:VAL:HG23 | 13:6:283:THR:HG23 | 1.94 | 0.49 |
| 1:G:86:TRP:NE1 | 14:G:1126:CLA:OBD | 2.43 | 0.49 |
| 1:G:441:VAL:HG11 | 14:G:1119:CLA:H192 | 1.94 | 0.49 |
| 14:G:1118:CLA:HBB1 | 17:U:4104:BCR:H342 | 1.94 | 0.49 |
| 2:H:127:ILE:HG12 | 2:H:190:TRP:HH2 | 1.77 | 0.49 |
| 13:Z:34:GLN:HG2 | 14:Z:509:CLA:HHB | 1.93 | 0.49 |
| 1:A:377:ILE:HG21 | 14:A:1117:CLA:H201 | 1.95 | 0.49 |
| 1:A:345:THR:HG21 | 18:A:5003:LHG:HC11 | 1.94 | 0.49 |
| 1:A:589:PRO:HB3 | 2:B:559:CYS:SG | 2.53 | 0.49 |
| 2:B:687:LEU:HB2 | 17:L:4020:BCR:H282 | 1.93 | 0.49 |
| 1:G:377:ILE:HG21 | 14:G:1117:CLA:H201 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:Y:143:GLY:HA3 | 13:Y:222:ILE:HG13 | 1.94 | 0.49 |
| 14:A:1106:CLA:HMC3 | 14:A:1107:CLA:HMD2 | 1.94 | 0.49 |
| 13:5:221:HIS:CE1 | 14:5:506:CLA:NA | 2.81 | 0.49 |
| 18:G:5008:LHG:HC5 | 13:Z:13:TRP:NE1 | 2.28 | 0.49 |
| 2:H:158:GLN:HG3 | 21:H:1852:SQD:H1 | 1.94 | 0.49 |
| 14:H:1202:CLA:HBD | 14:H:1202:CLA:H122 | 1.93 | 0.49 |
| 6:F:143:SER:HB2 | 13:4:14:TRP:CH2 | 2.48 | 0.49 |
| 13:4:276:LEU:HG | 13:4:300:ARG:HD2 | 1.93 | 0.49 |
| 3:N:58:CYS:HB3 | 3:N:63:LEU:HD22 | 1.95 | 0.49 |
| 1:A:300:LEU:HD21 | 1:A:385:MET:HB3 | 1.95 | 0.48 |
| 13:1:143:GLY:HA3 | 13:1:222:ILE:HG13 | 1.94 | 0.48 |
| 1:G:429:ASP:O | 1:G:433:ASN:ND2 | 2.46 | 0.48 |
| 1:G:589:PRO:HB3 | 2:H:559:CYS:SG | 2.53 | 0.48 |
| 14:A:1137:CLA:H41 | 14:A:1137:CLA:H62 | 1.64 | 0.48 |
| 18:I:5001:LHG:HC62 | 21:V:5216:SQD:H242 | 1.95 | 0.48 |
| 9:K:43:GLY:HA3 | 9:K:58:PRO:HG2 | 1.94 | 0.48 |
| 13:2:148:PHE:CE2 | 14:2:512:CLA:HHB | 2.48 | 0.48 |
| 13:4:273:GLY:O | 13:4:300:ARG:NH2 | 2.39 | 0.48 |
| 13:5:67:LEU:HD22 | 13:5:89:LEU:HD13 | 1.95 | 0.48 |
| 17:L:4219:BCR:H14C | 18:L:5220:LHG:H331 | 1.95 | 0.48 |
| 1:A:692:ALA:HB3 | 14:A:1013:CLA:HBB2 | 1.94 | 0.48 |
| 18:A:5008:LHG:HC5 | 13:2:13:TRP:NE1 | 2.28 | 0.48 |
| 2:H:15:ASP:OD2 | 2:H:19:ARG:NH2 | 2.47 | 0.48 |
| 12:X:78:PHE:HB3 | 12:X:114:SER:HB3 | 1.95 | 0.48 |
| 2:B:151:PHE:CZ | 21:B:1852:SQD:H252 | 2.49 | 0.48 |
| 2:B:611:GLU:OE2 | 6:F:36:ARG:NH1 | 2.43 | 0.48 |
| 10:L:133:ILE:HG21 | 10:V:48:LEU:HD21 | 1.93 | 0.48 |
| 1:G:626:GLN:HE21 | 1:G:759:ILE:HD13 | 1.78 | 0.48 |
| 13:Z:30:ALA:HB2 | 14:Z:511:CLA:HMA1 | 1.94 | 0.48 |
| 2:B:498:LEU:HA | 2:B:501:ILE:HG22 | 1.95 | 0.48 |
| 2:B:714:THR:HG21 | 20:B:5002:LMG:H402 | 1.94 | 0.48 |
| 13:2:49:GLU:HB3 | 13:2:64:LEU:HD22 | 1.96 | 0.48 |
| 13:4:59:MET:HB2 | 13:4:271:PHE:HA | 1.96 | 0.48 |
| 13:5:148:PHE:CE2 | 14:5:512:CLA:HHB | 2.49 | 0.48 |
| 14:G:1108:CLA:HBB2 | 14:G:1111:CLA:HMA3 | 1.95 | 0.48 |
| 14:G:1129:CLA:HAB | 14:G:1137:CLA:HBB2 | 1.96 | 0.48 |
| 14:G:1101:CLA:HHC | 14:G:1101:CLA:HBB1 | 1.96 | 0.48 |
| 9:U:43:GLY:HA3 | 9:U:58:PRO:HG2 | 1.94 | 0.48 |
| 13:Z:49:GLU:HB3 | 13:Z:64:LEU:HD22 | 1.96 | 0.48 |
| 1:A:360:TRP:HB3 | 14:A:1103:CLA:HAC1 | 1.94 | 0.48 |
| 1:A:429:ASP:O | 1:A:433:ASN:ND2 | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L:21:ILE:HD13 | 18:L:5218:LHG:H302 | 1.96 | 0.48 |
| 13:6:20:PHE:HA | 13:6:23:LEU:HD12 | 1.94 | 0.48 |
| 14:6:519:CLA:HED2 | 14:6:519:CLA:H2A | 1.96 | 0.48 |
| 14:G:1121:CLA:HAB | 14:G:1801:CLA:HAB | 1.96 | 0.48 |
| 1:A:695:LEU:HB2 | 14:A:1013:CLA:HMC3 | 1.94 | 0.48 |
| 14:A:1104:CLA:H62 | 14:A:1104:CLA:H41 | 1.61 | 0.48 |
| 14:A:1121:CLA:HAB | 14:A:1801:CLA:HAB | 1.96 | 0.48 |
| 2:B:377:TYR:HB3 | 14:B:1224:CLA:HMC3 | 1.96 | 0.48 |
| 13:4:38:ILE:HG12 | 14:4:510:CLA:HMC2 | 1.96 | 0.48 |
| 13:6:78:GLY:N | 13:6:82:GLN:O | 2.47 | 0.48 |
| 1:G:573:LEU:O | 4:O:61:ARG:NH2 | 2.42 | 0.48 |
| 14:G:1115:CLA:H62 | 14:G:1115:CLA:H41 | 1.65 | 0.48 |
| 14:G:1237:CLA:HAB | 2:H:691:VAL:HG11 | 1.94 | 0.48 |
| 2:H:722:ALA:HB2 | 14:H:1224:CLA:HBB1 | 1.95 | 0.48 |
| 4:O:79:LYS:NZ | 12:X:92:VAL:HG13 | 2.29 | 0.48 |
| 13:Z:67:LEU:HD22 | 13:Z:89:LEU:HD13 | 1.95 | 0.48 |
| 2:B:493:TYR:HE1 | 14:B:1231:CLA:HED1 | 1.79 | 0.48 |
| 13:2:30:ALA:HB2 | 14:2:511:CLA:HMA1 | 1.94 | 0.48 |
| 14:G:1139:CLA:HMC2 | 17:H:4014:BCR:H381 | 1.96 | 0.48 |
| 4:O:101:ASP:OD1 | 4:O:101:ASP:N | 2.47 | 0.48 |
| 13:Z:148:PHE:CE2 | 14:Z:512:CLA:HHB | 2.48 | 0.48 |
| 14:A:1108:CLA:HBB2 | 14:A:1111:CLA:HMA3 | 1.95 | 0.48 |
| 6:F:118:VAL:HA | 8:J:10:SER:HA | 1.96 | 0.48 |
| 13:2:67:LEU:HD22 | 13:2:89:LEU:HD13 | 1.95 | 0.48 |
| 13:3:320:TRP:CH2 | 21:3:822:SQD:H462 | 2.49 | 0.48 |
| 13:4:276:LEU:HB3 | 13:4:286:PHE:HB3 | 1.96 | 0.48 |
| 13:5:282:VAL:HG23 | 13:5:283:THR:HG23 | 1.95 | 0.48 |
| 14:G:1117:CLA:H8 | 14:G:1117:CLA:HAB | 1.95 | 0.48 |
| 10:V:90:THR:HG21 | 10:V:133:ILE:HD12 | 1.96 | 0.48 |
| 17:V:4219:BCR:H14C | 18:V:5220:LHG:H331 | 1.95 | 0.48 |
| 14:A:1114:CLA:HBB1 | 18:A:5005:LHG:H301 | 1.95 | 0.47 |
| 4:D:79:LYS:NZ | 12:P:92:VAL:HG13 | 2.29 | 0.47 |
| 13:3:38:ILE:HG12 | 14:3:510:CLA:HMC2 | 1.96 | 0.47 |
| 13:4:147:LEU:HD12 | 13:4:215:ILE:HG12 | 1.96 | 0.47 |
| 1:G:219:VAL:HG13 | 1:G:252:PRO:HB3 | 1.96 | 0.47 |
| 1:G:616:ILE:HD12 | 14:G:1011:CLA:H122 | 1.96 | 0.47 |
| 14:G:1114:CLA:HBB1 | 18:G:5005:LHG:H301 | 1.95 | 0.47 |
| 1:A:577:LYS:NZ | 2:B:673:GLU:OE2 | 2.43 | 0.47 |
| 14:A:1109:CLA:H72 | 14:A:1101:CLA:HBB2 | 1.96 | 0.47 |
| 14:A:1115:CLA:HBC1 | 14:A:1116:CLA:H121 | 1.96 | 0.47 |
| 2:B:15:ASP:OD2 | 2:B:19:ARG:NH2 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:722:ALA:HB2 | 14:B:1224:CLA:HBB1 | 1.95 | 0.47 |
| 4:D:37:GLU:HA | 4:D:50:MET:O | 2.14 | 0.47 |
| 14:A:1139:CLA:HMC2 | 17:B:4014:BCR:H381 | 1.96 | 0.47 |
| 10:L:90:THR:HG21 | 10:L:133:ILE:HD12 | 1.96 | 0.47 |
| 13:3:267:TYR:O | 13:3:300:ARG:NH2 | 2.39 | 0.47 |
| 14:G:1103:CLA:H3A | 14:G:1103:CLA:HBA1 | 1.57 | 0.47 |
| 2:H:151:PHE:CZ | 21:H:1852:SQD:H252 | 2.49 | 0.47 |
| 5:Q:28:VAL:HG22 | 5:Q:37:VAL:HG13 | 1.96 | 0.47 |
| 1:A:485:ASP:OD1 | 1:A:491:GLN:NE2 | 2.45 | 0.47 |
| 2:B:114:ASN:ND2 | 14:B:1206:CLA:OBD | 2.47 | 0.47 |
| 14:B:1204:CLA:H3A | 14:B:1205:CLA:HMB3 | 1.97 | 0.47 |
| 2:H:493:TYR:HE1 | 14:H:1231:CLA:HED1 | 1.79 | 0.47 |
| 14:H:1227:CLA:HAB | 14:H:1236:CLA:HBB2 | 1.97 | 0.47 |
| 1:A:258:VAL:O | 1:A:262:SER:HB2 | 2.15 | 0.47 |
| 14:A:1124:CLA:HMB2 | 14:A:1137:CLA:HBA1 | 1.97 | 0.47 |
| 17:6:522:BCR:H352 | 13:Y:315:LEU:HD21 | 1.95 | 0.47 |
| 14:G:1130:CLA:H61 | 14:G:1130:CLA:H41 | 1.70 | 0.47 |
| 2:H:301:ILE:HG23 | 14:H:1216:CLA:HED2 | 1.97 | 0.47 |
| 2:H:498:LEU:HA | 2:H:501:ILE:HG22 | 1.94 | 0.47 |
| 14:H:1204:CLA:H3A | 14:H:1205:CLA:HMB3 | 1.97 | 0.47 |
| 6:R:118:VAL:HA | 8:T:10:SER:HA | 1.96 | 0.47 |
| 14:Y:518:CLA:HED2 | 14:Y:518:CLA:H2A | 1.96 | 0.47 |
| 13:Z:145:HIS:NE2 | 14:Z:512:CLA:NA | 2.62 | 0.47 |
| 14:Z:501:CLA:C4D | 14:Z:503:CLA:H2 | 2.44 | 0.47 |
| 2:B:142:LEU:HG | 17:B:4006:BCR:H382 | 1.96 | 0.47 |
| 13:1:261:ALA:HA | 13:1:276:LEU:HD12 | 1.96 | 0.47 |
| 14:2:501:CLA:C4D | 14:2:503:CLA:H2 | 2.44 | 0.47 |
| 13:4:249:ILE:HG12 | 14:4:502:CLA:HAC1 | 1.96 | 0.47 |
| 1:G:300:LEU:HD21 | 1:G:385:MET:HB3 | 1.95 | 0.47 |
| 1:G:440:ARG:O | 1:G:444:HIS:ND1 | 2.43 | 0.47 |
| 14:G:1130:CLA:H52 | 14:V:1502:CLA:H12 | 1.96 | 0.47 |
| 1:A:219:VAL:HG13 | 1:A:252:PRO:HB3 | 1.96 | 0.47 |
| 14:A:1119:CLA:H11 | 14:A:1125:CLA:H93 | 1.97 | 0.47 |
| 14:A:1130:CLA:H52 | 14:L:1502:CLA:H12 | 1.96 | 0.47 |
| 2:B:210:ASP:OD1 | 2:B:210:ASP:N | 2.48 | 0.47 |
| 2:B:301:ILE:HG21 | 14:B:1221:CLA:HAC1 | 1.97 | 0.47 |
| 14:B:1216:CLA:H43 | 14:B:1223:CLA:H111 | 1.96 | 0.47 |
| 12:P:57:TRP:NE1 | 22:P:170:FMN:O2P | 2.45 | 0.47 |
| 13:3:148:PHE:CE2 | 14:3:512:CLA:HHB | 2.50 | 0.47 |
| 13:5:305:ASN:HB3 | 17:5:521:BCR:HC8 | 1.95 | 0.47 |
| 1:G:66:GLU:HG3 | 1:G:187:LEU:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:66:GLU:OE2 | 1:G:70:ARG:NH2 | 2.48 | 0.47 |
| 1:G:490:LEU:HB2 | 1:G:541:THR:HG23 | 1.96 | 0.47 |
| 14:G:1115:CLA:HBC1 | 14:G:1116:CLA:H121 | 1.96 | 0.47 |
| 2:H:156:HIS:CE1 | 14:H:1208:CLA:NA | 2.83 | 0.47 |
| 2:H:301:ILE:HG21 | 14:H:1221:CLA:HAC1 | 1.97 | 0.47 |
| 4:O:37:GLU:HA | 4:O:50:MET:O | 2.14 | 0.47 |
| 10:V:21:ILE:HD13 | 18:V:5218:LHG:H302 | 1.96 | 0.47 |
| 14:A:1139:CLA:H143 | 14:A:1139:CLA:H111 | 1.75 | 0.47 |
| 13:6:42:ALA:O | 13:6:46:THR:OG1 | 2.30 | 0.47 |
| 14:G:1109:CLA:H72 | 14:G:1101:CLA:HBB2 | 1.95 | 0.47 |
| 2:H:142:LEU:HG | 17:H:4006:BCR:H382 | 1.96 | 0.47 |
| 2:H:326:LEU:HD13 | 2:H:332:PHE:CD2 | 2.50 | 0.47 |
| 14:Z:505:CLA:H43 | 17:Z:524:BCR:HC7 | 1.96 | 0.47 |
| 14:A:1129:CLA:HAB | 14:A:1137:CLA:HBB2 | 1.96 | 0.47 |
| 2:B:326:LEU:HD13 | 2:B:332:PHE:CD2 | 2.50 | 0.47 |
| 1:G:512:ASN:HB2 | 14:G:1134:CLA:HED2 | 1.97 | 0.47 |
| 13:Y:146:LEU:HG | 14:Y:507:CLA:HED1 | 1.97 | 0.47 |
| 13:Z:251:LEU:HD13 | 14:Z:505:CLA:H122 | 1.97 | 0.47 |
| 1:A:336:ILE:O | 1:A:340:HIS:ND1 | 2.38 | 0.47 |
| 1:A:522:GLY:HA2 | 1:A:536:PRO:HB3 | 1.97 | 0.47 |
| 2:B:301:ILE:HG23 | 14:B:1216:CLA:HED2 | 1.97 | 0.47 |
| 14:B:1227:CLA:HBB2 | 14:B:1236:CLA:HMC2 | 1.97 | 0.47 |
| 14:1:518:CLA:HED2 | 14:1:518:CLA:H2A | 1.96 | 0.47 |
| 13:4:30:ALA:HB2 | 14:4:511:CLA:HMA1 | 1.96 | 0.47 |
| 13:6:40:PHE:CE1 | 14:Y:519:CLA:HMB2 | 2.50 | 0.47 |
| 13:6:79:ASP:OD1 | 13:6:79:ASP:N | 2.48 | 0.47 |
| 13:Y:261:ALA:HA | 13:Y:276:LEU:HD12 | 1.96 | 0.47 |
| 14:Z:518:CLA:H3A | 14:Z:518:CLA:C2 | 2.45 | 0.47 |
| 1:A:66:GLU:OE2 | 1:A:70:ARG:NH2 | 2.48 | 0.46 |
| 14:A:1116:CLA:HBA2 | 14:A:1116:CLA:H3A | 1.57 | 0.46 |
| 13:6:30:ALA:HB2 | 14:6:511:CLA:HMA1 | 1.96 | 0.46 |
| 2:H:377:TYR:HB3 | 14:H:1224:CLA:HMC3 | 1.96 | 0.46 |
| 2:H:546:LEU:HD13 | 2:H:567:THR:HG22 | 1.97 | 0.46 |
| 13:Z:38:ILE:HG12 | 14:Z:510:CLA:HMC2 | 1.97 | 0.46 |
| 1:A:66:GLU:HG3 | 1:A:187:LEU:HB2 | 1.97 | 0.46 |
| 14:A:1128:CLA:H121 | 18:A:5001:LHG:H352 | 1.97 | 0.46 |
| 13:1:26:LEU:HB3 | 14:1:511:CLA:HMA2 | 1.96 | 0.46 |
| 13:2:182:LEU:O | 13:2:209:TYR:OH | 2.33 | 0.46 |
| 13:3:146:LEU:HD22 | 13:3:214:LEU:HD22 | 1.97 | 0.46 |
| 14:H:1216:CLA:H43 | 14:H:1223:CLA:H111 | 1.97 | 0.46 |
| 1:A:616:ILE:HD12 | 14:A:1011:CLA:H122 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:A:1122:CLA:H62 | 14:A:1122:CLA:H41 | 1.67 | 0.46 |
| 2:B:182:LEU:HD13 | 14:B:1210:CLA:HBB | 1.97 | 0.46 |
| 13:1:146:LEU:HG | 14:1:507:CLA:HED1 | 1.97 | 0.46 |
| 17:1:522:BCR:H351 | 17:1:522:BCR:H15C | 1.78 | 0.46 |
| 14:2:505:CLA:H43 | 17:2:524:BCR:HC7 | 1.96 | 0.46 |
| 13:3:143:GLY:HA3 | 13:3:222:ILE:HG13 | 1.96 | 0.46 |
| 13:4:34:GLN:HB2 | 14:4:509:CLA:HMB2 | 1.97 | 0.46 |
| 13:5:38:ILE:HG12 | 14:5:510:CLA:HMC2 | 1.96 | 0.46 |
| 13:5:213:MET:HG2 | 14:5:506:CLA:HMC1 | 1.96 | 0.46 |
| 14:G:1124:CLA:HMB2 | 14:G:1137:CLA:HBA1 | 1.97 | 0.46 |
| 1:A:239:ASN:HD22 | 1:A:263:GLN:HE22 | 1.63 | 0.46 |
| 1:A:512:ASN:HB2 | 14:A:1134:CLA:HED2 | 1.97 | 0.46 |
| 14:A:1101:CLA:HBB1 | 14:A:1101:CLA:HHC | 1.96 | 0.46 |
| 5:E:28:VAL:HG22 | 5:E:37:VAL:HG13 | 1.96 | 0.46 |
| 12:P:2:LYS:HG3 | 12:P:3:ILE:HG13 | 1.98 | 0.46 |
| 13:4:307:HIS:NE2 | 14:4:502:CLA:ND | 2.63 | 0.46 |
| 1:G:145:GLN:HB3 | 1:G:388:TYR:HB3 | 1.98 | 0.46 |
| 2:H:174:ARG:HB2 | 14:H:1210:CLA:HBC2 | 1.97 | 0.46 |
| 2:H:237:PRO:HB3 | 2:H:256:THR:HG21 | 1.98 | 0.46 |
| 13:Y:110:HIS:HA | 13:Y:114:ALA:HB3 | 1.97 | 0.46 |
| 13:Y:319:LEU:HD21 | 14:Y:505:CLA:HMB3 | 1.97 | 0.46 |
| 1:A:316:PHE:HZ | 14:A:1117:CLA:H112 | 1.81 | 0.46 |
| 14:A:1106:CLA:H161 | 14:A:1106:CLA:H122 | 1.60 | 0.46 |
| 2:B:510:LEU:HD22 | 2:B:601:VAL:HG21 | 1.98 | 0.46 |
| 7:I:4:ASP:OD1 | 7:I:4:ASP:N | 2.42 | 0.46 |
| 13:2:145:HIS:NE2 | 14:2:512:CLA:NA | 2.62 | 0.46 |
| 14:3:512:CLA:H3A | 14:3:512:CLA:HBA1 | 1.62 | 0.46 |
| 13:5:261:ALA:HA | 13:5:276:LEU:HD12 | 1.97 | 0.46 |
| 14:G:1121:CLA:HMB1 | 18:G:5002:LHG:H271 | 1.98 | 0.46 |
| 14:H:1202:CLA:H3A | 14:H:1202:CLA:HBA1 | 1.62 | 0.46 |
| 13:Y:26:LEU:HB3 | 14:Y:511:CLA:HMA2 | 1.96 | 0.46 |
| 13:Z:148:PHE:CD2 | 14:Z:512:CLA:H3A | 2.50 | 0.46 |
| 14:A:1106:CLA:HBA2 | 14:A:1106:CLA:H3A | 1.64 | 0.46 |
| 18:A:5008:LHG:HC5 | 13:2:13:TRP:CD1 | 2.51 | 0.46 |
| 18:A:5009:LHG:C13 | 17:1:521:BCR:H313 | 2.46 | 0.46 |
| 2:B:156:HIS:CE1 | 14:B:1208:CLA:NA | 2.83 | 0.46 |
| 1:G:522:GLY:HA2 | 1:G:536:PRO:HB3 | 1.97 | 0.46 |
| 8:T:21:ILE:HA | 14:T:1302:CLA:HBB2 | 1.97 | 0.46 |
| 2:B:237:PRO:HB3 | 2:B:256:THR:HG21 | 1.98 | 0.46 |
| 2:B:546:LEU:HD13 | 2:B:567:THR:HG22 | 1.97 | 0.46 |
| 14:2:518:CLA:H3A | 14:2:518:CLA:C2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:3:517:CLA:HBA1 | 14:3:517:CLA:H3A | 1.60 | 0.46 |
| 13:6:41:TRP:O | 13:6:45:PHE:HB2 | 2.16 | 0.46 |
| 1:G:258:VAL:O | 1:G:262:SER:HB2 | 2.15 | 0.46 |
| 2:H:450:GLU:OE2 | 6:R:52:ARG:NE | 2.43 | 0.46 |
| 2:H:577:TYR:OH | 2:H:664:LEU:HD22 | 2.15 | 0.46 |
| 14:H:1239:CLA:H91 | 14:H:1239:CLA:H112 | 1.81 | 0.46 |
| 18:H:1842:LHG:HC81 | 18:H:1842:LHG:H112 | 1.80 | 0.46 |
| 1:A:441:VAL:HA | 1:A:444:HIS:CE1 | 2.51 | 0.46 |
| 2:B:577:TYR:OH | 2:B:664:LEU:HD22 | 2.15 | 0.46 |
| 14:B:1234:CLA:HMB2 | 14:B:1236:CLA:HED1 | 1.98 | 0.46 |
| 13:2:251:LEU:HD13 | 14:2:505:CLA:H122 | 1.97 | 0.46 |
| 1:G:316:PHE:HZ | 14:G:1117:CLA:H112 | 1.81 | 0.46 |
| 14:G:1128:CLA:H121 | 18:G:5001:LHG:H352 | 1.97 | 0.46 |
| 14:H:1207:CLA:HAB | 7:S:19:GLY:HA3 | 1.98 | 0.46 |
| 7:S:23:PRO:O | 7:S:27:MET:HB2 | 2.16 | 0.46 |
| 13:Z:182:LEU:O | 13:Z:209:TYR:OH | 2.33 | 0.46 |
| 14:A:1121:CLA:HMB1 | 18:A:5002:LHG:H271 | 1.97 | 0.46 |
| 14:B:1227:CLA:HAB | 14:B:1236:CLA:HBB2 | 1.97 | 0.46 |
| 13:1:130:PHE:HA | 13:1:137:GLN:HG2 | 1.97 | 0.46 |
| 13:1:319:LEU:HD21 | 14:1:505:CLA:HMB3 | 1.97 | 0.46 |
| 14:1:516:CLA:H3A | 14:1:516:CLA:HBA1 | 1.44 | 0.46 |
| 13:5:73:LEU:O | 13:5:159:LYS:NZ | 2.49 | 0.46 |
| 2:H:182:LEU:HD13 | 14:H:1210:CLA:HBB | 1.97 | 0.46 |
| 7:S:30:LEU:HD13 | 17:V:4019:BCR:HC8 | 1.98 | 0.46 |
| 10:V:49:GLU:OE2 | 14:V:1501:CLA:ND | 2.49 | 0.46 |
| 13:Y:67:LEU:HD22 | 13:Y:89:LEU:HD13 | 1.98 | 0.46 |
| 13:Z:143:GLY:HA3 | 13:Z:222:ILE:HG13 | 1.98 | 0.46 |
| 2:B:73:ASN:HB2 | 2:B:76:GLN:HB2 | 1.97 | 0.46 |
| 14:B:1217:CLA:H3A | 14:B:1217:CLA:HBA2 | 1.49 | 0.46 |
| 14:B:1207:CLA:HAB | 7:I:19:GLY:HA3 | 1.98 | 0.46 |
| 6:F:75:LEU:HA | 6:F:78:ALA:HB2 | 1.98 | 0.46 |
| 13:1:67:LEU:HD22 | 13:1:89:LEU:HD13 | 1.98 | 0.46 |
| 18:G:5008:LHG:HC5 | 13:Z:13:TRP:CD1 | 2.51 | 0.46 |
| 2:H:114:ASN:ND2 | 14:H:1206:CLA:OBD | 2.47 | 0.46 |
| 2:H:410:ARG:NH2 | 14:H:1227:CLA:OBD | 2.49 | 0.46 |
| 2:H:510:LEU:HD22 | 2:H:601:VAL:HG21 | 1.98 | 0.46 |
| 14:H:1227:CLA:HBB2 | 14:H:1236:CLA:HMC2 | 1.97 | 0.46 |
| 13:Z:319:LEU:HD21 | 14:Z:505:CLA:HMB3 | 1.97 | 0.46 |
| 14:A:1139:CLA:H61 | 14:A:1139:CLA:H41 | 1.64 | 0.45 |
| 17:A:4002:BCR:H361 | 17:A:4002:BCR:H20C | 1.76 | 0.45 |
| 2:B:174:ARG:HB2 | 14:B:1210:CLA:HBC2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:340:SER:HB3 | 14:B:1221:CLA:H2 | 1.97 | 0.45 |
| 14:B:1210:CLA:H42 | 17:B:4005:BCR:H21C | 1.98 | 0.45 |
| 7:I:30:LEU:HD13 | 17:L:4019:BCR:HC8 | 1.98 | 0.45 |
| 10:L:163:TRP:CH2 | 17:L:4219:BCR:HC7 | 2.51 | 0.45 |
| 13:2:147:LEU:HD12 | 13:2:215:ILE:HG12 | 1.98 | 0.45 |
| 13:4:159:LYS:HA | 13:4:163:TRP:HB2 | 1.98 | 0.45 |
| 2:H:73:ASN:HB2 | 2:H:76:GLN:HB2 | 1.97 | 0.45 |
| 14:H:1210:CLA:H2 | 14:H:1210:CLA:H62 | 1.60 | 0.45 |
| 17:H:4006:BCR:H15C | 17:H:4006:BCR:H351 | 1.81 | 0.45 |
| 6:R:84:PRO:HB3 | 17:T:4015:BCR:H362 | 1.98 | 0.45 |
| 13:Z:301:ALA:O | 13:Z:305:ASN:ND2 | 2.42 | 0.45 |
| 1:A:490:LEU:HB2 | 1:A:541:THR:HG23 | 1.96 | 0.45 |
| 14:A:1120:CLA:HED2 | 9:K:38:LYS:HD2 | 1.98 | 0.45 |
| 10:L:149:THR:HG22 | 10:L:151:TYR:H | 1.81 | 0.45 |
| 13:1:110:HIS:HA | 13:1:114:ALA:HB3 | 1.98 | 0.45 |
| 13:2:34:GLN:HB2 | 14:2:509:CLA:HMB2 | 1.98 | 0.45 |
| 14:G:1104:CLA:H193 | 14:G:1104:CLA:H161 | 1.79 | 0.45 |
| 14:H:1210:CLA:H42 | 17:H:4005:BCR:H21C | 1.98 | 0.45 |
| 12:X:2:LYS:HG3 | 12:X:3:ILE:HG13 | 1.98 | 0.45 |
| 13:Z:147:LEU:HD12 | 13:Z:215:ILE:HG12 | 1.98 | 0.45 |
| 13:Z:149:LEU:HD21 | 14:Z:509:CLA:H61 | 1.97 | 0.45 |
| 1:A:595:CYS:HB2 | 2:B:667:TRP:HB3 | 1.98 | 0.45 |
| 14:A:1105:CLA:HMB3 | 14:A:1106:CLA:HMB | 1.99 | 0.45 |
| 14:B:1201:CLA:HMD2 | 17:L:4019:BCR:HC41 | 1.98 | 0.45 |
| 7:I:23:PRO:O | 7:I:27:MET:HB2 | 2.16 | 0.45 |
| 13:2:38:ILE:HG12 | 14:2:510:CLA:HMC2 | 1.97 | 0.45 |
| 13:2:148:PHE:CD2 | 14:2:512:CLA:H3A | 2.50 | 0.45 |
| 13:3:34:GLN:HB2 | 14:3:509:CLA:HMB2 | 1.99 | 0.45 |
| 13:4:178:THR:OG1 | 13:4:201:GLU:OE2 | 2.34 | 0.45 |
| 14:G:1105:CLA:HMB3 | 14:G:1106:CLA:HMB | 1.99 | 0.45 |
| 14:G:1119:CLA:H11 | 14:G:1125:CLA:H93 | 1.97 | 0.45 |
| 14:H:1216:CLA:HBA1 | 14:H:1216:CLA:H12 | 1.83 | 0.45 |
| 14:Y:512:CLA:H3A | 14:Y:512:CLA:HBA1 | 1.68 | 0.45 |
| 1:A:115:GLN:NE2 | 14:A:1107:CLA:OBD | 2.43 | 0.45 |
| 1:A:440:ARG:O | 1:A:444:HIS:ND1 | 2.43 | 0.45 |
| 6:F:71:VAL:HG12 | 6:F:81:PHE:HB2 | 1.98 | 0.45 |
| 10:L:7:ALA:HB3 | 10:L:18:ALA:HB3 | 1.97 | 0.45 |
| 13:2:229:TRP:HA | 13:2:232:LYS:HB2 | 1.98 | 0.45 |
| 13:3:68:PRO:HB3 | 13:3:271:PHE:HB3 | 1.97 | 0.45 |
| 13:5:267:TYR:O | 13:5:300:ARG:NH2 | 2.45 | 0.45 |
| 14:G:1120:CLA:HED2 | 9:U:38:LYS:HD2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:H:160:LYS:HB3 | 21:H:1852:SQD:O8 | 2.16 | 0.45 |
| 14:H:1219:CLA:HMA1 | 14:H:1240:CLA:HMD3 | 1.99 | 0.45 |
| 6:R:75:LEU:HA | 6:R:78:ALA:HB2 | 1.98 | 0.45 |
| 14:B:1210:CLA:H62 | 14:B:1210:CLA:H2 | 1.60 | 0.45 |
| 13:4:119:ALA:O | 13:4:126:LYS:NZ | 2.43 | 0.45 |
| 2:H:340:SER:HB3 | 14:H:1221:CLA:H2 | 1.97 | 0.45 |
| 14:H:1209:CLA:H3A | 14:H:1209:CLA:HBA2 | 1.47 | 0.45 |
| 1:A:220:SER:O | 1:A:224:ASN:HB2 | 2.16 | 0.45 |
| 17:A:4002:BCR:H15C | 17:A:4002:BCR:H351 | 1.86 | 0.45 |
| 13:2:149:LEU:HD21 | 14:2:509:CLA:H61 | 1.97 | 0.45 |
| 13:2:319:LEU:HD21 | 14:2:505:CLA:HMB3 | 1.97 | 0.45 |
| 1:G:220:SER:O | 1:G:224:ASN:HB2 | 2.16 | 0.45 |
| 1:G:591:ARG:HH21 | 1:G:594:THR:HG21 | 1.81 | 0.45 |
| 10:V:163:TRP:CH2 | 17:V:4219:BCR:HC7 | 2.51 | 0.45 |
| 14:V:1503:CLA:H93 | 14:V:1503:CLA:H61 | 1.88 | 0.45 |
| 14:A:1110:CLA:H2 | 14:A:1110:CLA:H62 | 1.83 | 0.45 |
| 14:B:1219:CLA:HMA1 | 14:B:1240:CLA:HMD3 | 1.99 | 0.45 |
| 17:L:4019:BCR:H11C | 17:L:4019:BCR:H341 | 1.81 | 0.45 |
| 14:2:519:CLA:HED2 | 14:2:519:CLA:H2A | 1.99 | 0.45 |
| 14:G:1126:CLA:HBA2 | 14:G:1126:CLA:H3A | 1.63 | 0.45 |
| 18:G:5009:LHG:C13 | 17:Y:521:BCR:H313 | 2.46 | 0.45 |
| 10:V:7:ALA:HB3 | 10:V:18:ALA:HB3 | 1.97 | 0.45 |
| 1:A:145:GLN:HB3 | 1:A:388:TYR:HB3 | 1.98 | 0.45 |
| 8:J:21:ILE:HA | 14:J:1302:CLA:HBB2 | 1.97 | 0.45 |
| 14:2:501:CLA:H62 | 14:2:501:CLA:H41 | 1.70 | 0.45 |
| 17:2:522:BCR:H15C | 17:2:522:BCR:H351 | 1.77 | 0.45 |
| 1:G:441:VAL:HA | 1:G:444:HIS:CE1 | 2.51 | 0.45 |
| 1:G:595:CYS:HB2 | 2:H:667:TRP:HB3 | 1.98 | 0.45 |
| 18:G:5005:LHG:HC82 | 17:Z:521:BCR:HC22 | 1.98 | 0.45 |
| 6:R:83:ILE:HG12 | 14:T:1303:CLA:HMB3 | 1.99 | 0.45 |
| 14:V:1501:CLA:HAA2 | 17:V:4022:BCR:H363 | 1.98 | 0.45 |
| 12:X:57:TRP:NE1 | 22:X:170:FMN:O2P | 2.45 | 0.45 |
| 2:B:576:PHE:HE1 | 14:B:1226:CLA:HAC2 | 1.82 | 0.45 |
| 14:B:1215:CLA:HBA2 | 14:B:1215:CLA:H3A | 1.63 | 0.45 |
| 5:E:18:TRP:HB3 | 5:E:21:GLU:HB2 | 1.99 | 0.45 |
| 17:1:522:BCR:H371 | 17:1:522:BCR:H24C | 1.86 | 0.45 |
| 13:2:130:PHE:HA | 13:2:137:GLN:HG2 | 1.99 | 0.45 |
| 13:2:143:GLY:HA3 | 13:2:222:ILE:HG13 | 1.98 | 0.45 |
| 17:H:4009:BCR:H11C | 17:H:4009:BCR:H341 | 1.81 | 0.45 |
| 3:N:6:LYS:HG3 | 4:O:139:TYR:HB2 | 1.99 | 0.45 |
| 3:N:26:LEU:HA | 3:N:41:ALA:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:Y:130:PHE:HA | 13:Y:137:GLN:HG2 | 1.97 | 0.45 |
| 17:A:4001:BCR:H23C | 9:K:66:PHE:HB2 | 1.99 | 0.45 |
| 18:A:5008:LHG:HC82 | 13:2:13:TRP:HZ2 | 1.82 | 0.45 |
| 17:B:4004:BCR:H11C | 17:B:4004:BCR:H341 | 1.83 | 0.45 |
| 10:L:49:GLU:OE2 | 14:L:1501:CLA:ND | 2.49 | 0.45 |
| 14:2:505:CLA:HBA2 | 14:2:505:CLA:H11 | 1.80 | 0.45 |
| 13:3:307:HIS:NE2 | 14:3:502:CLA:ND | 2.65 | 0.45 |
| 13:5:59:MET:HB2 | 13:5:271:PHE:HA | 1.99 | 0.45 |
| 5:Q:18:TRP:HB3 | 5:Q:21:GLU:HB2 | 1.99 | 0.45 |
| 2:B:321:GLY:O | 2:B:325:THR:OG1 | 2.34 | 0.44 |
| 14:B:1221:CLA:H151 | 14:B:1221:CLA:H112 | 1.81 | 0.44 |
| 6:F:125:VAL:HG12 | 13:3:13:TRP:HH2 | 1.80 | 0.44 |
| 10:L:30:PHE:CD1 | 21:L:5216:SQD:H122 | 2.53 | 0.44 |
| 10:L:163:TRP:HH2 | 17:L:4219:BCR:H311 | 1.83 | 0.44 |
| 14:G:1013:CLA:H143 | 14:G:1013:CLA:H161 | 1.85 | 0.44 |
| 14:G:1116:CLA:HBA2 | 14:G:1116:CLA:H3A | 1.57 | 0.44 |
| 14:G:1121:CLA:HAB | 14:G:1801:CLA:CAB | 2.47 | 0.44 |
| 14:G:1122:CLA:H41 | 14:G:1122:CLA:H62 | 1.67 | 0.44 |
| 14:H:1206:CLA:H122 | 14:H:1206:CLA:H162 | 1.84 | 0.44 |
| 17:H:4010:BCR:H351 | 17:H:4010:BCR:H15C | 1.72 | 0.44 |
| 13:Z:110:HIS:HA | 13:Z:114:ALA:HB3 | 2.00 | 0.44 |
| 1:A:148:ARG:HD3 | 1:A:389:PRO:HB2 | 1.99 | 0.44 |
| 1:A:199:HIS:CG | 14:A:1111:CLA:HMC2 | 2.53 | 0.44 |
| 1:A:440:ARG:NH1 | 14:A:1129:CLA:O1D | 2.50 | 0.44 |
| 14:A:1124:CLA:H2 | 14:A:1124:CLA:H61 | 1.76 | 0.44 |
| 6:F:83:ILE:HG12 | 14:J:1303:CLA:HMB3 | 1.99 | 0.44 |
| 13:3:17:ASN:ND2 | 14:3:510:CLA:O1A | 2.47 | 0.44 |
| 13:3:253:GLY:HA2 | 14:3:502:CLA:HMD3 | 2.00 | 0.44 |
| 17:3:523:BCR:H11C | 17:3:523:BCR:H341 | 1.84 | 0.44 |
| 13:6:143:GLY:HA3 | 13:6:222:ILE:HG13 | 1.98 | 0.44 |
| 1:G:588:GLY:HA2 | 2:H:562:PRO:HD3 | 1.99 | 0.44 |
| 18:G:5008:LHG:HC82 | 13:Z:13:TRP:HZ2 | 1.82 | 0.44 |
| 10:V:149:THR:HG22 | 10:V:151:TYR:H | 1.81 | 0.44 |
| 1:A:121:PHE:HB3 | 14:B:1230:CLA:HMD1 | 2.00 | 0.44 |
| 1:A:308:HIS:HE2 | 14:A:1117:CLA:C2B | 2.31 | 0.44 |
| 14:B:1023:CLA:H142 | 17:I:4018:BCR:H271 | 1.99 | 0.44 |
| 14:L:1501:CLA:HAA2 | 17:L:4022:BCR:H363 | 1.97 | 0.44 |
| 13:3:251:LEU:HB2 | 14:3:505:CLA:HMC1 | 1.99 | 0.44 |
| 13:5:307:HIS:NE2 | 14:5:502:CLA:NA | 2.65 | 0.44 |
| 1:G:239:ASN:HD22 | 1:G:263:GLN:HE22 | 1.63 | 0.44 |
| 1:G:308:HIS:HE2 | 14:G:1117:CLA:C2B | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:R:4016:BCR:H24C | 17:R:4016:BCR:H371 | 1.83 | 0.44 |
| 12:X:63:GLN:O | 12:X:67:GLU:N | 2.50 | 0.44 |
| 13:Y:190:TYR:HE2 | 13:Y:202:ASP:HB3 | 1.83 | 0.44 |
| 13:Z:34:GLN:HB2 | 14:Z:509:CLA:HMB2 | 1.98 | 0.44 |
| 17:Z:523:BCR:H15C | 17:Z:523:BCR:H351 | 1.82 | 0.44 |
| 14:A:1121:CLA:HAB | 14:A:1801:CLA:CAB | 2.47 | 0.44 |
| 14:A:1137:CLA:H143 | 14:A:1137:CLA:H112 | 1.83 | 0.44 |
| 18:A:5001:LHG:H341 | 18:A:5001:LHG:H372 | 1.84 | 0.44 |
| 14:B:1226:CLA:H91 | 20:B:5002:LMG:H372 | 2.00 | 0.44 |
| 13:1:307:HIS:NE2 | 14:1:502:CLA:ND | 2.66 | 0.44 |
| 17:2:521:BCR:H15C | 17:2:521:BCR:H351 | 1.83 | 0.44 |
| 14:G:1104:CLA:H191 | 18:G:5001:LHG:H211 | 1.99 | 0.44 |
| 2:H:44:GLN:NE2 | 2:H:163:PRO:O | 2.38 | 0.44 |
| 2:H:91:ILE:HB | 2:H:112:PRO:HB2 | 2.00 | 0.44 |
| 14:H:1023:CLA:H142 | 17:S:4018:BCR:H271 | 1.99 | 0.44 |
| 14:H:1201:CLA:HMD2 | 17:V:4019:BCR:HC41 | 1.98 | 0.44 |
| 14:H:1215:CLA:H13 | 14:H:1221:CLA:H162 | 2.00 | 0.44 |
| 5:Q:53:ASP:OD1 | 5:Q:53:ASP:N | 2.43 | 0.44 |
| 10:V:20:PRO:HB3 | 18:V:5218:LHG:HC82 | 1.99 | 0.44 |
| 14:Z:505:CLA:HBC2 | 17:Z:524:BCR:H341 | 2.00 | 0.44 |
| 1:A:312:ILE:HD13 | 1:A:312:ILE:HA | 1.85 | 0.44 |
| 14:A:1110:CLA:HBA2 | 14:A:1110:CLA:H3A | 1.63 | 0.44 |
| 18:A:5005:LHG:HC82 | 17:2:521:BCR:HC22 | 1.98 | 0.44 |
| 2:B:160:LYS:HB3 | 21:B:1852:SQD:O8 | 2.16 | 0.44 |
| 14:2:505:CLA:HBC2 | 17:2:524:BCR:H341 | 2.00 | 0.44 |
| 13:6:38:ILE:HG12 | 14:6:510:CLA:HMC2 | 1.99 | 0.44 |
| 13:6:243:SER:O | 13:6:318:HIS:ND1 | 2.50 | 0.44 |
| 1:G:199:HIS:CG | 14:G:1111:CLA:HMC2 | 2.53 | 0.44 |
| 1:G:440:ARG:NH1 | 14:G:1129:CLA:O1D | 2.50 | 0.44 |
| 18:G:5005:LHG:C6 | 17:Z:521:BCR:HC22 | 2.48 | 0.44 |
| 14:H:1234:CLA:HMB2 | 14:H:1236:CLA:HED1 | 1.98 | 0.44 |
| 13:Z:229:TRP:HA | 13:Z:232:LYS:HB2 | 1.98 | 0.44 |
| 1:A:404:HIS:CE1 | 14:A:1126:CLA:ND | 2.86 | 0.44 |
| 1:A:440:ARG:HD2 | 14:A:1129:CLA:HED3 | 1.99 | 0.44 |
| 14:A:1108:CLA:HBA2 | 14:A:1108:CLA:H3A | 1.75 | 0.44 |
| 14:A:1022:CLA:H13 | 17:B:4017:BCR:H10C | 2.00 | 0.44 |
| 2:B:380:THR:HG22 | 2:B:583:ALA:HB1 | 2.00 | 0.44 |
| 6:F:125:VAL:HG12 | 13:3:13:TRP:CH2 | 2.53 | 0.44 |
| 17:1:521:BCR:H15C | 17:1:521:BCR:H351 | 1.82 | 0.44 |
| 13:3:73:LEU:HD11 | 14:3:503:CLA:HAA2 | 1.99 | 0.44 |
| 13:4:101:ALA:HB1 | 14:5:505:CLA:HAB | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:5:51:SER:HB2 | 13:6:279:LYS:HG3 | 2.00 | 0.44 |
| 13:5:110:HIS:NE2 | 14:5:513:CLA:NB | 2.65 | 0.44 |
| 13:5:309:PHE:HD2 | 17:5:521:BCR:H10C | 1.83 | 0.44 |
| 13:6:31:HIS:NE2 | 14:6:509:CLA:ND | 2.65 | 0.44 |
| 13:6:101:ALA:HB1 | 14:Y:505:CLA:HAB | 1.99 | 0.44 |
| 1:G:364:LEU:HD11 | 14:G:1128:CLA:HBB1 | 2.00 | 0.44 |
| 2:H:310:PRO:HA | 2:H:311:PRO:HD3 | 1.88 | 0.44 |
| 2:H:380:THR:HG22 | 2:H:583:ALA:HB1 | 2.00 | 0.44 |
| 14:H:1221:CLA:H151 | 14:H:1221:CLA:H112 | 1.81 | 0.44 |
| 3:N:13:GLY:O | 3:N:38:GLN:NE2 | 2.47 | 0.44 |
| 14:Z:519:CLA:H2A | 14:Z:519:CLA:HED2 | 1.99 | 0.44 |
| 14:A:1126:CLA:H3A | 14:A:1126:CLA:HBA2 | 1.63 | 0.44 |
| 15:A:2001:PQN:H111 | 15:A:2001:PQN:H2M1 | 1.82 | 0.44 |
| 2:B:236:ASN:OD1 | 2:B:252:THR:OG1 | 2.36 | 0.44 |
| 2:B:415:LYS:HD2 | 2:B:539:LEU:HB3 | 2.00 | 0.44 |
| 3:C:13:GLY:O | 3:C:38:GLN:NE2 | 2.46 | 0.44 |
| 13:3:274:ALA:HB3 | 13:3:290:VAL:HG22 | 2.00 | 0.44 |
| 13:4:110:HIS:NE2 | 14:4:513:CLA:NB | 2.66 | 0.44 |
| 14:6:517:CLA:HBA1 | 14:6:517:CLA:H3A | 1.55 | 0.44 |
| 1:G:440:ARG:HD2 | 14:G:1129:CLA:HED3 | 1.99 | 0.44 |
| 2:H:690:ILE:HG13 | 10:V:36:ILE:HG12 | 1.99 | 0.44 |
| 15:H:2002:PQN:H111 | 15:H:2002:PQN:H2M1 | 1.82 | 0.44 |
| 6:R:71:VAL:HG12 | 6:R:81:PHE:HB2 | 1.98 | 0.44 |
| 10:V:163:TRP:HH2 | 17:V:4219:BCR:H311 | 1.83 | 0.44 |
| 14:V:1501:CLA:H11 | 14:V:1501:CLA:H52 | 1.84 | 0.44 |
| 13:Y:307:HIS:NE2 | 14:Y:502:CLA:ND | 2.66 | 0.44 |
| 1:A:591:ARG:HH21 | 1:A:594:THR:HG21 | 1.81 | 0.44 |
| 14:A:1013:CLA:H93 | 14:A:1013:CLA:H61 | 1.83 | 0.44 |
| 14:A:1128:CLA:H91 | 14:A:1128:CLA:H112 | 1.82 | 0.44 |
| 2:B:410:ARG:O | 2:B:414:HIS:ND1 | 2.44 | 0.44 |
| 2:B:690:ILE:HG13 | 10:L:36:ILE:HG12 | 1.99 | 0.44 |
| 3:C:26:LEU:HA | 3:C:41:ALA:O | 2.17 | 0.44 |
| 1:G:404:HIS:CE1 | 14:G:1126:CLA:ND | 2.86 | 0.44 |
| 14:G:1022:CLA:H13 | 17:H:4017:BCR:H10C | 2.00 | 0.44 |
| 17:G:4001:BCR:H23C | 9:U:66:PHE:HB2 | 1.99 | 0.44 |
| 2:H:376:GLN:O | 2:H:380:THR:OG1 | 2.30 | 0.44 |
| 14:H:1215:CLA:HBA2 | 14:H:1215:CLA:H3A | 1.63 | 0.44 |
| 1:A:31:PRO:HB3 | 14:A:1101:CLA:HAC1 | 2.00 | 0.44 |
| 1:A:474:ARG:HD2 | 1:A:653:THR:HG21 | 2.00 | 0.44 |
| 14:A:1013:CLA:H143 | 14:A:1013:CLA:H161 | 1.85 | 0.44 |
| 2:B:196:HIS:NE2 | 14:B:1212:CLA:ND | 2.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:B:1206:CLA:H3A | 14:B:1207:CLA:CBB | 2.48 | 0.44 |
| 3:C:6:LYS:HG3 | 4:D:139:TYR:HB2 | 1.99 | 0.44 |
| 6:F:84:PRO:HB3 | 17:J:4015:BCR:H362 | 1.98 | 0.44 |
| 13:1:190:TYR:HD2 | 17:1:524:BCR:H401 | 1.83 | 0.44 |
| 17:2:521:BCR:H24C | 17:2:521:BCR:H371 | 1.77 | 0.44 |
| 14:3:505:CLA:H62 | 14:3:505:CLA:H41 | 1.75 | 0.44 |
| 13:4:282:VAL:HG23 | 13:4:283:THR:HG23 | 2.00 | 0.44 |
| 14:5:513:CLA:HBB1 | 17:5:523:BCR:H24C | 1.99 | 0.44 |
| 14:6:513:CLA:HBB1 | 17:6:523:BCR:H371 | 2.00 | 0.44 |
| 1:G:115:GLN:NE2 | 14:G:1107:CLA:OBD | 2.43 | 0.44 |
| 1:G:312:ILE:HD13 | 1:G:312:ILE:HA | 1.85 | 0.44 |
| 14:G:1116:CLA:H93 | 14:G:1116:CLA:H61 | 1.89 | 0.44 |
| 2:H:478:LEU:HD21 | 14:H:1231:CLA:HED2 | 2.00 | 0.44 |
| 2:H:713:PHE:O | 2:H:717:TYR:HB2 | 2.18 | 0.44 |
| 18:H:1855:LHG:H261 | 18:H:1855:LHG:H131 | 2.00 | 0.44 |
| 18:A:5005:LHG:HC41 | 17:2:521:BCR:HC31 | 2.00 | 0.43 |
| 13:4:137:GLN:HE22 | 14:4:516:CLA:HED1 | 1.83 | 0.43 |
| 1:G:202:ALA:HB2 | 1:G:320:GLY:HA3 | 2.00 | 0.43 |
| 14:G:1124:CLA:H2 | 14:G:1124:CLA:H61 | 1.76 | 0.43 |
| 17:U:4104:BCR:H15C | 17:U:4104:BCR:H351 | 1.90 | 0.43 |
| 13:Z:130:PHE:HA | 13:Z:137:GLN:HG2 | 1.99 | 0.43 |
| 2:B:478:LEU:HD21 | 14:B:1231:CLA:HED2 | 2.00 | 0.43 |
| 13:2:16:GLY:HA3 | 14:2:511:CLA:HMD3 | 2.00 | 0.43 |
| 13:3:182:LEU:O | 13:3:209:TYR:OH | 2.35 | 0.43 |
| 13:4:4:TYR:OH | 13:4:328:PHE:O | 2.31 | 0.43 |
| 13:5:146:LEU:HD22 | 13:5:214:LEU:HD22 | 2.00 | 0.43 |
| 13:6:148:PHE:CD2 | 14:6:512:CLA:H3A | 2.51 | 0.43 |
| 1:G:148:ARG:HD3 | 1:G:389:PRO:HB2 | 1.99 | 0.43 |
| 14:G:1104:CLA:H62 | 14:G:1104:CLA:H41 | 1.61 | 0.43 |
| 2:H:455:ILE:HD13 | 6:R:69:LEU:HB2 | 2.00 | 0.43 |
| 2:H:576:PHE:HE1 | 14:H:1226:CLA:HAC2 | 1.82 | 0.43 |
| 14:H:1206:CLA:H3A | 14:H:1207:CLA:CBB | 2.48 | 0.43 |
| 10:V:30:PHE:CD1 | 21:V:5216:SQD:H122 | 2.53 | 0.43 |
| 17:V:4219:BCR:H15C | 17:V:4219:BCR:H351 | 1.75 | 0.43 |
| 13:Z:16:GLY:HA3 | 14:Z:511:CLA:HMD3 | 2.00 | 0.43 |
| 14:Z:501:CLA:H41 | 14:Z:501:CLA:H62 | 1.70 | 0.43 |
| 1:A:202:ALA:HB2 | 1:A:320:GLY:HA3 | 2.00 | 0.43 |
| 1:A:221:LEU:HD23 | 1:A:221:LEU:HA | 1.84 | 0.43 |
| 14:A:1134:CLA:H61 | 14:A:1134:CLA:H41 | 1.87 | 0.43 |
| 2:B:91:ILE:HB | 2:B:112:PRO:HB2 | 2.00 | 0.43 |
| 14:B:1218:CLA:H61 | 14:B:1218:CLA:H2 | 1.75 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:K:4104:BCR:H15C | 17:K:4104:BCR:H351 | 1.90 | 0.43 |
| 13:2:110:HIS:HA | 13:2:114:ALA:HB3 | 2.00 | 0.43 |
| 17:2:524:BCR:H15C | 17:2:524:BCR:H351 | 1.78 | 0.43 |
| 13:3:62:GLN:HB2 | 13:3:64:LEU:HG | 2.01 | 0.43 |
| 13:3:261:ALA:HA | 13:3:276:LEU:HD12 | 2.00 | 0.43 |
| 13:5:309:PHE:CD2 | 17:5:521:BCR:H10C | 2.53 | 0.43 |
| 1:G:31:PRO:HB3 | 14:G:1101:CLA:HAC1 | 2.00 | 0.43 |
| 2:H:196:HIS:NE2 | 14:H:1212:CLA:ND | 2.66 | 0.43 |
| 14:H:1226:CLA:H91 | 20:H:5002:LMG:H372 | 2.00 | 0.43 |
| 9:U:46:LEU:H | 9:U:56:GLY:HA2 | 1.84 | 0.43 |
| 1:A:364:LEU:HD11 | 14:A:1128:CLA:HBB1 | 2.00 | 0.43 |
| 1:A:588:GLY:HA2 | 2:B:562:PRO:HD3 | 1.99 | 0.43 |
| 14:A:1121:CLA:HBB | 14:A:1801:CLA:HBC3 | 2.01 | 0.43 |
| 2:B:713:PHE:O | 2:B:717:TYR:HB2 | 2.18 | 0.43 |
| 14:B:1240:CLA:H62 | 14:B:1240:CLA:H41 | 1.87 | 0.43 |
| 17:B:4005:BCR:H15C | 17:B:4005:BCR:H351 | 1.84 | 0.43 |
| 10:L:20:PRO:HB3 | 18:L:5218:LHG:HC82 | 1.99 | 0.43 |
| 17:L:4022:BCR:H11C | 17:L:4022:BCR:H341 | 1.81 | 0.43 |
| 11:M:11:LEU:HD21 | 17:M:4021:BCR:H272 | 2.01 | 0.43 |
| 14:2:512:CLA:H3A | 14:2:512:CLA:HBA1 | 1.54 | 0.43 |
| 2:H:481:ALA:HA | 2:H:486:THR:HG21 | 2.00 | 0.43 |
| 11:W:1:MET:HE2 | 11:W:6:VAL:HG22 | 2.00 | 0.43 |
| 13:Y:190:TYR:HD2 | 17:Y:524:BCR:H401 | 1.83 | 0.43 |
| 14:A:1133:CLA:H111 | 14:A:1133:CLA:H91 | 1.81 | 0.43 |
| 17:A:4001:BCR:H19C | 9:K:69:ILE:HD11 | 2.00 | 0.43 |
| 14:B:1215:CLA:H13 | 14:B:1221:CLA:H162 | 2.00 | 0.43 |
| 14:B:1221:CLA:H141 | 14:B:1221:CLA:H161 | 1.78 | 0.43 |
| 14:B:1229:CLA:HMB2 | 17:B:4014:BCR:H10C | 1.99 | 0.43 |
| 18:B:1842:LHG:H112 | 18:B:1842:LHG:HC81 | 1.80 | 0.43 |
| 8:J:40:PRO:HD2 | 17:J:4015:BCR:H382 | 2.01 | 0.43 |
| 1:G:441:VAL:HG23 | 14:G:1129:CLA:HMD3 | 2.00 | 0.43 |
| 14:H:1208:CLA:HAB | 19:H:1843:LMU:H111 | 2.00 | 0.43 |
| 1:A:441:VAL:HG23 | 14:A:1129:CLA:HMD3 | 2.00 | 0.43 |
| 14:A:1131:CLA:HBB2 | 10:L:65:LEU:HD13 | 2.00 | 0.43 |
| 2:B:410:ARG:NH2 | 14:B:1227:CLA:OBD | 2.49 | 0.43 |
| 18:B:1855:LHG:H261 | 18:B:1855:LHG:H131 | 2.00 | 0.43 |
| 17:F:4016:BCR:H341 | 17:F:4016:BCR:H11C | 1.75 | 0.43 |
| 13:1:148:PHE:CE1 | 14:1:516:CLA:HBC2 | 2.54 | 0.43 |
| 17:6:522:BCR:H24C | 17:6:522:BCR:H371 | 1.84 | 0.43 |
| 1:G:485:ASP:OD1 | 1:G:491:GLN:NE2 | 2.45 | 0.43 |
| 14:G:1137:CLA:H62 | 14:G:1137:CLA:H41 | 1.63 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:317:ILE:O | 1:A:321:HIS:ND1 | 2.46 | 0.43 |
| 12:P:82:LYS:HB3 | 12:P:117:VAL:HG21 | 2.01 | 0.43 |
| 14:1:513:CLA:HBB1 | 17:1:523:BCR:H402 | 2.01 | 0.43 |
| 13:4:307:HIS:NE2 | 14:4:502:CLA:NA | 2.67 | 0.43 |
| 13:6:190:TYR:HE2 | 13:6:202:ASP:HB3 | 1.83 | 0.43 |
| 1:G:745:LEU:HD22 | 14:G:1140:CLA:HMA1 | 2.00 | 0.43 |
| 18:G:5005:LHG:HC41 | 17:Z:521:BCR:HC31 | 2.00 | 0.43 |
| 2:H:236:ASN:OD1 | 2:H:236:ASN:N | 2.51 | 0.43 |
| 14:H:1229:CLA:HMB2 | 17:H:4014:BCR:H10C | 1.99 | 0.43 |
| 17:V:4019:BCR:H15C | 17:V:4019:BCR:H351 | 1.86 | 0.43 |
| 14:Y:505:CLA:HBC2 | 17:Y:524:BCR:H341 | 2.01 | 0.43 |
| 13:Z:190:TYR:HE2 | 13:Z:202:ASP:HB3 | 1.83 | 0.43 |
| 1:A:572:ARG:HD3 | 3:C:80:ALA:HB3 | 2.01 | 0.43 |
| 14:A:1104:CLA:H191 | 18:A:5001:LHG:H211 | 1.99 | 0.43 |
| 2:B:455:ILE:HD13 | 6:F:69:LEU:HB2 | 2.00 | 0.43 |
| 14:1:505:CLA:HBC2 | 17:1:524:BCR:H341 | 2.01 | 0.43 |
| 13:2:190:TYR:HE2 | 13:2:202:ASP:HB3 | 1.83 | 0.43 |
| 13:5:16:GLY:HA3 | 14:5:511:CLA:HMD3 | 2.00 | 0.43 |
| 13:6:91:VAL:HG22 | 17:6:523:BCR:HC22 | 2.01 | 0.43 |
| 13:6:109:PHE:HB2 | 14:Y:505:CLA:HAA2 | 2.01 | 0.43 |
| 1:G:121:PHE:HB3 | 14:H:1230:CLA:HMD1 | 2.00 | 0.43 |
| 1:G:388:TYR:HB2 | 1:G:391:LEU:HB2 | 2.01 | 0.43 |
| 18:G:5005:LHG:O7 | 17:Z:521:BCR:HC22 | 2.19 | 0.43 |
| 2:H:585:ASN:HB2 | 14:H:1012:CLA:HBC2 | 2.00 | 0.43 |
| 17:R:4016:BCR:H341 | 17:R:4016:BCR:H11C | 1.75 | 0.43 |
| 8:T:8:LEU:HA | 8:T:13:ILE:HG21 | 2.01 | 0.43 |
| 14:Z:518:CLA:H61 | 14:Z:518:CLA:H41 | 1.70 | 0.43 |
| 17:I:4018:BCR:H20C | 17:I:4018:BCR:H361 | 1.89 | 0.43 |
| 18:I:5001:LHG:H242 | 21:V:5216:SQD:H242 | 2.01 | 0.43 |
| 17:J:4015:BCR:H20C | 17:J:4015:BCR:H361 | 1.88 | 0.43 |
| 13:1:190:TYR:HE2 | 13:1:202:ASP:HB3 | 1.83 | 0.43 |
| 1:G:371:LEU:HD12 | 1:G:371:LEU:HA | 1.88 | 0.43 |
| 1:G:600:TRP:CD1 | 14:G:1128:CLA:HMD1 | 2.54 | 0.43 |
| 14:G:1121:CLA:HHB | 14:G:1801:CLA:HBC3 | 2.01 | 0.43 |
| 14:G:1131:CLA:HBB2 | 10:V:65:LEU:HD13 | 2.00 | 0.43 |
| 14:G:1133:CLA:H192 | 14:G:1133:CLA:H162 | 1.88 | 0.43 |
| 2:H:299:HIS:HB3 | 2:H:304:ILE:HD11 | 2.01 | 0.43 |
| 14:Z:512:CLA:H3A | 14:Z:512:CLA:HBA1 | 1.54 | 0.43 |
| 1:A:745:LEU:HD22 | 14:A:1140:CLA:HMA1 | 2.00 | 0.43 |
| 14:A:1102:CLA:HBA2 | 14:A:1102:CLA:H3A | 1.81 | 0.43 |
| 14:A:1104:CLA:H161 | 14:A:1104:CLA:H193 | 1.79 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:A:5005:LHG:C6 | 17:2:521:BCR:HC22 | 2.48 | 0.43 |
| 2:B:257:PHE:CD1 | 14:B:1214:CLA:HMB2 | 2.54 | 0.43 |
| 14:B:1229:CLA:H2 | 14:B:1229:CLA:H62 | 1.81 | 0.43 |
| 4:D:101:ASP:OD1 | 4:D:101:ASP:N | 2.47 | 0.43 |
| 17:J:4015:BCR:H11C | 17:J:4015:BCR:H341 | 1.83 | 0.43 |
| 17:M:4021:BCR:H24C | 17:M:4021:BCR:H371 | 1.83 | 0.43 |
| 12:P:63:GLN:O | 12:P:67:GLU:N | 2.50 | 0.43 |
| 13:1:177:VAL:HG13 | 13:1:201:GLU:HG2 | 2.01 | 0.43 |
| 14:3:502:CLA:HMB1 | 14:3:504:CLA:HMC3 | 2.01 | 0.43 |
| 13:4:160:ALA:HA | 13:4:165:GLY:HA2 | 2.01 | 0.43 |
| 1:G:474:ARG:HD2 | 1:G:653:THR:HG21 | 2.00 | 0.43 |
| 1:G:572:ARG:HD3 | 3:N:80:ALA:HB3 | 2.00 | 0.43 |
| 1:G:734:GLN:HG3 | 18:G:5001:LHG:C7 | 2.49 | 0.43 |
| 14:G:1104:CLA:H201 | 18:G:5001:LHG:H221 | 2.01 | 0.43 |
| 14:G:1116:CLA:C4D | 14:G:1125:CLA:HBB1 | 2.48 | 0.43 |
| 14:G:1123:CLA:H141 | 14:G:1123:CLA:H161 | 1.82 | 0.43 |
| 14:G:1128:CLA:H91 | 14:G:1128:CLA:H112 | 1.82 | 0.43 |
| 14:G:1133:CLA:H91 | 14:G:1133:CLA:H111 | 1.81 | 0.43 |
| 2:H:270:LEU:HD23 | 2:H:270:LEU:HA | 1.89 | 0.43 |
| 2:H:415:LYS:HD2 | 2:H:539:LEU:HB3 | 2.00 | 0.43 |
| 14:H:1221:CLA:H112 | 14:H:1221:CLA:H72 | 1.73 | 0.43 |
| 10:V:18:ALA:HB2 | 10:V:110:VAL:HG21 | 2.00 | 0.43 |
| 14:Y:505:CLA:HMD2 | 17:Y:524:BCR:H343 | 2.01 | 0.43 |
| 1:A:600:TRP:CD1 | 14:A:1128:CLA:HMD1 | 2.54 | 0.42 |
| 2:B:194:LEU:HA | 2:B:198:ALA:HB3 | 2.00 | 0.42 |
| 2:B:236:ASN:OD1 | 2:B:236:ASN:N | 2.51 | 0.42 |
| 17:B:4009:BCR:H15C | 17:B:4009:BCR:H351 | 1.83 | 0.42 |
| 14:1:505:CLA:HMD2 | 17:1:524:BCR:H343 | 2.01 | 0.42 |
| 13:4:57:GLN:HB3 | 13:4:61:GLU:HB2 | 2.00 | 0.42 |
| 1:G:336:ILE:O | 1:G:340:HIS:ND1 | 2.38 | 0.42 |
| 17:G:4002:BCR:H11C | 17:G:4002:BCR:H341 | 1.83 | 0.42 |
| 2:H:7:LYS:HD2 | 11:W:28:TYR:CZ | 2.54 | 0.42 |
| 1:A:94:GLY:O | 1:A:98:SER:OG | 2.33 | 0.42 |
| 1:A:388:TYR:HB2 | 1:A:391:LEU:HB2 | 2.01 | 0.42 |
| 14:A:1116:CLA:C4D | 14:A:1125:CLA:HBB1 | 2.48 | 0.42 |
| 17:A:4008:BCR:H11C | 17:A:4008:BCR:H341 | 1.90 | 0.42 |
| 14:B:1220:CLA:HED3 | 14:B:1220:CLA:H2A | 2.01 | 0.42 |
| 10:L:18:ALA:HB2 | 10:L:110:VAL:HG21 | 2.00 | 0.42 |
| 13:1:207:HIS:CE1 | 17:1:524:BCR:H381 | 2.54 | 0.42 |
| 14:2:502:CLA:HBD | 14:2:503:CLA:H43 | 2.01 | 0.42 |
| 14:2:518:CLA:H61 | 14:2:518:CLA:H41 | 1.70 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:4:17:ASN:OD1 | 14:4:511:CLA:NC | 2.52 | 0.42 |
| 14:G:1131:CLA:H111 | 15:H:2002:PQN:H201 | 2.01 | 0.42 |
| 2:H:236:ASN:OD1 | 2:H:252:THR:OG1 | 2.36 | 0.42 |
| 2:H:428:PHE:CZ | 17:T:4015:BCR:HC41 | 2.55 | 0.42 |
| 8:T:40:PRO:HD2 | 17:T:4015:BCR:H382 | 2.01 | 0.42 |
| 13:Y:177:VAL:HG13 | 13:Y:201:GLU:HG2 | 2.01 | 0.42 |
| 14:Y:513:CLA:HBB1 | 17:Y:523:BCR:H402 | 2.01 | 0.42 |
| 17:A:4002:BCR:H24C | 17:A:4002:BCR:H371 | 1.85 | 0.42 |
| 2:B:450:GLU:OE2 | 6:F:52:ARG:NE | 2.43 | 0.42 |
| 2:B:585:ASN:HB2 | 14:B:1012:CLA:HBC2 | 2.00 | 0.42 |
| 14:B:1239:CLA:H112 | 14:B:1239:CLA:H91 | 1.81 | 0.42 |
| 14:B:1207:CLA:H91 | 14:B:1207:CLA:H112 | 1.87 | 0.42 |
| 9:K:46:LEU:H | 9:K:56:GLY:HA2 | 1.84 | 0.42 |
| 17:K:4104:BCR:H11C | 17:K:4104:BCR:H341 | 1.94 | 0.42 |
| 11:M:1:MET:HE2 | 11:M:6:VAL:HG22 | 2.00 | 0.42 |
| 13:1:34:GLN:HB2 | 14:1:509:CLA:HMB2 | 2.01 | 0.42 |
| 13:5:50:ILE:HD11 | 13:5:89:LEU:HB2 | 2.00 | 0.42 |
| 14:5:509:CLA:HBA1 | 14:5:509:CLA:H3A | 1.81 | 0.42 |
| 14:G:1106:CLA:H91 | 14:G:1106:CLA:H112 | 1.85 | 0.42 |
| 17:G:4001:BCR:H19C | 9:U:69:ILE:HD11 | 2.00 | 0.42 |
| 2:H:527:LEU:HD12 | 14:H:1236:CLA:HED3 | 2.02 | 0.42 |
| 14:H:1220:CLA:HED3 | 14:H:1220:CLA:H2A | 2.01 | 0.42 |
| 12:X:82:LYS:HB3 | 12:X:117:VAL:HG21 | 2.01 | 0.42 |
| 14:Z:502:CLA:HBD | 14:Z:503:CLA:H43 | 2.01 | 0.42 |
| 14:A:1113:CLA:HMA2 | 18:A:5006:LHG:H292 | 2.01 | 0.42 |
| 14:A:1131:CLA:H111 | 15:B:2002:PQN:H201 | 2.01 | 0.42 |
| 17:3:524:BCR:H15C | 17:3:524:BCR:H351 | 1.79 | 0.42 |
| 13:4:168:ASP:HB3 | 13:4:171:SER:HB2 | 2.00 | 0.42 |
| 1:G:749:VAL:HG21 | 17:G:4011:BCR:HC8 | 2.01 | 0.42 |
| 14:G:1113:CLA:HMA2 | 18:G:5006:LHG:H292 | 2.01 | 0.42 |
| 15:G:2001:PQN:H111 | 15:G:2001:PQN:H2M1 | 1.82 | 0.42 |
| 14:H:1229:CLA:H2 | 14:H:1229:CLA:H62 | 1.81 | 0.42 |
| 13:Y:34:GLN:HB2 | 14:Y:509:CLA:HMB2 | 2.01 | 0.42 |
| 13:Y:148:PHE:CE1 | 14:Y:516:CLA:HBC2 | 2.54 | 0.42 |
| 17:A:4002:BCR:H11C | 17:A:4002:BCR:H341 | 1.83 | 0.42 |
| 2:B:276:HIS:HE2 | 14:B:1215:CLA:C2B | 2.32 | 0.42 |
| 2:B:657:TRP:CZ3 | 14:B:1021:CLA:HBB | 2.55 | 0.42 |
| 14:B:1012:CLA:H122 | 14:B:1012:CLA:H8 | 1.86 | 0.42 |
| 14:B:1209:CLA:H3A | 14:B:1209:CLA:HBA2 | 1.47 | 0.42 |
| 14:B:1234:CLA:H143 | 14:B:1234:CLA:H111 | 1.81 | 0.42 |
| 17:1:523:BCR:H15C | 17:1:523:BCR:H351 | 1.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:4:309:PHE:CD1 | 17:4:521:BCR:H12C | 2.54 | 0.42 |
| 14:G:1237:CLA:H202 | 17:V:4019:BCR:H391 | 2.02 | 0.42 |
| 2:H:167:TRP:CZ2 | 14:H:1208:CLA:HHB | 2.54 | 0.42 |
| 14:H:1021:CLA:H62 | 14:H:1021:CLA:H102 | 1.83 | 0.42 |
| 17:H:4004:BCR:H361 | 17:H:4004:BCR:H20C | 1.79 | 0.42 |
| 13:Y:148:PHE:HD2 | 14:Y:512:CLA:H3A | 1.85 | 0.42 |
| 17:Z:524:BCR:H15C | 17:Z:524:BCR:H351 | 1.78 | 0.42 |
| 1:A:544:PHE:CZ | 17:L:4219:BCR:H332 | 2.55 | 0.42 |
| 1:A:734:GLN:HG3 | 18:A:5001:LHG:C7 | 2.49 | 0.42 |
| 18:A:5005:LHG:O7 | 17:2:521:BCR:HC22 | 2.19 | 0.42 |
| 2:B:7:LYS:HD2 | 11:M:28:TYR:CZ | 2.54 | 0.42 |
| 2:B:299:HIS:HB3 | 2:B:304:ILE:HD11 | 2.01 | 0.42 |
| 2:B:428:PHE:CZ | 17:J:4015:BCR:HC41 | 2.54 | 0.42 |
| 17:4:521:BCR:H11C | 17:4:521:BCR:H341 | 1.88 | 0.42 |
| 14:G:1136:CLA:H92 | 14:G:1136:CLA:H62 | 1.81 | 0.42 |
| 14:G:1101:CLA:H51 | 8:T:19:PHE:HE2 | 1.85 | 0.42 |
| 17:H:4004:BCR:H11C | 17:H:4004:BCR:H341 | 1.83 | 0.42 |
| 9:U:78:LEU:HD22 | 9:U:83:ASN:HB2 | 2.01 | 0.42 |
| 1:A:691:TRP:CE2 | 14:A:1011:CLA:HBA2 | 2.54 | 0.42 |
| 14:A:1237:CLA:H202 | 17:L:4019:BCR:H391 | 2.02 | 0.42 |
| 18:A:5008:LHG:C8 | 13:2:13:TRP:CZ2 | 3.03 | 0.42 |
| 2:B:218:HIS:HD2 | 2:B:220:ALA:H | 1.67 | 0.42 |
| 14:B:1204:CLA:HMC2 | 14:B:1204:CLA:H92 | 2.02 | 0.42 |
| 14:B:1221:CLA:H112 | 14:B:1221:CLA:H72 | 1.72 | 0.42 |
| 14:B:1229:CLA:H112 | 14:B:1229:CLA:H152 | 1.81 | 0.42 |
| 13:1:148:PHE:HD2 | 14:1:512:CLA:H3A | 1.85 | 0.42 |
| 17:3:522:BCR:H24C | 17:3:522:BCR:H371 | 1.87 | 0.42 |
| 13:6:59:MET:HA | 13:6:62:GLN:HB2 | 2.02 | 0.42 |
| 14:6:505:CLA:H111 | 14:6:517:CLA:HBB2 | 2.02 | 0.42 |
| 14:G:1013:CLA:H141 | 14:H:1012:CLA:H151 | 2.02 | 0.42 |
| 14:G:1108:CLA:HBA2 | 14:G:1108:CLA:H3A | 1.75 | 0.42 |
| 14:G:1237:CLA:H13 | 10:V:89:LEU:HD21 | 2.02 | 0.42 |
| 2:H:111:SER:HB3 | 7:S:3:GLY:HA2 | 2.01 | 0.42 |
| 2:H:531:THR:HG21 | 14:H:1236:CLA:HMB3 | 2.02 | 0.42 |
| 2:H:657:TRP:CZ3 | 14:H:1021:CLA:HHB | 2.55 | 0.42 |
| 14:H:1221:CLA:H141 | 14:H:1221:CLA:H161 | 1.78 | 0.42 |
| 13:Y:207:HIS:CE1 | 17:Y:524:BCR:H381 | 2.54 | 0.42 |
| 13:Z:138:LEU:HA | 13:Z:141:ILE:HD12 | 2.01 | 0.42 |
| 1:A:430:PRO:HG2 | 4:D:41:GLU:HB2 | 2.02 | 0.42 |
| 2:B:460:ALA:HB1 | 14:B:1234:CLA:HBD | 2.02 | 0.42 |
| 2:B:481:ALA:HA | 2:B:486:THR:HG21 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:E:10:ARG:HD3 | 5:E:21:GLU:O | 2.20 | 0.42 |
| 14:J:1303:CLA:HMD3 | 17:J:4015:BCR:H402 | 2.02 | 0.42 |
| 15:G:2001:PQN:H142 | 15:G:2001:PQN:H112 | 1.82 | 0.42 |
| 18:G:5001:LHG:H341 | 18:G:5001:LHG:H372 | 1.84 | 0.42 |
| 17:V:4022:BCR:H341 | 17:V:4022:BCR:H11C | 1.82 | 0.42 |
| 2:B:167:TRP:CZ2 | 14:B:1208:CLA:HBB | 2.54 | 0.42 |
| 2:B:177:HIS:CG | 14:B:1210:CLA:HMC2 | 2.55 | 0.42 |
| 14:B:1206:CLA:H3A | 14:B:1206:CLA:HBA1 | 1.63 | 0.42 |
| 14:B:1208:CLA:HAB | 19:B:1843:LMU:H111 | 2.00 | 0.42 |
| 14:B:1224:CLA:HBA2 | 14:B:1224:CLA:H3A | 1.67 | 0.42 |
| 18:L:5220:LHG:H151 | 18:L:5220:LHG:H292 | 2.02 | 0.42 |
| 13:5:221:HIS:HE1 | 14:5:506:CLA:NA | 2.18 | 0.42 |
| 1:G:544:PHE:CZ | 17:V:4219:BCR:H332 | 2.55 | 0.42 |
| 2:H:177:HIS:CG | 14:H:1210:CLA:HMC2 | 2.55 | 0.42 |
| 2:H:194:LEU:HA | 2:H:198:ALA:HB3 | 2.00 | 0.42 |
| 2:H:257:PHE:CD1 | 14:H:1214:CLA:HMB2 | 2.54 | 0.42 |
| 17:H:4006:BCR:H24C | 17:H:4006:BCR:H371 | 1.79 | 0.42 |
| 14:A:1104:CLA:H201 | 18:A:5001:LHG:H221 | 2.01 | 0.42 |
| 14:A:1128:CLA:H142 | 14:A:1128:CLA:H111 | 1.83 | 0.42 |
| 17:A:4001:BCR:H11C | 17:A:4001:BCR:H341 | 1.88 | 0.42 |
| 17:A:4008:BCR:H20C | 17:A:4008:BCR:H361 | 1.83 | 0.42 |
| 2:B:192:GLY:O | 2:B:196:HIS:HB2 | 2.20 | 0.42 |
| 14:B:1208:CLA:H61 | 14:B:1208:CLA:H2 | 1.84 | 0.42 |
| 12:P:36:ILE:HD12 | 12:P:36:ILE:HA | 1.96 | 0.42 |
| 13:2:301:ALA:O | 13:2:305:ASN:ND2 | 2.42 | 0.42 |
| 13:3:54:THR:H | 13:3:62:GLN:HE22 | 1.68 | 0.42 |
| 13:4:65:ILE:HB | 13:4:303:LEU:HD21 | 2.02 | 0.42 |
| 14:4:512:CLA:HAB | 14:4:516:CLA:HMD3 | 2.02 | 0.42 |
| 14:G:1011:CLA:H62 | 14:G:1011:CLA:H102 | 1.82 | 0.42 |
| 14:G:1119:CLA:H111 | 14:G:1119:CLA:H152 | 1.81 | 0.42 |
| 14:G:1131:CLA:H142 | 14:G:1237:CLA:HMC1 | 2.02 | 0.42 |
| 17:G:4007:BCR:H11C | 17:G:4007:BCR:H341 | 1.90 | 0.42 |
| 18:G:5008:LHG:C8 | 13:Z:13:TRP:CZ2 | 3.03 | 0.42 |
| 2:H:59:LEU:HD23 | 2:H:59:LEU:HA | 1.92 | 0.42 |
| 2:H:276:HIS:HE2 | 14:H:1215:CLA:C2B | 2.32 | 0.42 |
| 18:A:5006:LHG:H241 | 13:1:52:TRP:CH2 | 2.55 | 0.41 |
| 17:B:4006:BCR:H15C | 17:B:4006:BCR:H351 | 1.81 | 0.41 |
| 3:C:61:ASP:HA | 3:C:62:PHE:HA | 1.81 | 0.41 |
| 6:F:87:LEU:HD21 | 14:J:1303:CLA:HMC3 | 2.02 | 0.41 |
| 17:F:4016:BCR:H24C | 17:F:4016:BCR:H371 | 1.83 | 0.41 |
| 8:J:8:LEU:HA | 8:J:13:ILE:HG21 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:K:68:HIS:O | 9:K:72:ILE:HG12 | 2.20 | 0.41 |
| 17:6:523:BCR:H11C | 17:6:523:BCR:H341 | 1.91 | 0.41 |
| 1:G:430:PRO:HG2 | 4:O:41:GLU:HB2 | 2.02 | 0.41 |
| 1:G:691:TRP:CE2 | 14:G:1011:CLA:HBA2 | 2.54 | 0.41 |
| 14:G:1112:CLA:HBC3 | 18:G:5006:LHG:H352 | 2.02 | 0.41 |
| 3:N:61:ASP:HA | 3:N:62:PHE:HA | 1.81 | 0.41 |
| 20:T:5104:LMG:H292 | 20:T:5104:LMG:H321 | 1.89 | 0.41 |
| 17:U:4104:BCR:H11C | 17:U:4104:BCR:H341 | 1.94 | 0.41 |
| 12:X:59:VAL:O | 12:X:59:VAL:HG12 | 2.20 | 0.41 |
| 13:Y:79:ASP:OD1 | 13:Y:79:ASP:N | 2.52 | 0.41 |
| 17:Y:521:BCR:H371 | 17:Y:521:BCR:H24C | 1.78 | 0.41 |
| 1:A:749:VAL:HG21 | 17:A:4011:BCR:HC8 | 2.01 | 0.41 |
| 15:A:2001:PQN:H162 | 15:A:2001:PQN:H193 | 1.89 | 0.41 |
| 17:A:4008:BCR:H15C | 17:A:4008:BCR:H351 | 1.77 | 0.41 |
| 2:B:126:THR:HG22 | 2:B:270:LEU:HD21 | 2.02 | 0.41 |
| 13:3:267:TYR:OH | 14:3:502:CLA:O1D | 2.36 | 0.41 |
| 14:5:509:CLA:H92 | 14:5:509:CLA:H62 | 1.81 | 0.41 |
| 1:G:205:LEU:HD11 | 14:G:1127:CLA:H192 | 2.03 | 0.41 |
| 1:G:554:ILE:HD11 | 14:G:1135:CLA:HBB1 | 2.02 | 0.41 |
| 14:G:1116:CLA:H91 | 14:G:1116:CLA:H111 | 1.82 | 0.41 |
| 14:G:1137:CLA:H143 | 14:G:1137:CLA:H112 | 1.83 | 0.41 |
| 17:G:4011:BCR:H20C | 17:G:4011:BCR:H361 | 1.87 | 0.41 |
| 2:H:192:GLY:O | 2:H:196:HIS:HB2 | 2.20 | 0.41 |
| 11:W:11:LEU:HD21 | 17:W:4021:BCR:H272 | 2.01 | 0.41 |
| 17:W:4021:BCR:H15C | 17:W:4021:BCR:H351 | 1.81 | 0.41 |
| 17:Y:521:BCR:H11C | 17:Y:521:BCR:H341 | 1.86 | 0.41 |
| 14:A:1112:CLA:HBC3 | 18:A:5006:LHG:H352 | 2.02 | 0.41 |
| 14:A:1131:CLA:H142 | 14:A:1237:CLA:HMC1 | 2.02 | 0.41 |
| 2:B:527:LEU:HD12 | 14:B:1236:CLA:HED3 | 2.02 | 0.41 |
| 14:B:1228:CLA:H12 | 14:B:1228:CLA:H52 | 1.77 | 0.41 |
| 17:B:4014:BCR:H24C | 17:B:4014:BCR:H371 | 1.84 | 0.41 |
| 12:P:132:ALA:HB1 | 12:P:139:VAL:HG22 | 2.03 | 0.41 |
| 13:3:263:ASN:HD21 | 13:3:266:ALA:H | 1.67 | 0.41 |
| 17:4:523:BCR:H351 | 17:4:523:BCR:H15C | 1.79 | 0.41 |
| 17:6:522:BCR:H15C | 17:6:522:BCR:H351 | 1.79 | 0.41 |
| 17:6:524:BCR:H351 | 17:6:524:BCR:H15C | 1.80 | 0.41 |
| 14:G:1128:CLA:H142 | 14:G:1128:CLA:H111 | 1.83 | 0.41 |
| 14:H:1210:CLA:H111 | 17:H:4005:BCR:H381 | 2.03 | 0.41 |
| 14:H:1234:CLA:H143 | 14:H:1234:CLA:H111 | 1.81 | 0.41 |
| 5:Q:10:ARG:HD3 | 5:Q:21:GLU:O | 2.20 | 0.41 |
| 1:A:205:LEU:HD11 | 14:A:1127:CLA:H192 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:A:2001:PQN:H112 | 15:A:2001:PQN:H142 | 1.82 | 0.41 |
| 18:A:5008:LHG:C8 | 13:2:13:TRP:HZ2 | 2.34 | 0.41 |
| 2:B:326:LEU:O | 2:B:326:LEU:HD12 | 2.20 | 0.41 |
| 2:B:700:LEU:HD22 | 2:B:704:GLN:NE2 | 2.35 | 0.41 |
| 14:B:1229:CLA:H193 | 14:B:1229:CLA:H162 | 1.88 | 0.41 |
| 17:B:4014:BCR:H15C | 17:B:4014:BCR:H351 | 1.95 | 0.41 |
| 9:K:78:LEU:HD22 | 9:K:83:ASN:HB2 | 2.01 | 0.41 |
| 13:2:73:LEU:HD11 | 14:2:503:CLA:HAA2 | 2.03 | 0.41 |
| 13:2:138:LEU:HA | 13:2:141:ILE:HD12 | 2.01 | 0.41 |
| 13:3:323:LEU:HD22 | 14:3:518:CLA:HMD1 | 2.02 | 0.41 |
| 13:4:26:LEU:HB3 | 14:4:511:CLA:HMA2 | 2.01 | 0.41 |
| 14:G:1115:CLA:H142 | 14:G:1115:CLA:H112 | 1.92 | 0.41 |
| 14:G:1126:CLA:H72 | 14:G:1126:CLA:H111 | 1.88 | 0.41 |
| 14:G:1130:CLA:HMC2 | 14:V:1502:CLA:H151 | 2.02 | 0.41 |
| 2:H:159:PRO:HD2 | 21:H:1852:SQD:H5 | 2.02 | 0.41 |
| 2:H:326:LEU:HD12 | 2:H:326:LEU:O | 2.20 | 0.41 |
| 14:H:1204:CLA:H92 | 14:H:1204:CLA:HMC2 | 2.02 | 0.41 |
| 14:H:1206:CLA:H3A | 14:H:1206:CLA:HBA1 | 1.63 | 0.41 |
| 14:H:1218:CLA:H61 | 14:H:1218:CLA:H2 | 1.75 | 0.41 |
| 1:A:141:SER:HB3 | 14:A:1126:CLA:HAA2 | 2.02 | 0.41 |
| 1:A:601:ASP:HA | 1:A:604:PHE:HB3 | 2.03 | 0.41 |
| 14:A:1106:CLA:H61 | 14:A:1106:CLA:H92 | 1.78 | 0.41 |
| 2:B:339:ALA:HB2 | 17:B:4010:BCR:H372 | 2.03 | 0.41 |
| 15:B:2002:PQN:H261 | 15:B:2002:PQN:H222 | 1.78 | 0.41 |
| 7:I:17:LEU:HD23 | 7:I:17:LEU:HA | 1.84 | 0.41 |
| 10:L:85:LEU:HD12 | 10:L:85:LEU:HA | 1.89 | 0.41 |
| 17:1:524:BCR:H15C | 17:1:524:BCR:H351 | 1.79 | 0.41 |
| 17:3:521:BCR:H351 | 17:3:521:BCR:H15C | 1.77 | 0.41 |
| 13:4:54:THR:HG22 | 13:4:56:ASP:H | 1.86 | 0.41 |
| 1:G:197:LEU:O | 1:G:201:LEU:HB2 | 2.21 | 0.41 |
| 14:G:1129:CLA:H51 | 14:G:1129:CLA:H11 | 1.84 | 0.41 |
| 18:G:5008:LHG:C8 | 13:Z:13:TRP:HZ2 | 2.33 | 0.41 |
| 14:H:1223:CLA:H13 | 17:H:4010:BCR:H15C | 2.02 | 0.41 |
| 17:H:4004:BCR:H15C | 17:H:4004:BCR:H351 | 1.83 | 0.41 |
| 6:R:87:LEU:HD21 | 14:T:1303:CLA:HMC3 | 2.02 | 0.41 |
| 1:A:354:GLU:HA | 1:A:357:THR:HG22 | 2.03 | 0.41 |
| 14:A:1237:CLA:H13 | 10:L:89:LEU:HD21 | 2.02 | 0.41 |
| 2:B:323:TYR:O | 2:B:327:ASN:HB2 | 2.20 | 0.41 |
| 14:B:1207:CLA:C4 | 18:V:5221:LHG:H252 | 2.42 | 0.41 |
| 13:1:57:GLN:HB2 | 13:1:62:GLN:HE21 | 1.85 | 0.41 |
| 13:5:26:LEU:HB3 | 14:5:511:CLA:HMA2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:315:LEU:CD2 | 14:G:1119:CLA:HMC1 | 2.50 | 0.41 |
| 2:H:218:HIS:HD2 | 2:H:220:ALA:H | 1.67 | 0.41 |
| 17:T:4015:BCR:H15C | 17:T:4015:BCR:H351 | 1.81 | 0.41 |
| 9:U:68:HIS:O | 9:U:72:ILE:HG12 | 2.20 | 0.41 |
| 17:Z:521:BCR:H371 | 17:Z:521:BCR:H24C | 1.77 | 0.41 |
| 17:Z:524:BCR:H20C | 17:Z:524:BCR:H361 | 1.91 | 0.41 |
| 14:A:1013:CLA:H122 | 14:A:1140:CLA:H101 | 2.03 | 0.41 |
| 14:A:1133:CLA:H192 | 14:A:1133:CLA:H162 | 1.88 | 0.41 |
| 14:B:1207:CLA:HMA1 | 18:V:5221:LHG:H121 | 2.02 | 0.41 |
| 5:E:53:ASP:OD1 | 5:E:53:ASP:N | 2.43 | 0.41 |
| 13:3:110:HIS:HA | 13:3:114:ALA:HB3 | 2.02 | 0.41 |
| 13:3:183:ASN:HD22 | 13:3:186:VAL:HG23 | 1.86 | 0.41 |
| 14:4:507:CLA:HED2 | 14:4:507:CLA:H2A | 2.03 | 0.41 |
| 14:6:513:CLA:HMC2 | 17:6:523:BCR:H372 | 2.02 | 0.41 |
| 1:G:23:THR:HG21 | 18:G:5008:LHG:C9 | 2.51 | 0.41 |
| 1:G:366:ILE:HD11 | 17:G:4007:BCR:HC7 | 2.03 | 0.41 |
| 14:G:1106:CLA:H92 | 14:G:1106:CLA:H61 | 1.78 | 0.41 |
| 14:G:1119:CLA:H122 | 14:G:1122:CLA:H101 | 2.03 | 0.41 |
| 14:H:1207:CLA:H91 | 14:H:1207:CLA:H112 | 1.87 | 0.41 |
| 15:H:2002:PQN:H261 | 15:H:2002:PQN:H222 | 1.78 | 0.41 |
| 14:T:1303:CLA:HMD3 | 17:T:4015:BCR:H402 | 2.02 | 0.41 |
| 12:X:132:ALA:HB1 | 12:X:139:VAL:HG22 | 2.03 | 0.41 |
| 13:Z:73:LEU:HD11 | 14:Z:503:CLA:HAA2 | 2.03 | 0.41 |
| 14:Z:505:CLA:H11 | 14:Z:505:CLA:HBA2 | 1.80 | 0.41 |
| 19:A:1849:LMU:H62 | 19:A:1849:LMU:H91 | 1.81 | 0.41 |
| 2:B:142:LEU:HD23 | 2:B:142:LEU:HA | 1.88 | 0.41 |
| 2:B:150:LEU:HD22 | 11:M:20:ALA:HA | 2.03 | 0.41 |
| 2:B:262:HIS:HA | 2:B:263:PRO:HD3 | 1.96 | 0.41 |
| 14:B:1223:CLA:H13 | 17:B:4010:BCR:H15C | 2.02 | 0.41 |
| 17:J:4013:BCR:H15C | 17:J:4013:BCR:H351 | 1.87 | 0.41 |
| 13:1:206:GLY:HA3 | 17:1:524:BCR:H402 | 2.02 | 0.41 |
| 14:G:1123:CLA:H193 | 14:G:1123:CLA:H162 | 1.84 | 0.41 |
| 2:H:339:ALA:HB2 | 17:H:4010:BCR:H372 | 2.03 | 0.41 |
| 2:H:697:PRO:O | 3:N:81:TYR:OH | 2.30 | 0.41 |
| 14:H:1201:CLA:H2A | 14:H:1201:CLA:HED2 | 2.03 | 0.41 |
| 4:O:127:ASN:O | 4:O:130:THR:OG1 | 2.34 | 0.41 |
| 17:W:4021:BCR:H24C | 17:W:4021:BCR:H371 | 1.83 | 0.41 |
| 13:Y:326:MET:H | 13:Y:326:MET:HG2 | 1.72 | 0.41 |
| 17:Z:522:BCR:H24C | 17:Z:522:BCR:H371 | 1.84 | 0.41 |
| 1:A:366:ILE:HD11 | 17:A:4007:BCR:HC7 | 2.03 | 0.41 |
| 14:A:1129:CLA:H11 | 14:A:1129:CLA:H51 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:A:1130:CLA:HMC2 | 14:L:1502:CLA:H151 | 2.02 | 0.41 |
| 14:B:1205:CLA:H51 | 14:B:1205:CLA:H8 | 1.87 | 0.41 |
| 17:B:4006:BCR:H371 | 17:B:4006:BCR:H24C | 1.79 | 0.41 |
| 8:J:13:ILE:HD11 | 17:J:4013:BCR:H281 | 2.02 | 0.41 |
| 13:1:79:ASP:OD1 | 13:1:79:ASP:N | 2.52 | 0.41 |
| 13:6:16:GLY:HA3 | 14:6:511:CLA:HMD3 | 2.02 | 0.41 |
| 14:6:512:CLA:H2A | 14:6:512:CLA:HED2 | 2.03 | 0.41 |
| 1:G:217:ILE:HD11 | 1:G:287:LEU:HD21 | 2.02 | 0.41 |
| 1:G:468:ILE:HG23 | 14:G:1022:CLA:H61 | 2.03 | 0.41 |
| 17:G:4003:BCR:H361 | 17:G:4003:BCR:H20C | 1.82 | 0.41 |
| 18:G:5006:LHG:H241 | 13:Y:52:TRP:CH2 | 2.55 | 0.41 |
| 23:G:909:HOH:O | 2:H:682:HIS:HB2 | 2.21 | 0.41 |
| 2:H:126:THR:HG22 | 2:H:270:LEU:HD21 | 2.02 | 0.41 |
| 2:H:142:LEU:HD23 | 2:H:142:LEU:HA | 1.88 | 0.41 |
| 2:H:531:THR:O | 2:H:535:VAL:HB | 2.21 | 0.41 |
| 2:H:700:LEU:HD22 | 2:H:704:GLN:NE2 | 2.35 | 0.41 |
| 14:H:1234:CLA:H161 | 14:H:1234:CLA:H193 | 1.86 | 0.41 |
| 13:Y:206:GLY:HA3 | 17:Y:524:BCR:H402 | 2.02 | 0.41 |
| 17:Z:522:BCR:H15C | 17:Z:522:BCR:H351 | 1.77 | 0.41 |
| 1:A:470:ASN:HB3 | 1:A:653:THR:HG22 | 2.02 | 0.41 |
| 14:A:1013:CLA:H141 | 14:B:1012:CLA:H151 | 2.02 | 0.41 |
| 14:A:1237:CLA:HAA2 | 14:A:1130:CLA:HMB1 | 2.03 | 0.41 |
| 2:B:111:SER:HB3 | 7:I:3:GLY:HA2 | 2.02 | 0.41 |
| 2:B:293:THR:OG1 | 2:B:294:ASN:N | 2.54 | 0.41 |
| 14:B:1204:CLA:H142 | 14:B:1204:CLA:H112 | 1.93 | 0.41 |
| 17:B:4017:BCR:H371 | 17:B:4017:BCR:H24C | 1.81 | 0.41 |
| 12:P:59:VAL:O | 12:P:59:VAL:HG12 | 2.20 | 0.41 |
| 17:2:523:BCR:H20C | 17:2:523:BCR:H361 | 1.94 | 0.41 |
| 13:3:16:GLY:HA3 | 14:3:511:CLA:HMD3 | 2.03 | 0.41 |
| 13:4:34:GLN:HG2 | 14:4:509:CLA:HHB | 2.03 | 0.41 |
| 14:4:509:CLA:O1A | 14:4:510:CLA:HBB1 | 2.21 | 0.41 |
| 13:6:47:LEU:HD21 | 13:6:90:PHE:HD1 | 1.86 | 0.41 |
| 1:G:470:ASN:HB3 | 1:G:653:THR:HG22 | 2.02 | 0.41 |
| 14:G:1106:CLA:H161 | 14:G:1106:CLA:H122 | 1.60 | 0.41 |
| 14:H:1216:CLA:H111 | 14:H:1216:CLA:H91 | 1.84 | 0.41 |
| 17:Y:524:BCR:H351 | 17:Y:524:BCR:H15C | 1.79 | 0.41 |
| 13:Z:243:SER:O | 13:Z:318:HIS:ND1 | 2.44 | 0.41 |
| 1:A:217:ILE:HD11 | 1:A:287:LEU:HD21 | 2.03 | 0.40 |
| 14:A:1237:CLA:HED3 | 2:B:681:ALA:HB1 | 2.03 | 0.40 |
| 14:B:1211:CLA:H12 | 14:B:1211:CLA:H52 | 1.90 | 0.40 |
| 14:B:1219:CLA:HBC2 | 14:B:1220:CLA:HBA1 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L:3:GLN:N | 10:L:3:GLN:OE1 | 2.54 | 0.40 |
| 13:3:148:PHE:CD2 | 14:3:512:CLA:H3A | 2.53 | 0.40 |
| 17:4:524:BCR:H11C | 17:4:524:BCR:H341 | 1.79 | 0.40 |
| 17:5:523:BCR:H15C | 17:5:523:BCR:H351 | 1.82 | 0.40 |
| 1:G:141:SER:HB3 | 14:G:1126:CLA:HAA2 | 2.02 | 0.40 |
| 1:G:173:LEU:HD12 | 1:G:173:LEU:HA | 1.95 | 0.40 |
| 1:G:440:ARG:NH2 | 10:V:4:ASP:OD1 | 2.54 | 0.40 |
| 1:G:728:ARG:HH11 | 1:G:728:ARG:HD3 | 1.77 | 0.40 |
| 14:G:1237:CLA:HED3 | 2:H:681:ALA:HB1 | 2.03 | 0.40 |
| 2:H:118:SER:HA | 14:H:1224:CLA:HMA2 | 2.03 | 0.40 |
| 2:H:323:TYR:O | 2:H:327:ASN:HB2 | 2.20 | 0.40 |
| 2:H:704:GLN:HG3 | 20:H:5002:LMG:H131 | 2.03 | 0.40 |
| 14:H:1215:CLA:H142 | 14:H:1215:CLA:H112 | 1.90 | 0.40 |
| 6:R:91:ILE:O | 6:R:94:TRP:HB3 | 2.21 | 0.40 |
| 14:Y:516:CLA:H3A | 14:Y:516:CLA:HBA1 | 1.45 | 0.40 |
| 13:Z:148:PHE:HE2 | 14:Z:512:CLA:HBB | 1.86 | 0.40 |
| 1:A:315:LEU:CD2 | 14:A:1119:CLA:HMC1 | 2.50 | 0.40 |
| 1:A:360:TRP:HE3 | 14:A:1103:CLA:HMD2 | 1.86 | 0.40 |
| 2:B:558:PRO:HB3 | 2:B:702:ILE:HB | 2.03 | 0.40 |
| 12:P:51:ILE:HG12 | 12:P:84:ALA:HB3 | 2.04 | 0.40 |
| 13:1:305:ASN:HB3 | 17:1:521:BCR:HC8 | 2.03 | 0.40 |
| 14:1:512:CLA:H3A | 14:1:512:CLA:HBA1 | 1.68 | 0.40 |
| 17:1:521:BCR:H24C | 17:1:521:BCR:H371 | 1.79 | 0.40 |
| 13:4:143:GLY:HA3 | 13:4:222:ILE:HG23 | 2.03 | 0.40 |
| 1:G:354:GLU:HA | 1:G:357:THR:HG22 | 2.03 | 0.40 |
| 19:G:1849:LMU:H62 | 19:G:1849:LMU:H91 | 1.81 | 0.40 |
| 13:Y:57:GLN:HB2 | 13:Y:62:GLN:HE21 | 1.86 | 0.40 |
| 1:A:197:LEU:O | 1:A:201:LEU:HB2 | 2.21 | 0.40 |
| 23:A:909:HOH:O | 2:B:682:HIS:HB2 | 2.21 | 0.40 |
| 2:B:270:LEU:HD23 | 2:B:270:LEU:HA | 1.89 | 0.40 |
| 14:B:1201:CLA:H143 | 14:B:1201:CLA:H111 | 1.90 | 0.40 |
| 17:B:4009:BCR:H24C | 17:B:4009:BCR:H371 | 1.94 | 0.40 |
| 7:I:16:PRO:HB2 | 17:V:4219:BCR:H291 | 2.02 | 0.40 |
| 17:4:524:BCR:H15C | 17:4:524:BCR:H351 | 1.82 | 0.40 |
| 17:5:522:BCR:H15C | 17:5:522:BCR:H351 | 1.77 | 0.40 |
| 13:6:246:LEU:HD23 | 13:6:246:LEU:HA | 1.87 | 0.40 |
| 1:G:601:ASP:HA | 1:G:604:PHE:HB3 | 2.03 | 0.40 |
| 14:G:1110:CLA:H3A | 14:G:1110:CLA:HBA2 | 1.63 | 0.40 |
| 17:G:4008:BCR:H20C | 17:G:4008:BCR:H361 | 1.83 | 0.40 |
| 2:H:460:ALA:HB1 | 14:H:1234:CLA:HBD | 2.02 | 0.40 |
| 14:H:1023:CLA:H92 | 14:H:1023:CLA:H62 | 1.92 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:H:4010:BCR:H20C | 17:H:4010:BCR:H361 | 1.86 | 0.40 |
| 7:S:10:LEU:HD23 | 7:S:10:LEU:HA | 1.89 | 0.40 |
| 8:T:13:ILE:HD11 | 17:T:4013:BCR:H281 | 2.03 | 0.40 |
| 17:T:4013:BCR:H15C | 17:T:4013:BCR:H351 | 1.87 | 0.40 |
| 18:V:5220:LHG:H151 | 18:V:5220:LHG:H292 | 2.02 | 0.40 |
| 17:Z:521:BCR:H351 | 17:Z:521:BCR:H15C | 1.83 | 0.40 |
| 1:A:336:ILE:HG21 | 1:A:336:ILE:HD13 | 1.89 | 0.40 |
| 1:A:371:LEU:HD12 | 1:A:371:LEU:HA | 1.88 | 0.40 |
| 1:A:554:ILE:HD11 | 14:A:1135:CLA:HBB1 | 2.02 | 0.40 |
| 14:A:1115:CLA:H41 | 14:A:1115:CLA:H62 | 1.65 | 0.40 |
| 14:A:1101:CLA:H51 | 8:J:19:PHE:HE2 | 1.85 | 0.40 |
| 2:B:531:THR:O | 2:B:535:VAL:HB | 2.21 | 0.40 |
| 4:D:89:PHE:HB2 | 4:D:93:ASP:HB3 | 2.02 | 0.40 |
| 17:2:524:BCR:H20C | 17:2:524:BCR:H361 | 1.91 | 0.40 |
| 13:5:110:HIS:HA | 13:5:114:ALA:HB3 | 2.04 | 0.40 |
| 13:5:148:PHE:CD2 | 14:5:512:CLA:H3A | 2.53 | 0.40 |
| 17:5:522:BCR:H371 | 17:5:522:BCR:H24C | 1.88 | 0.40 |
| 13:6:26:LEU:HD22 | 14:6:511:CLA:HAA2 | 2.03 | 0.40 |
| 1:G:317:ILE:O | 1:G:321:HIS:ND1 | 2.46 | 0.40 |
| 1:G:577:LYS:NZ | 2:H:673:GLU:OE2 | 2.43 | 0.40 |
| 2:H:658:ALA:HB3 | 14:H:1023:CLA:HBB2 | 2.04 | 0.40 |
| 14:H:1205:CLA:H8 | 14:H:1205:CLA:H51 | 1.87 | 0.40 |
| 14:H:1219:CLA:HBC2 | 14:H:1220:CLA:HBA1 | 2.03 | 0.40 |
| 14:H:1230:CLA:H102 | 14:H:1230:CLA:H61 | 1.83 | 0.40 |
| 13:Y:282:VAL:HG23 | 13:Y:283:THR:HG23 | 2.04 | 0.40 |
| 13:Y:305:ASN:HB3 | 17:Y:521:BCR:HC8 | 2.03 | 0.40 |
| 1:A:468:ILE:HG23 | 14:A:1022:CLA:H61 | 2.03 | 0.40 |
| 18:A:5004:LHG:H271 | 18:A:5005:LHG:H291 | 2.04 | 0.40 |
| 14:B:1210:CLA:H111 | 17:B:4005:BCR:H381 | 2.03 | 0.40 |
| 14:B:1216:CLA:H91 | 14:B:1216:CLA:H111 | 1.84 | 0.40 |
| 17:B:4010:BCR:H15C | 17:B:4010:BCR:H351 | 1.72 | 0.40 |
| 5:E:56:VAL:HG12 | 5:E:58:THR:H | 1.87 | 0.40 |
| 17:2:522:BCR:H24C | 17:2:522:BCR:H371 | 1.84 | 0.40 |
| 13:3:77:VAL:HG12 | 13:3:83:VAL:HA | 2.03 | 0.40 |
| 17:4:522:BCR:H24C | 17:4:522:BCR:H371 | 1.90 | 0.40 |
| 13:6:221:HIS:CE1 | 14:6:506:CLA:NA | 2.89 | 0.40 |
| 1:G:329:ILE:HD13 | 9:U:62:ALA:HB2 | 2.03 | 0.40 |
| 14:G:1013:CLA:H122 | 14:G:1140:CLA:H101 | 2.03 | 0.40 |
| 14:G:1237:CLA:HAA2 | 14:G:1130:CLA:HMB1 | 2.03 | 0.40 |
| 17:G:4003:BCR:H15C | 17:G:4003:BCR:H351 | 1.80 | 0.40 |
| 14:H:1222:CLA:HBA2 | 14:H:1222:CLA:H3A | 1.90 | 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 | 749/763 (98%) | 724 (97%) | 25 (3%) | 0 | 100 | 100 |
| 1 | G | 749/763 (98%) | 724 (97%) | 25 (3%) | 0 | 100 | 100 |
| 1 | e | 749/763 (98%) | 724 (97%) | 25 (3%) | 0 | 100 | 100 |
| 2 | B | 731/734 (100%) | 710 (97%) | 21 (3%) | 0 | 100 | 100 |
| 2 | H | 731/734 (100%) | 710 (97%) | 21 (3%) | 0 | 100 | 100 |
| 2 | f | 731/734 (100%) | 710 (97%) | 21 (3%) | 0 | 100 | 100 |
| 3 | C | 78/81 (96%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | N | 78/81 (96%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | g | 78/81 (96%) | 77 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | D | 139/141 (99%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 4 | O | 139/141 (99%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 4 | h | 139/141 (99%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 5 | E | 69/75 (92%) | 68 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | Q | 69/75 (92%) | 68 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | i | 69/75 (92%) | 68 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | F | 134/159 (84%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 6 | R | 134/159 (84%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 6 | j | 134/159 (84%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 7 | I | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 7 | S | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 7 | k | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 8 | J | 39/41 (95%) | 39 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 8 | T | 39/41 (95%) | 39 (100%) | 0 | 0 | 100 | 100 |
| 8 | l | 39/41 (95%) | 39 (100%) | 0 | 0 | 100 | 100 |
| 9 | K | 76/84 (90%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 9 | U | 76/84 (90%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 9 | m | 76/84 (90%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 10 | L | 162/166 (98%) | 158 (98%) | 4 (2%) | 0 | 100 | 100 |
| 10 | V | 162/166 (98%) | 158 (98%) | 4 (2%) | 0 | 100 | 100 |
| 10 | n | 162/166 (98%) | 158 (98%) | 4 (2%) | 0 | 100 | 100 |
| 11 | M | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 11 | W | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 11 | o | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 12 | P | 167/172 (97%) | 159 (95%) | 8 (5%) | 0 | 100 | 100 |
| 12 | X | 167/172 (97%) | 159 (95%) | 8 (5%) | 0 | 100 | 100 |
| 12 | p | 167/172 (97%) | 159 (95%) | 8 (5%) | 0 | 100 | 100 |
| 13 | 1 | 337/342 (98%) | 328 (97%) | 9 (3%) | 0 | 100 | 100 |
| 13 | 2 | 337/342 (98%) | 330 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | 3 | 337/342 (98%) | 330 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | 4 | 337/342 (98%) | 326 (97%) | 11 (3%) | 0 | 100 | 100 |
| 13 | 5 | 337/342 (98%) | 326 (97%) | 11 (3%) | 0 | 100 | 100 |
| 13 | 6 | 337/342 (98%) | 328 (97%) | 9 (3%) | 0 | 100 | 100 |
| 13 | Y | 337/342 (98%) | 328 (97%) | 9 (3%) | 0 | 100 | 100 |
| 13 | Z | 337/342 (98%) | 330 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | a | 337/342 (98%) | 330 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | b | 337/342 (98%) | 326 (97%) | 11 (3%) | 0 | 100 | 100 |
| 13 | c | 337/342 (98%) | 326 (97%) | 11 (3%) | 0 | 100 | 100 |
| 13 | d | 337/342 (98%) | 328 (97%) | 9 (3%) | 0 | 100 | 100 |
| 13 | q | 337/342 (98%) | 328 (97%) | 9 (3%) | 0 | 100 | 100 |
| 13 | r | 337/342 (98%) | 330 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | s | 337/342 (98%) | 330 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | t | 337/342 (98%) | 326 (97%) | 11 (3%) | 0 | 100 | 100 |
| 13 | u | 337/342 (98%) | 326 (97%) | 11 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 13 | v | 337/342 (98%) | 328 (97%) | 9 (3%) | 0 | 100 | 100 |
| All | All | 13287/13605 (98%) | 12906 (97%) | 381 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 600/611 (98%) | 597 (100%) | 3 (0%) | 86 | 91 |
| 1 | G | 600/611 (98%) | 597 (100%) | 3 (0%) | 86 | 91 |
| 1 | e | 600/611 (98%) | 597 (100%) | 3 (0%) | 86 | 91 |
| 2 | B | 583/584 (100%) | 582 (100%) | 1 (0%) | 92 | 95 |
| 2 | H | 583/584 (100%) | 582 (100%) | 1 (0%) | 92 | 95 |
| 2 | f | 583/584 (100%) | 582 (100%) | 1 (0%) | 92 | 95 |
| 3 | C | 67/68 (98%) | 67 (100%) | 0 | 100 | 100 |
| 3 | N | 67/68 (98%) | 67 (100%) | 0 | 100 | 100 |
| 3 | g | 67/68 (98%) | 67 (100%) | 0 | 100 | 100 |
| 4 | D | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 4 | O | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 4 | h | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 5 | E | 56/59 (95%) | 56 (100%) | 0 | 100 | 100 |
| 5 | Q | 56/59 (95%) | 56 (100%) | 0 | 100 | 100 |
| 5 | i | 56/59 (95%) | 56 (100%) | 0 | 100 | 100 |
| 6 | F | 105/121 (87%) | 105 (100%) | 0 | 100 | 100 |
| 6 | R | 105/121 (87%) | 105 (100%) | 0 | 100 | 100 |
| 6 | j | 105/121 (87%) | 105 (100%) | 0 | 100 | 100 |
| 7 | I | 30/30 (100%) | 30 (100%) | 0 | 100 | 100 |
| 7 | S | 30/30 (100%) | 30 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 7 | k | 30/30 (100%) | 30 (100%) | 0 | 100 | 100 |
| 8 | J | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 8 | T | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 8 | l | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 9 | K | 56/61 (92%) | 56 (100%) | 0 | 100 | 100 |
| 9 | U | 56/61 (92%) | 56 (100%) | 0 | 100 | 100 |
| 9 | m | 56/61 (92%) | 56 (100%) | 0 | 100 | 100 |
| 10 | L | 127/128 (99%) | 127 (100%) | 0 | 100 | 100 |
| 10 | V | 127/128 (99%) | 127 (100%) | 0 | 100 | 100 |
| 10 | n | 127/128 (99%) | 127 (100%) | 0 | 100 | 100 |
| 11 | M | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| 11 | W | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| 11 | o | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| 12 | P | 140/142 (99%) | 140 (100%) | 0 | 100 | 100 |
| 12 | X | 140/142 (99%) | 140 (100%) | 0 | 100 | 100 |
| 12 | p | 140/142 (99%) | 140 (100%) | 0 | 100 | 100 |
| 13 | 1 | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | 2 | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | 3 | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | 4 | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | 5 | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | 6 | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | Y | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | Z | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | a | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | b | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | c | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | d | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | q | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | r | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | s | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 13 | t | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | u | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| 13 | v | 257/259 (99%) | 257 (100%) | 0 | 100 | 100 |
| All | All | 10437/10593 (98%) | 10425 (100%) | 12 (0%) | 92 | 96 |

All (12) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 13 | LYS |
| 1 | A | 36 | ARG |
| 1 | A | 383 | TYR |
| 2 | B | 443 | VAL |
| 1 | G | 13 | LYS |
| 1 | G | 36 | ARG |
| 1 | G | 383 | TYR |
| 2 | H | 443 | VAL |
| 1 | e | 13 | LYS |
| 1 | e | 36 | ARG |
| 1 | e | 383 | TYR |
| 2 | f | 443 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 19 | ASN |
| 1 | A | 179 | HIS |
| 1 | A | 181 | HIS |
| 1 | A | 216 | GLN |
| 1 | A | 239 | ASN |
| 1 | A | 253 | HIS |
| 1 | A | 612 | ASN |
| 1 | A | 626 | GLN |
| 2 | B | 34 | HIS |
| 2 | B | 122 | HIS |
| 2 | B | 156 | HIS |
| 2 | B | 218 | HIS |
| 2 | B | 452 | GLN |
| 2 | B | 603 | GLN |
| 4 | D | 71 | GLN |
| 5 | E | 67 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 58 | GLN |
| 13 | 1 | 57 | GLN |
| 13 | 4 | 62 | GLN |
| 13 | 4 | 137 | GLN |
| 13 | 4 | 263 | ASN |
| 1 | G | 19 | ASN |
| 1 | G | 179 | HIS |
| 1 | G | 216 | GLN |
| 1 | G | 239 | ASN |
| 1 | G | 253 | HIS |
| 1 | G | 612 | ASN |
| 1 | G | 626 | GLN |
| 2 | H | 34 | HIS |
| 2 | H | 122 | HIS |
| 2 | H | 156 | HIS |
| 2 | H | 218 | HIS |
| 2 | H | 452 | GLN |
| 2 | H | 603 | GLN |
| 4 | O | 71 | GLN |
| 5 | Q | 67 | GLN |
| 6 | R | 58 | GLN |
| 13 | Y | 57 | GLN |
| 13 | b | 62 | GLN |
| 13 | b | 137 | GLN |
| 13 | b | 263 | ASN |
| 1 | e | 19 | ASN |
| 1 | e | 179 | HIS |
| 1 | e | 181 | HIS |
| 1 | e | 216 | GLN |
| 1 | e | 239 | ASN |
| 1 | e | 253 | HIS |
| 1 | e | 612 | ASN |
| 1 | e | 626 | GLN |
| 2 | f | 34 | HIS |
| 2 | f | 122 | HIS |
| 2 | f | 156 | HIS |
| 2 | f | 218 | HIS |
| 2 | f | 452 | GLN |
| 2 | f | 603 | GLN |
| 4 | h | 71 | GLN |
| 5 | i | 67 | GLN |
| 6 | j | 58 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | q | 57 | GLN |
| 13 | t | 62 | GLN |
| 13 | t | 137 | GLN |
| 13 | t | 263 | 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

843 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 | $\# Z > 2$ |
| 14 | CLA | B | 1203 | 2 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.53 | 9 (11%) |
| 14 | CLA | B | 1219 | 2 | 63,71,73 | 1.52 | 8 (12%) | 73,110,113 | 1.44 | 10 (13%) |
| 21 | SQD | n | 5216 | - | 45,46,54 | 1.02 | 5 (11%) | 54,57,65 | 1.68 | 11 (20%) |
| 14 | CLA | 3 | 501 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.66 | 9 (17%) |
| 17 | BCR | b | 523 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.77 | 14 (25%) |
| 14 | CLA | A | 1011 | 1 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.73 | 14 (18%) |
| 17 | BCR | l | 4013 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.93 | 16 (28%) |
| 14 | CLA | Y | 508 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.92 | 8 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | 6 | 502 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.66 | 8 (15%) |
| 14 | CLA | G | 1136 | 1 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.54 | 10 (13%) |
| 14 | CLA | e | 1122 | 1 | 60,68,73 | 1.51 | 11 (18%) | 70,107,113 | 1.54 | 9 (12%) |
| 14 | CLA | Z | 501 | 13 | 60,68,73 | 1.50 | 8 (13%) | 70,107,113 | 1.57 | 7 (10%) |
| 17 | BCR | 3 | 522 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 2.04 | 18 (32%) |
| 14 | CLA | H | 1206 | 2 | 65,73,73 | 1.49 | 11 (16%) | 76,113,113 | 1.61 | 10 (13%) |
| 14 | CLA | Y | 506 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.64 | 6 (11%) |
| 17 | BCR | 2 | 522 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.85 | 17 (30%) |
| 14 | CLA | v | 506 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 6 (11%) |
| 16 | SF4 | C | 3002 | 3 | 0,12,12 | - | - | - | - | - |
| 14 | CLA | B | 1225 | 2 | 65,73,73 | 1.44 | 10 (15%) | 76,113,113 | 1.49 | 8 (10%) |
| 14 | CLA | A | 1126 | 1 | 65,73,73 | 1.39 | 8 (12%) | 76,113,113 | 1.57 | 8 (10%) |
| 14 | CLA | 6 | 513 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.59 | 6 (11%) |
| 14 | CLA | f | 1240 | 18 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.45 | 8 (10%) |
| 14 | CLA | r | 518 | 13 | 55,63,73 | 1.55 | 7 (12%) | 64,101,113 | 1.53 | 8 (12%) |
| 14 | CLA | 3 | 511 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.71 | 9 (17%) |
| 14 | CLA | q | 505 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.64 | 6 (11%) |
| 14 | CLA | Y | 511 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | G | 1140 | 1 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.56 | 10 (13%) |
| 14 | CLA | e | 1013 | - | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.88 | 13 (17%) |
| 14 | CLA | B | 1216 | 23 | 60,68,73 | 1.60 | 10 (16%) | 70,107,113 | 1.56 | 11 (15%) |
| 14 | CLA | a | 503 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.64 | 8 (15%) |
| 14 | CLA | 4 | 512 | 13 | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.59 | 6 (11%) |
| 17 | BCR | Z | 522 | - | 41,41,41 | 0.75 | 0 | 56,56,56 | 1.86 | 17 (30%) |
| 14 | CLA | A | 1108 | 1 | 54,62,73 | 1.58 | 9 (16%) | 62,99,113 | 1.58 | 8 (12%) |
| 17 | BCR | f | 4005 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.72 | 12 (21%) |
| 14 | CLA | c | 516 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.58 | 6 (11%) |
| 14 | CLA | G | 1137 | 1 | 60,68,73 | 1.52 | 9 (15%) | 70,107,113 | 1.57 | 10 (14%) |
| 14 | CLA | c | 517 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.56 | 6 (11%) |
| 14 | CLA | 3 | 517 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.58 | 6 (11%) |
| 18 | LHG | e | 5008 | - | 34,34,48 | 0.71 | 1 (2%) | 37,40,54 | 1.25 | 4 (10%) |
| 17 | BCR | q | 523 | - | 41,41,41 | 0.75 | 0 | 56,56,56 | 1.68 | 13 (23%) |
| 14 | CLA | 1 | 506 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.64 | 6 (11%) |
| 14 | CLA | H | 1219 | 2 | 63,71,73 | 1.52 | 9 (14%) | 73,110,113 | 1.43 | 10 (13%) |
| 14 | CLA | G | 1118 | 1 | 60,68,73 | 1.47 | 9 (15%) | 70,107,113 | 1.56 | 8 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | t | 501 | 13 | 45,53,73 | 1.79 | 6 (13%) | 52,89,113 | 1.63 | 7 (13%) |
| 14 | CLA | G | 1122 | 1 | 60,68,73 | 1.51 | 11 (18%) | 70,107,113 | 1.54 | 9 (12%) |
| 14 | CLA | t | 517 | - | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.66 | 8 (15%) |
| 14 | CLA | Z | 503 | 13 | 65,73,73 | 1.45 | 6 (9%) | 76,113,113 | 1.47 | 8 (10%) |
| 17 | BCR | s | 523 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 1.82 | 15 (26%) |
| 14 | CLA | u | 502 | 13 | 45,53,73 | 1.79 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | f | 1236 | 2 | 50,58,73 | 1.70 | 9 (18%) | 58,95,113 | 1.55 | 10 (17%) |
| 14 | CLA | t | 509 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.75 | 9 (17%) |
| 14 | CLA | a | 509 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.78 | 7 (13%) |
| 14 | CLA | v | 512 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.58 | 6 (11%) |
| 14 | CLA | r | 501 | 13 | 60,68,73 | 1.50 | 8 (13%) | 70,107,113 | 1.57 | 8 (11%) |
| 14 | CLA | c | 519 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.62 | 7 (13%) |
| 22 | FMN | X | 170 | - | 33,33,33 | 1.12 | 2 (6%) | 48,50,50 | 1.24 | 6 (12%) |
| 14 | CLA | H | 1214 | 2 | 65,73,73 | 1.49 | 9 (13%) | 76,113,113 | 1.52 | 8 (10%) |
| 14 | CLA | d | 512 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.58 | 6 (11%) |
| 17 | BCR | 6 | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.79 | 12 (21%) |
| 14 | CLA | u | 508 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.85 | 7 (13%) |
| 14 | CLA | 3 | 505 | 13 | 55,63,73 | 1.56 | 8 (14%) | 64,101,113 | 1.49 | 7 (10%) |
| 16 | SF4 | e | 3001 | 1,2 | 0,12,12 | - | - | - | - | - |
| 14 | CLA | l | 511 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | A | 1138 | 1 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.55 | 7 (9%) |
| 14 | CLA | e | 1123 | 23 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.53 | 8 (10%) |
| 14 | CLA | f | 1023 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.89 | 11 (14%) |
| 17 | BCR | 3 | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.83 | 11 (19%) |
| 14 | CLA | 2 | 506 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | 1 | 510 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | 4 | 506 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.66 | 6 (11%) |
| 14 | CLA | t | 511 | 13 | 45,53,73 | 1.79 | 6 (13%) | 52,89,113 | 1.67 | 9 (17%) |
| 17 | BCR | H | 4004 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.85 | 14 (25%) |
| 14 | CLA | b | 508 | 13 | 45,53,73 | 1.81 | 10 (22%) | 52,89,113 | 1.80 | 9 (17%) |
| 18 | LHG | e | 5003 | 14 | 39,39,48 | 0.86 | 1 (2%) | 42,45,54 | 1.38 | 6 (14%) |
| 14 | CLA | 2 | 512 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.50 | 5 (9%) |
| 17 | BCR | t | 522 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.91 | 19 (33%) |
| 14 | CLA | b | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.61 | 6 (11%) |
| 17 | BCR | o | 4021 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.91 | 15 (26%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | A | 1134 | 1 | 56,64,73 | 1.56 | 8 (14%) | 65,102,113 | 1.64 | 11 (16%) |
| 14 | CLA | u | 505 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | d | 503 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.68 | 6 (11%) |
| 17 | BCR | t | 523 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.77 | 14 (25%) |
| 14 | CLA | A | 1131 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.42 | 9 (11%) |
| 20 | LMG | f | 5002 | - | 53,53,55 | 0.85 | 2 (3%) | 61,61,63 | 1.51 | 12 (19%) |
| 14 | CLA | 4 | 511 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.67 | 9 (17%) |
| 21 | SQD | v | 822 | - | 25,26,54 | 1.31 | 4 (16%) | 34,37,65 | 2.00 | 10 (29%) |
| 14 | CLA | e | 1120 | 1 | 50,58,73 | 1.58 | 8 (16%) | 58,95,113 | 1.73 | 10 (17%) |
| 17 | BCR | 6 | 524 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.85 | 15 (26%) |
| 17 | BCR | Y | 522 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.91 | 20 (35%) |
| 17 | BCR | r | 522 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.85 | 17 (30%) |
| 14 | CLA | G | 1237 | 23 | 65,73,73 | 1.47 | 12 (18%) | 76,113,113 | 1.57 | 9 (11%) |
| 17 | BCR | B | 4004 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.85 | 14 (25%) |
| 14 | CLA | d | 513 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.58 | 6 (11%) |
| 14 | CLA | K | 1103 | 9 | 48,56,73 | 1.66 | 8 (16%) | 55,92,113 | 1.62 | 8 (14%) |
| 14 | CLA | 3 | 519 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.61 | 7 (13%) |
| 14 | CLA | b | 513 | 13 | 45,53,73 | 1.78 | 6 (13%) | 52,89,113 | 1.63 | 6 (11%) |
| 14 | CLA | 2 | 502 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.70 | 9 (17%) |
| 14 | CLA | v | 503 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.69 | 6 (11%) |
| 17 | BCR | Z | 523 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.76 | 17 (30%) |
| 15 | PQN | A | 2001 | - | 34,34,34 | 2.81 | 11 (32%) | 42,45,45 | 2.19 | 6 (14%) |
| 17 | BCR | r | 521 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.90 | 13 (23%) |
| 14 | CLA | f | 1201 | 2 | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.65 | 9 (12%) |
| 14 | CLA | 4 | 508 | 13 | 45,53,73 | 1.80 | 9 (20%) | 52,89,113 | 1.80 | 9 (17%) |
| 14 | CLA | B | 1230 | 2 | 60,68,73 | 1.53 | 10 (16%) | 70,107,113 | 1.47 | 7 (10%) |
| 14 | CLA | 6 | 510 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.63 | 6 (11%) |
| 14 | CLA | G | 1128 | 1 | 65,73,73 | 1.58 | 11 (16%) | 76,113,113 | 1.69 | 9 (11%) |
| 14 | CLA | B | 1012 | 23 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.58 | 9 (11%) |
| 14 | CLA | G | 1123 | 23 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.52 | 8 (10%) |
| 14 | CLA | r | 519 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.59 | 8 (15%) |
| 15 | PQN | H | 2002 | - | 34,34,34 | 2.84 | 11 (32%) | 42,45,45 | 2.30 | 6 (14%) |
| 17 | BCR | r | 524 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.76 | 13 (23%) |
| 14 | CLA | H | 1215 | 2 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.71 | 10 (13%) |
| 17 | BCR | m | 4104 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.88 | 16 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | B | 1220 | 2 | 55,63,73 | 1.58 | 10 (18%) | 64,101,113 | 1.64 | 10 (15%) |
| 18 | LHG | V | 5220 | - | 40,40,48 | 0.70 | 1 (2%) | 43,46,54 | 1.30 | 5 (11%) |
| 14 | CLA | c | 504 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | A | 1109 | 1 | 65,73,73 | 1.41 | 9 (13%) | 76,113,113 | 1.60 | 8 (10%) |
| 14 | CLA | 2 | 513 | 13 | 45,53,73 | 1.78 | 9 (20%) | 52,89,113 | 1.55 | 6 (11%) |
| 14 | CLA | f | 1215 | 2 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.72 | 10 (13%) |
| 14 | CLA | r | 517 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.65 | 7 (13%) |
| 16 | SF4 | g | 3003 | 3 | 0,12,12 | - | - | - | | |
| 14 | CLA | 5 | 516 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.58 | 6 (11%) |
| 14 | CLA | 5 | 506 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.62 | 7 (13%) |
| 17 | BCR | 3 | 523 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 1.82 | 15 (26%) |
| 14 | CLA | H | 1225 | 2 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.49 | 9 (11%) |
| 14 | CLA | 4 | 505 | 13 | 45,53,73 | 1.75 | 9 (20%) | 52,89,113 | 1.54 | 6 (11%) |
| 14 | CLA | e | 1137 | 1 | 60,68,73 | 1.52 | 9 (15%) | 70,107,113 | 1.56 | 10 (14%) |
| 14 | CLA | f | 1210 | 2 | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.48 | 9 (11%) |
| 18 | LHG | G | 5004 | - | 34,34,48 | 0.67 | 0 | 37,40,54 | 1.28 | 4 (10%) |
| 20 | LMG | T | 5104 | - | 32,32,55 | 0.96 | 2 (6%) | 40,40,63 | 1.26 | 4 (10%) |
| 14 | CLA | B | 1202 | 2 | 65,73,73 | 1.41 | 7 (10%) | 76,113,113 | 1.58 | 8 (10%) |
| 19 | LMU | G | 1849 | - | 23,23,36 | 1.18 | 1 (4%) | 28,28,47 | 1.39 | 4 (14%) |
| 17 | BCR | T | 4015 | - | 41,41,41 | 0.80 | 0 | 56,56,56 | 1.73 | 12 (21%) |
| 14 | CLA | e | 1117 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.57 | 10 (13%) |
| 15 | PQN | B | 2002 | - | 34,34,34 | 2.84 | 11 (32%) | 42,45,45 | 2.31 | 6 (14%) |
| 14 | CLA | f | 1225 | 2 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.49 | 9 (11%) |
| 14 | CLA | 2 | 511 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.70 | 7 (13%) |
| 14 | CLA | 5 | 512 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.56 | 6 (11%) |
| 14 | CLA | q | 508 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.93 | 8 (15%) |
| 14 | CLA | H | 1222 | 23 | 50,58,73 | 1.61 | 9 (18%) | 58,95,113 | 1.73 | 9 (15%) |
| 14 | CLA | e | 1103 | 1 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.73 | 10 (13%) |
| 21 | SQD | d | 822 | - | 25,26,54 | 1.31 | 4 (16%) | 34,37,65 | 2.00 | 10 (29%) |
| 14 | CLA | f | 1222 | 23 | 50,58,73 | 1.61 | 9 (18%) | 58,95,113 | 1.73 | 9 (15%) |
| 14 | CLA | B | 1214 | 2 | 65,73,73 | 1.49 | 9 (13%) | 76,113,113 | 1.51 | 7 (9%) |
| 14 | CLA | q | 513 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.63 | 7 (13%) |
| 17 | BCR | A | 4002 | - | 41,41,41 | 0.88 | 1 (2%) | 56,56,56 | 1.94 | 16 (28%) |
| 14 | CLA | R | 1301 | 23 | 45,53,73 | 1.72 | 9 (20%) | 52,89,113 | 1.59 | 6 (11%) |
| 14 | CLA | B | 1023 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.89 | 11 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | LMU | T | 5105 | - | 22,22,36 | 1.21 | 1 (4%) | 27,27,47 | 1.43 | 5 (18%) |
| 14 | CLA | v | 508 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.78 | 11 (21%) |
| 17 | BCR | a | 523 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 1.82 | 15 (26%) |
| 14 | CLA | e | 1124 | 23 | 60,68,73 | 1.53 | 9 (15%) | 70,107,113 | 1.59 | 10 (14%) |
| 19 | LMU | G | 1848 | - | 36,36,36 | 1.15 | 2 (5%) | 47,47,47 | 1.02 | 2 (4%) |
| 14 | CLA | e | 1136 | 1 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.54 | 10 (13%) |
| 14 | CLA | e | 1114 | 23 | 45,53,73 | 1.80 | 8 (17%) | 52,89,113 | 1.68 | 9 (17%) |
| 14 | CLA | 5 | 502 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.70 | 7 (13%) |
| 17 | BCR | Z | 521 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.90 | 13 (23%) |
| 14 | CLA | 4 | 509 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.76 | 9 (17%) |
| 17 | BCR | r | 523 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.75 | 17 (30%) |
| 17 | BCR | u | 523 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.79 | 15 (26%) |
| 17 | BCR | G | 4003 | - | 41,41,41 | 0.87 | 1 (2%) | 56,56,56 | 1.78 | 14 (25%) |
| 17 | BCR | R | 4016 | - | 41,41,41 | 0.81 | 0 | 56,56,56 | 1.91 | 12 (21%) |
| 14 | CLA | q | 510 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.59 | 6 (11%) |
| 14 | CLA | B | 1229 | 2 | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.59 | 8 (10%) |
| 14 | CLA | B | 1226 | 2 | 55,63,73 | 1.71 | 10 (18%) | 64,101,113 | 1.98 | 15 (23%) |
| 14 | CLA | u | 519 | 13 | 45,53,73 | 1.78 | 6 (13%) | 52,89,113 | 1.60 | 7 (13%) |
| 14 | CLA | c | 512 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.56 | 6 (11%) |
| 15 | PQN | G | 2001 | - | 34,34,34 | 2.82 | 11 (32%) | 42,45,45 | 2.20 | 6 (14%) |
| 17 | BCR | G | 4008 | - | 41,41,41 | 0.95 | 2 (4%) | 56,56,56 | 2.17 | 16 (28%) |
| 14 | CLA | a | 510 | 13 | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.65 | 7 (13%) |
| 14 | CLA | 5 | 513 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.55 | 6 (11%) |
| 14 | CLA | r | 509 | 13 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.51 | 7 (9%) |
| 14 | CLA | Y | 509 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.66 | 9 (17%) |
| 17 | BCR | K | 4104 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.88 | 16 (28%) |
| 14 | CLA | e | 1115 | 1 | 60,68,73 | 1.50 | 9 (15%) | 70,107,113 | 1.58 | 7 (10%) |
| 14 | CLA | e | 1116 | 1 | 60,68,73 | 1.52 | 8 (13%) | 70,107,113 | 1.50 | 7 (10%) |
| 18 | LHG | n | 5221 | - | 48,48,48 | 0.62 | 0 | 51,54,54 | 1.28 | 7 (13%) |
| 18 | LHG | A | 5003 | 14 | 39,39,48 | 0.86 | 1 (2%) | 42,45,54 | 1.38 | 6 (14%) |
| 14 | CLA | K | 1401 | - | 55,63,73 | 1.58 | 7 (12%) | 64,101,113 | 1.63 | 10 (15%) |
| 14 | CLA | f | 1021 | 2 | 65,73,73 | 1.47 | 9 (13%) | 76,113,113 | 1.45 | 9 (11%) |
| 14 | CLA | d | 510 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.62 | 6 (11%) |
| 14 | CLA | n | 1502 | 10 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.54 | 8 (10%) |
| 18 | LHG | A | 5004 | - | 34,34,48 | 0.67 | 0 | 37,40,54 | 1.28 | 4 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | b | 510 | 13 | 45,53,73 | 1.72 | 6 (13%) | 52,89,113 | 1.65 | 6 (11%) |
| 14 | CLA | b | 507 | - | 45,53,73 | 1.72 | 6 (13%) | 52,89,113 | 1.72 | 8 (15%) |
| 14 | CLA | 5 | 511 | 13 | 45,53,73 | 1.76 | 5 (11%) | 52,89,113 | 1.71 | 7 (13%) |
| 14 | CLA | a | 507 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.68 | 9 (17%) |
| 19 | LMU | J | 5105 | - | 22,22,36 | 1.21 | 1 (4%) | 27,27,47 | 1.43 | 5 (18%) |
| 14 | CLA | 2 | 505 | 13 | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.47 | 8 (10%) |
| 14 | CLA | B | 1215 | 2 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.71 | 10 (13%) |
| 14 | CLA | e | 1102 | 1 | 55,63,73 | 1.56 | 9 (16%) | 64,101,113 | 1.62 | 7 (10%) |
| 14 | CLA | Z | 504 | - | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.64 | 8 (15%) |
| 14 | CLA | e | 1131 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.42 | 9 (11%) |
| 18 | LHG | e | 5002 | - | 42,42,48 | 0.76 | 1 (2%) | 45,48,54 | 1.23 | 4 (8%) |
| 21 | SQD | l | 822 | - | 31,32,54 | 1.20 | 5 (16%) | 40,43,65 | 2.05 | 13 (32%) |
| 17 | BCR | n | 4019 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.95 | 15 (26%) |
| 14 | CLA | j | 1302 | 6 | 45,53,73 | 1.76 | 9 (20%) | 52,89,113 | 1.57 | 8 (15%) |
| 21 | SQD | r | 822 | - | 27,28,54 | 1.22 | 4 (14%) | 36,39,65 | 1.86 | 10 (27%) |
| 14 | CLA | 2 | 510 | 13 | 45,53,73 | 1.72 | 7 (15%) | 52,89,113 | 1.62 | 6 (11%) |
| 14 | CLA | s | 506 | 13 | 45,53,73 | 1.79 | 7 (15%) | 52,89,113 | 1.69 | 6 (11%) |
| 14 | CLA | c | 510 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | B | 1238 | 23 | 65,73,73 | 1.40 | 7 (10%) | 76,113,113 | 1.63 | 10 (13%) |
| 14 | CLA | Z | 507 | - | 45,53,73 | 1.72 | 7 (15%) | 52,89,113 | 1.71 | 10 (19%) |
| 14 | CLA | G | 1139 | 23 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.36 | 6 (7%) |
| 14 | CLA | c | 513 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.56 | 6 (11%) |
| 17 | BCR | Y | 523 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.69 | 14 (25%) |
| 14 | CLA | H | 1210 | 2 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.48 | 9 (11%) |
| 17 | BCR | 2 | 523 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.75 | 17 (30%) |
| 17 | BCR | e | 4001 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.69 | 11 (19%) |
| 17 | BCR | s | 521 | - | 41,41,41 | 0.66 | 0 | 56,56,56 | 1.83 | 11 (19%) |
| 17 | BCR | L | 4219 | - | 41,41,41 | 1.09 | 5 (12%) | 56,56,56 | 2.26 | 23 (41%) |
| 21 | SQD | B | 1852 | - | 39,40,54 | 1.18 | 6 (15%) | 48,51,65 | 1.84 | 12 (25%) |
| 14 | CLA | 4 | 517 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 8 (15%) |
| 17 | BCR | f | 4010 | - | 41,41,41 | 0.91 | 1 (2%) | 56,56,56 | 2.30 | 21 (37%) |
| 17 | BCR | u | 522 | - | 41,41,41 | 0.75 | 0 | 56,56,56 | 1.94 | 21 (37%) |
| 14 | CLA | 4 | 501 | 13 | 45,53,73 | 1.78 | 5 (11%) | 52,89,113 | 1.63 | 7 (13%) |
| 17 | BCR | n | 4219 | - | 41,41,41 | 1.09 | 5 (12%) | 56,56,56 | 2.26 | 23 (41%) |
| 21 | SQD | f | 1852 | - | 39,40,54 | 1.18 | 6 (15%) | 48,51,65 | 1.84 | 12 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | 2 | 519 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.60 | 8 (15%) |
| 14 | CLA | B | 1231 | 23 | 65,73,73 | 1.38 | 7 (10%) | 76,113,113 | 1.52 | 9 (11%) |
| 14 | CLA | v | 516 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.60 | 8 (15%) |
| 18 | LHG | H | 1855 | - | 40,40,48 | 0.69 | 1 (2%) | 43,46,54 | 1.24 | 5 (11%) |
| 14 | CLA | r | 512 | 13 | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.51 | 5 (9%) |
| 14 | CLA | 3 | 504 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.73 | 9 (17%) |
| 18 | LHG | f | 1855 | - | 40,40,48 | 0.69 | 1 (2%) | 43,46,54 | 1.24 | 5 (11%) |
| 17 | BCR | J | 4015 | - | 41,41,41 | 0.80 | 0 | 56,56,56 | 1.73 | 12 (21%) |
| 14 | CLA | 3 | 507 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.68 | 9 (17%) |
| 14 | CLA | u | 504 | - | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.67 | 7 (13%) |
| 14 | CLA | G | 1106 | 1 | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.53 | 9 (11%) |
| 14 | CLA | 6 | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.71 | 7 (13%) |
| 14 | CLA | q | 516 | 13 | 45,53,73 | 1.72 | 9 (20%) | 52,89,113 | 1.64 | 9 (17%) |
| 17 | BCR | B | 4010 | - | 41,41,41 | 0.91 | 1 (2%) | 56,56,56 | 2.30 | 21 (37%) |
| 14 | CLA | A | 1127 | 1 | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | V | 1501 | 10 | 60,68,73 | 1.57 | 10 (16%) | 70,107,113 | 1.51 | 9 (12%) |
| 14 | CLA | t | 508 | 13 | 45,53,73 | 1.81 | 10 (22%) | 52,89,113 | 1.79 | 9 (17%) |
| 16 | SF4 | N | 3002 | 3 | 0,12,12 | - | - | - | - | - |
| 14 | CLA | H | 1205 | 2 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.58 | 11 (14%) |
| 15 | PQN | e | 2001 | - | 34,34,34 | 2.81 | 11 (32%) | 42,45,45 | 2.19 | 6 (14%) |
| 14 | CLA | c | 502 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.69 | 7 (13%) |
| 17 | BCR | l | 524 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.85 | 17 (30%) |
| 18 | LHG | e | 5005 | - | 42,42,48 | 0.65 | 1 (2%) | 45,48,54 | 1.21 | 4 (8%) |
| 14 | CLA | e | 1105 | 1 | 55,63,73 | 1.50 | 9 (16%) | 64,101,113 | 1.67 | 8 (12%) |
| 14 | CLA | Y | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.64 | 7 (13%) |
| 18 | LHG | G | 5008 | - | 34,34,48 | 0.71 | 1 (2%) | 37,40,54 | 1.25 | 3 (8%) |
| 18 | LHG | k | 5001 | - | 47,47,48 | 0.62 | 0 | 50,53,54 | 1.24 | 5 (10%) |
| 21 | SQD | 3 | 822 | - | 27,28,54 | 1.29 | 5 (18%) | 36,39,65 | 1.80 | 11 (30%) |
| 14 | CLA | Y | 519 | 13 | 45,53,73 | 1.80 | 8 (17%) | 52,89,113 | 1.55 | 7 (13%) |
| 14 | CLA | 3 | 506 | 13 | 45,53,73 | 1.79 | 7 (15%) | 52,89,113 | 1.70 | 6 (11%) |
| 18 | LHG | e | 5001 | - | 48,48,48 | 0.80 | 1 (2%) | 51,54,54 | 1.30 | 7 (13%) |
| 14 | CLA | U | 1103 | 9 | 48,56,73 | 1.67 | 8 (16%) | 55,92,113 | 1.62 | 8 (14%) |
| 14 | CLA | A | 1111 | 1 | 65,73,73 | 1.43 | 9 (13%) | 76,113,113 | 1.53 | 8 (10%) |
| 14 | CLA | B | 1234 | 2 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.65 | 10 (13%) |
| 14 | CLA | G | 1133 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.49 | 6 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | f | 1228 | 2 | 55,63,73 | 1.52 | 7 (12%) | 64,101,113 | 1.70 | 8 (12%) |
| 17 | BCR | 4 | 523 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.77 | 14 (25%) |
| 14 | CLA | H | 1227 | 2 | 60,68,73 | 1.54 | 10 (16%) | 70,107,113 | 1.50 | 8 (11%) |
| 14 | CLA | v | 519 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.58 | 7 (13%) |
| 14 | CLA | l | 508 | 13 | 45,53,73 | 1.77 | 10 (22%) | 52,89,113 | 1.92 | 7 (13%) |
| 14 | CLA | Z | 506 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.61 | 7 (13%) |
| 14 | CLA | e | 1118 | 1 | 60,68,73 | 1.47 | 10 (16%) | 70,107,113 | 1.56 | 8 (11%) |
| 14 | CLA | r | 506 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.63 | 7 (13%) |
| 14 | CLA | l | 1302 | 8 | 55,63,73 | 1.55 | 9 (16%) | 64,101,113 | 1.56 | 9 (14%) |
| 17 | BCR | e | 4008 | - | 41,41,41 | 0.95 | 2 (4%) | 56,56,56 | 2.17 | 16 (28%) |
| 14 | CLA | 2 | 518 | 13 | 55,63,73 | 1.55 | 6 (10%) | 64,101,113 | 1.53 | 7 (10%) |
| 14 | CLA | 5 | 510 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | s | 518 | 13 | 55,63,73 | 1.59 | 7 (12%) | 64,101,113 | 1.47 | 7 (10%) |
| 14 | CLA | f | 1227 | 2 | 60,68,73 | 1.54 | 10 (16%) | 70,107,113 | 1.51 | 8 (11%) |
| 14 | CLA | H | 1230 | 2 | 60,68,73 | 1.54 | 10 (16%) | 70,107,113 | 1.46 | 7 (10%) |
| 14 | CLA | e | 1011 | 1 | 65,73,73 | 1.45 | 10 (15%) | 76,113,113 | 1.73 | 14 (18%) |
| 14 | CLA | f | 1230 | 2 | 60,68,73 | 1.54 | 10 (16%) | 70,107,113 | 1.46 | 7 (10%) |
| 17 | BCR | A | 4001 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.69 | 11 (19%) |
| 14 | CLA | t | 516 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | Z | 516 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.66 | 8 (15%) |
| 14 | CLA | H | 1229 | 2 | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.59 | 9 (11%) |
| 14 | CLA | A | 1128 | 1 | 65,73,73 | 1.58 | 11 (16%) | 76,113,113 | 1.69 | 9 (11%) |
| 14 | CLA | H | 1203 | 2 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.53 | 9 (11%) |
| 14 | CLA | r | 511 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.71 | 8 (15%) |
| 14 | CLA | A | 1114 | 23 | 45,53,73 | 1.80 | 8 (17%) | 52,89,113 | 1.69 | 9 (17%) |
| 14 | CLA | l | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.63 | 7 (13%) |
| 17 | BCR | c | 524 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.74 | 12 (21%) |
| 21 | SQD | 5 | 822 | - | 25,26,54 | 1.29 | 4 (16%) | 34,37,65 | 1.95 | 11 (32%) |
| 17 | BCR | S | 4018 | - | 41,41,41 | 0.93 | 2 (4%) | 56,56,56 | 1.93 | 16 (28%) |
| 14 | CLA | G | 1130 | 1 | 56,64,73 | 1.52 | 8 (14%) | 65,102,113 | 1.74 | 9 (13%) |
| 14 | CLA | t | 512 | 13 | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.60 | 6 (11%) |
| 18 | LHG | A | 5007 | - | 46,46,48 | 0.60 | 0 | 49,52,54 | 1.20 | 4 (8%) |
| 14 | CLA | l | 513 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | H | 1208 | 2 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.39 | 7 (9%) |
| 14 | CLA | u | 510 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.63 | 7 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | A | 1105 | 1 | 55,63,73 | 1.50 | 9 (16%) | 64,101,113 | 1.67 | 8 (12%) |
| 17 | BCR | v | 522 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.89 | 19 (33%) |
| 14 | CLA | e | 1140 | 1 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.56 | 10 (13%) |
| 18 | LHG | G | 5001 | - | 48,48,48 | 0.80 | 1 (2%) | 51,54,54 | 1.30 | 7 (13%) |
| 14 | CLA | 5 | 503 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.67 | 10 (19%) |
| 17 | BCR | n | 4022 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.82 | 10 (17%) |
| 14 | CLA | n | 1503 | 23 | 60,68,73 | 1.48 | 8 (13%) | 70,107,113 | 1.57 | 7 (10%) |
| 14 | CLA | e | 1139 | 23 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.36 | 7 (9%) |
| 18 | LHG | e | 5006 | - | 39,39,48 | 0.67 | 1 (2%) | 42,45,54 | 1.22 | 5 (11%) |
| 14 | CLA | Z | 512 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.49 | 5 (9%) |
| 14 | CLA | l | 507 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.70 | 9 (17%) |
| 14 | CLA | e | 1113 | 1 | 45,53,73 | 1.67 | 7 (15%) | 52,89,113 | 1.81 | 7 (13%) |
| 14 | CLA | s | 519 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.61 | 7 (13%) |
| 17 | BCR | 4 | 522 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.91 | 19 (33%) |
| 14 | CLA | r | 508 | 13 | 45,53,73 | 1.78 | 9 (20%) | 52,89,113 | 1.76 | 10 (19%) |
| 14 | CLA | J | 1302 | 8 | 55,63,73 | 1.56 | 9 (16%) | 64,101,113 | 1.56 | 9 (14%) |
| 14 | CLA | t | 503 | 13 | 45,53,73 | 1.80 | 7 (15%) | 52,89,113 | 1.71 | 8 (15%) |
| 14 | CLA | 3 | 516 | 13 | 45,53,73 | 1.75 | 5 (11%) | 52,89,113 | 1.87 | 11 (21%) |
| 17 | BCR | T | 4012 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.76 | 13 (23%) |
| 14 | CLA | Z | 508 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.77 | 10 (19%) |
| 17 | BCR | a | 522 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 2.03 | 17 (30%) |
| 14 | CLA | a | 518 | 13 | 55,63,73 | 1.58 | 8 (14%) | 64,101,113 | 1.48 | 7 (10%) |
| 14 | CLA | b | 519 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.64 | 7 (13%) |
| 14 | CLA | 3 | 512 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.52 | 5 (9%) |
| 14 | CLA | u | 503 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.68 | 10 (19%) |
| 14 | CLA | B | 1205 | 2 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.59 | 11 (14%) |
| 14 | CLA | v | 505 | 13 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.45 | 8 (10%) |
| 14 | CLA | v | 509 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | G | 1111 | 1 | 65,73,73 | 1.43 | 10 (15%) | 76,113,113 | 1.53 | 7 (9%) |
| 14 | CLA | d | 518 | 13 | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.63 | 6 (11%) |
| 14 | CLA | 4 | 516 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | G | 1132 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | A | 1140 | 1 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.57 | 10 (13%) |
| 18 | LHG | H | 1842 | 14 | 36,36,48 | 0.81 | 1 (2%) | 39,42,54 | 1.26 | 3 (7%) |
| 14 | CLA | d | 511 | 13 | 45,53,73 | 1.77 | 5 (11%) | 52,89,113 | 1.70 | 7 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | H | 1211 | 2 | 55,63,73 | 1.53 | 8 (14%) | 64,101,113 | 1.69 | 8 (12%) |
| 14 | CLA | f | 1202 | 2 | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.58 | 8 (10%) |
| 14 | CLA | 6 | 503 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.69 | 6 (11%) |
| 14 | CLA | m | 1105 | 9 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.84 | 11 (21%) |
| 17 | BCR | L | 4019 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.95 | 15 (26%) |
| 14 | CLA | Z | 513 | 13 | 45,53,73 | 1.78 | 9 (20%) | 52,89,113 | 1.55 | 6 (11%) |
| 14 | CLA | B | 1222 | 23 | 50,58,73 | 1.61 | 9 (18%) | 58,95,113 | 1.72 | 9 (15%) |
| 17 | BCR | L | 4020 | - | 41,41,41 | 0.98 | 2 (4%) | 56,56,56 | 1.67 | 15 (26%) |
| 14 | CLA | 3 | 502 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.72 | 9 (17%) |
| 14 | CLA | A | 1137 | 1 | 60,68,73 | 1.53 | 9 (15%) | 70,107,113 | 1.56 | 10 (14%) |
| 14 | CLA | B | 1223 | 2 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.63 | 7 (9%) |
| 14 | CLA | t | 502 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.67 | 7 (13%) |
| 18 | LHG | A | 5005 | - | 42,42,48 | 0.65 | 1 (2%) | 45,48,54 | 1.21 | 4 (8%) |
| 14 | CLA | r | 516 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.65 | 8 (15%) |
| 17 | BCR | H | 4017 | - | 41,41,41 | 0.97 | 4 (9%) | 56,56,56 | 1.82 | 12 (21%) |
| 14 | CLA | A | 1118 | 1 | 60,68,73 | 1.48 | 10 (16%) | 70,107,113 | 1.55 | 8 (11%) |
| 19 | LMU | e | 1848 | - | 36,36,36 | 1.15 | 2 (5%) | 47,47,47 | 1.02 | 2 (4%) |
| 14 | CLA | 3 | 508 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.75 | 7 (13%) |
| 14 | CLA | H | 1231 | 23 | 65,73,73 | 1.39 | 7 (10%) | 76,113,113 | 1.52 | 9 (11%) |
| 17 | BCR | H | 4006 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 2.09 | 18 (32%) |
| 17 | BCR | H | 4009 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.90 | 20 (35%) |
| 14 | CLA | f | 1208 | 2 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.39 | 7 (9%) |
| 14 | CLA | a | 508 | 13 | 45,53,73 | 1.78 | 9 (20%) | 52,89,113 | 1.75 | 7 (13%) |
| 14 | CLA | e | 1237 | 23 | 65,73,73 | 1.46 | 12 (18%) | 76,113,113 | 1.57 | 9 (11%) |
| 14 | CLA | H | 1224 | 2 | 60,68,73 | 1.50 | 7 (11%) | 70,107,113 | 1.54 | 9 (12%) |
| 17 | BCR | v | 523 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.72 | 15 (26%) |
| 14 | CLA | v | 502 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.66 | 8 (15%) |
| 17 | BCR | f | 4006 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 2.09 | 18 (32%) |
| 18 | LHG | B | 1855 | - | 40,40,48 | 0.69 | 1 (2%) | 43,46,54 | 1.24 | 5 (11%) |
| 14 | CLA | 3 | 513 | 13 | 45,53,73 | 1.78 | 8 (17%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | A | 1135 | 1 | 55,63,73 | 1.49 | 10 (18%) | 64,101,113 | 1.76 | 11 (17%) |
| 14 | CLA | f | 1224 | 2 | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.54 | 9 (12%) |
| 14 | CLA | j | 1301 | 23 | 45,53,73 | 1.73 | 9 (20%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | e | 1801 | 18 | 45,53,73 | 1.65 | 7 (15%) | 52,89,113 | 1.73 | 7 (13%) |
| 14 | CLA | e | 1127 | 1 | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.55 | 11 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | H | 1023 | - | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.90 | 11 (14%) |
| 14 | CLA | A | 1112 | 1 | 50,58,73 | 1.62 | 10 (20%) | 58,95,113 | 1.68 | 8 (13%) |
| 14 | CLA | n | 1501 | 10 | 60,68,73 | 1.56 | 10 (16%) | 70,107,113 | 1.50 | 9 (12%) |
| 14 | CLA | b | 502 | 13 | 45,53,73 | 1.80 | 8 (17%) | 52,89,113 | 1.67 | 8 (15%) |
| 14 | CLA | H | 1213 | 2 | 61,69,73 | 1.46 | 7 (11%) | 71,108,113 | 1.60 | 9 (12%) |
| 14 | CLA | d | 509 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.69 | 7 (13%) |
| 14 | CLA | A | 1013 | - | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.88 | 13 (17%) |
| 17 | BCR | V | 4020 | - | 41,41,41 | 0.99 | 2 (4%) | 56,56,56 | 1.67 | 15 (26%) |
| 14 | CLA | c | 503 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.68 | 10 (19%) |
| 17 | BCR | Y | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.83 | 11 (19%) |
| 14 | CLA | q | 518 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.62 | 7 (13%) |
| 17 | BCR | B | 4009 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.90 | 18 (32%) |
| 14 | CLA | l | 501 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.67 | 6 (11%) |
| 14 | CLA | B | 1224 | 2 | 60,68,73 | 1.50 | 7 (11%) | 70,107,113 | 1.54 | 9 (12%) |
| 14 | CLA | B | 1209 | 2 | 53,61,73 | 1.62 | 8 (15%) | 61,98,113 | 1.68 | 8 (13%) |
| 14 | CLA | q | 519 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.56 | 7 (13%) |
| 17 | BCR | G | 4011 | - | 41,41,41 | 0.81 | 0 | 56,56,56 | 1.78 | 12 (21%) |
| 14 | CLA | G | 1013 | - | 65,73,73 | 1.43 | 8 (12%) | 76,113,113 | 1.88 | 13 (17%) |
| 18 | LHG | L | 5220 | - | 40,40,48 | 0.70 | 1 (2%) | 43,46,54 | 1.30 | 5 (11%) |
| 14 | CLA | H | 1236 | 2 | 50,58,73 | 1.70 | 9 (18%) | 58,95,113 | 1.54 | 10 (17%) |
| 14 | CLA | v | 518 | 13 | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.62 | 6 (11%) |
| 14 | CLA | V | 1502 | 10 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.53 | 8 (10%) |
| 17 | BCR | u | 524 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.74 | 11 (19%) |
| 18 | LHG | I | 5001 | - | 47,47,48 | 0.62 | 0 | 50,53,54 | 1.24 | 5 (10%) |
| 14 | CLA | e | 1101 | 1 | 65,73,73 | 1.50 | 9 (13%) | 76,113,113 | 1.61 | 13 (17%) |
| 19 | LMU | e | 1849 | - | 23,23,36 | 1.17 | 1 (4%) | 28,28,47 | 1.39 | 4 (14%) |
| 14 | CLA | G | 1112 | 1 | 50,58,73 | 1.62 | 10 (20%) | 58,95,113 | 1.67 | 8 (13%) |
| 14 | CLA | f | 1214 | 2 | 65,73,73 | 1.49 | 9 (13%) | 76,113,113 | 1.51 | 7 (9%) |
| 14 | CLA | f | 1219 | 2 | 63,71,73 | 1.51 | 9 (14%) | 73,110,113 | 1.44 | 10 (13%) |
| 14 | CLA | q | 503 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.66 | 7 (13%) |
| 14 | CLA | 2 | 516 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.66 | 8 (15%) |
| 14 | CLA | s | 516 | 13 | 45,53,73 | 1.75 | 5 (11%) | 52,89,113 | 1.87 | 11 (21%) |
| 14 | CLA | A | 1237 | 23 | 65,73,73 | 1.46 | 12 (18%) | 76,113,113 | 1.57 | 9 (11%) |
| 17 | BCR | 5 | 521 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.97 | 18 (32%) |
| 17 | BCR | d | 522 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.89 | 19 (33%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 16 | SF4 | A | 3001 | 1,2 | 0,12,12 | - | - | - | | |
| 14 | CLA | B | 1236 | 2 | 50,58,73 | 1.70 | 9 (18%) | 58,95,113 | 1.54 | 10 (17%) |
| 14 | CLA | a | 519 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.61 | 7 (13%) |
| 14 | CLA | A | 1801 | 18 | 45,53,73 | 1.65 | 7 (15%) | 52,89,113 | 1.73 | 7 (13%) |
| 14 | CLA | A | 1122 | 1 | 60,68,73 | 1.50 | 10 (16%) | 70,107,113 | 1.54 | 9 (12%) |
| 17 | BCR | a | 524 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.93 | 18 (32%) |
| 17 | BCR | e | 4002 | - | 41,41,41 | 0.87 | 1 (2%) | 56,56,56 | 1.94 | 16 (28%) |
| 14 | CLA | Y | 502 | 13 | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.65 | 8 (15%) |
| 14 | CLA | b | 501 | 13 | 45,53,73 | 1.79 | 6 (13%) | 52,89,113 | 1.63 | 7 (13%) |
| 14 | CLA | U | 1401 | - | 55,63,73 | 1.58 | 7 (12%) | 64,101,113 | 1.62 | 10 (15%) |
| 14 | CLA | H | 1218 | 2 | 60,68,73 | 1.51 | 8 (13%) | 70,107,113 | 1.44 | 7 (10%) |
| 14 | CLA | H | 1228 | 2 | 55,63,73 | 1.52 | 7 (12%) | 64,101,113 | 1.71 | 8 (12%) |
| 17 | BCR | f | 4017 | - | 41,41,41 | 0.97 | 3 (7%) | 56,56,56 | 1.82 | 12 (21%) |
| 14 | CLA | c | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.70 | 8 (15%) |
| 17 | BCR | d | 524 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.84 | 15 (26%) |
| 20 | LMG | J | 5104 | - | 32,32,55 | 0.96 | 2 (6%) | 40,40,63 | 1.26 | 4 (10%) |
| 14 | CLA | Z | 519 | 13 | 45,53,73 | 1.76 | 9 (20%) | 52,89,113 | 1.60 | 8 (15%) |
| 14 | CLA | f | 1231 | 23 | 65,73,73 | 1.38 | 7 (10%) | 76,113,113 | 1.52 | 9 (11%) |
| 14 | CLA | l | 517 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.59 | 7 (13%) |
| 14 | CLA | Y | 507 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.70 | 9 (17%) |
| 14 | CLA | H | 1226 | 2 | 55,63,73 | 1.71 | 10 (18%) | 64,101,113 | 1.99 | 16 (25%) |
| 14 | CLA | c | 506 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | d | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.71 | 7 (13%) |
| 14 | CLA | s | 504 | - | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.74 | 9 (17%) |
| 17 | BCR | u | 521 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.97 | 18 (32%) |
| 14 | CLA | l | 509 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.65 | 9 (17%) |
| 18 | LHG | n | 5220 | - | 40,40,48 | 0.70 | 1 (2%) | 43,46,54 | 1.30 | 5 (11%) |
| 14 | CLA | 6 | 518 | 13 | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.63 | 6 (11%) |
| 14 | CLA | Y | 503 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.66 | 7 (13%) |
| 14 | CLA | f | 1207 | 2 | 65,73,73 | 1.44 | 8 (12%) | 76,113,113 | 1.38 | 6 (7%) |
| 17 | BCR | B | 4017 | - | 41,41,41 | 0.97 | 3 (7%) | 56,56,56 | 1.82 | 12 (21%) |
| 14 | CLA | B | 1206 | 2 | 65,73,73 | 1.49 | 11 (16%) | 76,113,113 | 1.61 | 10 (13%) |
| 14 | CLA | 2 | 503 | 13 | 65,73,73 | 1.45 | 6 (9%) | 76,113,113 | 1.47 | 8 (10%) |
| 17 | BCR | c | 521 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.97 | 18 (32%) |
| 14 | CLA | G | 1126 | 1 | 65,73,73 | 1.39 | 8 (12%) | 76,113,113 | 1.57 | 8 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | LMU | A | 1849 | - | 23,23,36 | 1.17 | 1 (4%) | 28,28,47 | 1.39 | 4 (14%) |
| 14 | CLA | B | 1218 | 2 | 60,68,73 | 1.51 | 8 (13%) | 70,107,113 | 1.43 | 7 (10%) |
| 18 | LHG | A | 5002 | - | 42,42,48 | 0.76 | 1 (2%) | 45,48,54 | 1.22 | 4 (8%) |
| 14 | CLA | t | 505 | 13 | 45,53,73 | 1.75 | 9 (20%) | 52,89,113 | 1.54 | 6 (11%) |
| 17 | BCR | 2 | 521 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.90 | 13 (23%) |
| 17 | BCR | b | 521 | - | 41,41,41 | 0.68 | 0 | 56,56,56 | 1.78 | 11 (19%) |
| 14 | CLA | c | 511 | 13 | 45,53,73 | 1.75 | 5 (11%) | 52,89,113 | 1.71 | 8 (15%) |
| 14 | CLA | Y | 513 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.63 | 7 (13%) |
| 14 | CLA | 3 | 510 | 13 | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.64 | 7 (13%) |
| 14 | CLA | A | 1120 | 1 | 50,58,73 | 1.58 | 8 (16%) | 58,95,113 | 1.73 | 10 (17%) |
| 17 | BCR | a | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.83 | 11 (19%) |
| 14 | CLA | A | 1139 | 23 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.36 | 7 (9%) |
| 14 | CLA | r | 505 | 13 | 65,73,73 | 1.42 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 18 | LHG | e | 5009 | - | 41,41,48 | 0.67 | 0 | 44,47,54 | 1.22 | 4 (9%) |
| 14 | CLA | f | 1232 | 23 | 55,63,73 | 1.54 | 8 (14%) | 64,101,113 | 1.70 | 7 (10%) |
| 14 | CLA | v | 513 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.59 | 6 (11%) |
| 22 | FMN | P | 170 | - | 33,33,33 | 1.13 | 2 (6%) | 48,50,50 | 1.24 | 6 (12%) |
| 14 | CLA | e | 1129 | 1 | 53,61,73 | 1.62 | 10 (18%) | 61,98,113 | 1.59 | 9 (14%) |
| 19 | LMU | A | 1848 | - | 36,36,36 | 1.15 | 2 (5%) | 47,47,47 | 1.02 | 2 (4%) |
| 17 | BCR | d | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.79 | 12 (21%) |
| 14 | CLA | 6 | 517 | - | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.61 | 7 (13%) |
| 17 | BCR | 1 | 522 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.91 | 20 (35%) |
| 14 | CLA | a | 517 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.58 | 6 (11%) |
| 14 | CLA | m | 1401 | - | 55,63,73 | 1.59 | 7 (12%) | 64,101,113 | 1.63 | 10 (15%) |
| 17 | BCR | 1 | 523 | - | 41,41,41 | 0.75 | 0 | 56,56,56 | 1.69 | 13 (23%) |
| 14 | CLA | 6 | 509 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | r | 502 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.70 | 9 (17%) |
| 14 | CLA | A | 1107 | 1 | 65,73,73 | 1.52 | 10 (15%) | 76,113,113 | 1.49 | 10 (13%) |
| 17 | BCR | d | 523 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.72 | 14 (25%) |
| 17 | BCR | f | 4009 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.89 | 18 (32%) |
| 17 | BCR | V | 4019 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.95 | 15 (26%) |
| 17 | BCR | J | 4012 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.75 | 12 (21%) |
| 17 | BCR | Y | 524 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.85 | 17 (30%) |
| 17 | BCR | l | 4012 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.75 | 12 (21%) |
| 18 | LHG | G | 5009 | - | 41,41,48 | 0.67 | 0 | 44,47,54 | 1.22 | 4 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | q | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.66 | 6 (11%) |
| 14 | CLA | A | 1117 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.58 | 10 (13%) |
| 14 | CLA | d | 517 | - | 45,53,73 | 1.72 | 6 (13%) | 52,89,113 | 1.61 | 7 (13%) |
| 14 | CLA | H | 1216 | 23 | 60,68,73 | 1.60 | 10 (16%) | 70,107,113 | 1.57 | 11 (15%) |
| 17 | BCR | 5 | 522 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.94 | 20 (35%) |
| 14 | CLA | b | 512 | 13 | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | 2 | 508 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.76 | 10 (19%) |
| 14 | CLA | 6 | 504 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.69 | 7 (13%) |
| 14 | CLA | Z | 517 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.65 | 7 (13%) |
| 14 | CLA | F | 1302 | 6 | 45,53,73 | 1.76 | 9 (20%) | 52,89,113 | 1.58 | 8 (15%) |
| 14 | CLA | e | 1121 | 1 | 55,63,73 | 1.57 | 10 (18%) | 64,101,113 | 1.65 | 12 (18%) |
| 14 | CLA | s | 508 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.75 | 7 (13%) |
| 17 | BCR | l | 4015 | - | 41,41,41 | 0.80 | 0 | 56,56,56 | 1.73 | 12 (21%) |
| 14 | CLA | U | 1105 | 9 | 45,53,73 | 1.78 | 8 (17%) | 52,89,113 | 1.85 | 11 (21%) |
| 14 | CLA | G | 1119 | 23 | 65,73,73 | 1.49 | 11 (16%) | 76,113,113 | 1.67 | 13 (17%) |
| 14 | CLA | Z | 509 | 13 | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.52 | 7 (9%) |
| 14 | CLA | e | 1106 | 1 | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.53 | 9 (11%) |
| 14 | CLA | u | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.57 | 8 (15%) |
| 17 | BCR | A | 4008 | - | 41,41,41 | 0.95 | 2 (4%) | 56,56,56 | 2.17 | 16 (28%) |
| 17 | BCR | 1 | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.83 | 11 (19%) |
| 14 | CLA | H | 1221 | 23 | 62,70,73 | 1.50 | 8 (12%) | 72,109,113 | 1.70 | 11 (15%) |
| 21 | SQD | H | 1852 | - | 39,40,54 | 1.18 | 6 (15%) | 48,51,65 | 1.84 | 12 (25%) |
| 17 | BCR | f | 4004 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.85 | 14 (25%) |
| 14 | CLA | G | 1102 | 1 | 55,63,73 | 1.57 | 9 (16%) | 64,101,113 | 1.61 | 7 (10%) |
| 17 | BCR | 2 | 524 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.76 | 12 (21%) |
| 14 | CLA | e | 1126 | 1 | 65,73,73 | 1.39 | 8 (12%) | 76,113,113 | 1.57 | 8 (10%) |
| 17 | BCR | q | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.83 | 11 (19%) |
| 14 | CLA | f | 1223 | 2 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.64 | 7 (9%) |
| 14 | CLA | B | 1240 | 18 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.46 | 8 (10%) |
| 14 | CLA | 5 | 509 | 13 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.49 | 7 (9%) |
| 14 | CLA | B | 1232 | 23 | 55,63,73 | 1.54 | 8 (14%) | 64,101,113 | 1.70 | 7 (10%) |
| 14 | CLA | 5 | 507 | - | 45,53,73 | 1.73 | 6 (13%) | 52,89,113 | 1.71 | 9 (17%) |
| 14 | CLA | r | 503 | 13 | 65,73,73 | 1.45 | 6 (9%) | 76,113,113 | 1.47 | 8 (10%) |
| 14 | CLA | e | 1133 | 1 | 65,73,73 | 1.41 | 10 (15%) | 76,113,113 | 1.48 | 6 (7%) |
| 14 | CLA | 4 | 502 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.67 | 7 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 17 | BCR | H | 4010 | - | 41,41,41 | 0.91 | 1 (2%) | 56,56,56 | 2.31 | 21 (37%) |
| 14 | CLA | Y | 510 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | l | 1303 | 8 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.74 | 9 (17%) |
| 14 | CLA | m | 1103 | 9 | 48,56,73 | 1.66 | 8 (16%) | 55,92,113 | 1.61 | 8 (14%) |
| 14 | CLA | G | 1127 | 1 | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.54 | 11 (14%) |
| 17 | BCR | H | 4014 | - | 41,41,41 | 0.83 | 0 | 56,56,56 | 1.89 | 23 (41%) |
| 14 | CLA | q | 517 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.60 | 7 (13%) |
| 14 | CLA | 6 | 516 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.60 | 8 (15%) |
| 14 | CLA | H | 1204 | 2 | 65,73,73 | 1.40 | 8 (12%) | 76,113,113 | 1.47 | 9 (11%) |
| 14 | CLA | H | 1217 | 2 | 60,68,73 | 1.53 | 6 (10%) | 70,107,113 | 1.42 | 7 (10%) |
| 14 | CLA | H | 1201 | 2 | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.65 | 9 (12%) |
| 14 | CLA | K | 1105 | 9 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.85 | 11 (21%) |
| 17 | BCR | f | 4014 | - | 41,41,41 | 0.83 | 1 (2%) | 56,56,56 | 1.90 | 23 (41%) |
| 14 | CLA | f | 1204 | 2 | 65,73,73 | 1.40 | 8 (12%) | 76,113,113 | 1.47 | 9 (11%) |
| 14 | CLA | f | 1217 | 2 | 60,68,73 | 1.52 | 6 (10%) | 70,107,113 | 1.41 | 7 (10%) |
| 14 | CLA | a | 504 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.72 | 9 (17%) |
| 14 | CLA | s | 512 | 13 | 45,53,73 | 1.78 | 8 (17%) | 52,89,113 | 1.52 | 5 (9%) |
| 14 | CLA | u | 501 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.71 | 8 (15%) |
| 17 | BCR | T | 4013 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.93 | 16 (28%) |
| 17 | BCR | e | 4011 | - | 41,41,41 | 0.83 | 0 | 56,56,56 | 1.78 | 12 (21%) |
| 17 | BCR | v | 524 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.84 | 15 (26%) |
| 17 | BCR | M | 4021 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.91 | 15 (26%) |
| 14 | CLA | G | 1107 | 1 | 65,73,73 | 1.52 | 10 (15%) | 76,113,113 | 1.50 | 10 (13%) |
| 22 | FMN | p | 170 | - | 33,33,33 | 1.12 | 2 (6%) | 48,50,50 | 1.24 | 6 (12%) |
| 14 | CLA | v | 504 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.69 | 7 (13%) |
| 14 | CLA | u | 506 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.63 | 7 (13%) |
| 18 | LHG | B | 1842 | 14 | 36,36,48 | 0.81 | 1 (2%) | 39,42,54 | 1.26 | 3 (7%) |
| 17 | BCR | B | 4014 | - | 41,41,41 | 0.83 | 1 (2%) | 56,56,56 | 1.89 | 23 (41%) |
| 14 | CLA | d | 508 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.78 | 11 (21%) |
| 14 | CLA | v | 510 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.63 | 6 (11%) |
| 14 | CLA | B | 1204 | 2 | 65,73,73 | 1.40 | 8 (12%) | 76,113,113 | 1.47 | 9 (11%) |
| 14 | CLA | B | 1217 | 2 | 60,68,73 | 1.53 | 6 (10%) | 70,107,113 | 1.42 | 7 (10%) |
| 14 | CLA | H | 1239 | 2 | 65,73,73 | 1.48 | 8 (12%) | 76,113,113 | 1.73 | 14 (18%) |
| 14 | CLA | G | 1138 | 1 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.55 | 7 (9%) |
| 14 | CLA | H | 1234 | 2 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.65 | 10 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | f | 1216 | 23 | 60,68,73 | 1.60 | 10 (16%) | 70,107,113 | 1.55 | 11 (15%) |
| 14 | CLA | q | 502 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.66 | 8 (15%) |
| 14 | CLA | c | 505 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.62 | 6 (11%) |
| 14 | CLA | u | 507 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.71 | 9 (17%) |
| 17 | BCR | 5 | 523 | - | 41,41,41 | 0.78 | 1 (2%) | 56,56,56 | 1.78 | 15 (26%) |
| 14 | CLA | e | 1022 | 23 | 65,73,73 | 1.54 | 11 (16%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | f | 1238 | 23 | 65,73,73 | 1.41 | 7 (10%) | 76,113,113 | 1.63 | 10 (13%) |
| 14 | CLA | G | 1131 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.42 | 9 (11%) |
| 14 | CLA | s | 502 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.72 | 9 (17%) |
| 14 | CLA | t | 506 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.65 | 6 (11%) |
| 14 | CLA | Z | 518 | 13 | 55,63,73 | 1.55 | 7 (12%) | 64,101,113 | 1.53 | 7 (10%) |
| 14 | CLA | a | 506 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.70 | 6 (11%) |
| 14 | CLA | a | 516 | 13 | 45,53,73 | 1.74 | 5 (11%) | 52,89,113 | 1.87 | 11 (21%) |
| 14 | CLA | f | 1239 | 2 | 65,73,73 | 1.48 | 8 (12%) | 76,113,113 | 1.73 | 14 (18%) |
| 14 | CLA | q | 507 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.70 | 9 (17%) |
| 14 | CLA | s | 517 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.59 | 6 (11%) |
| 14 | CLA | t | 513 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.63 | 6 (11%) |
| 14 | CLA | A | 1133 | 1 | 65,73,73 | 1.41 | 10 (15%) | 76,113,113 | 1.48 | 6 (7%) |
| 14 | CLA | A | 1136 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.54 | 10 (13%) |
| 14 | CLA | u | 511 | 13 | 45,53,73 | 1.76 | 5 (11%) | 52,89,113 | 1.72 | 8 (15%) |
| 14 | CLA | f | 1218 | 2 | 60,68,73 | 1.51 | 8 (13%) | 70,107,113 | 1.43 | 7 (10%) |
| 17 | BCR | 5 | 524 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.74 | 12 (21%) |
| 14 | CLA | e | 1111 | 1 | 65,73,73 | 1.42 | 9 (13%) | 76,113,113 | 1.53 | 8 (10%) |
| 17 | BCR | V | 4022 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.81 | 10 (17%) |
| 14 | CLA | f | 1229 | 2 | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.60 | 8 (10%) |
| 14 | CLA | a | 512 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.53 | 5 (9%) |
| 14 | CLA | d | 504 | - | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.69 | 7 (13%) |
| 14 | CLA | f | 1221 | 23 | 62,70,73 | 1.50 | 8 (12%) | 72,109,113 | 1.69 | 11 (15%) |
| 18 | LHG | L | 5218 | - | 36,36,48 | 0.76 | 2 (5%) | 39,42,54 | 1.20 | 4 (10%) |
| 14 | CLA | r | 513 | 13 | 45,53,73 | 1.78 | 9 (20%) | 52,89,113 | 1.55 | 6 (11%) |
| 14 | CLA | e | 1108 | 1 | 54,62,73 | 1.57 | 7 (12%) | 62,99,113 | 1.58 | 8 (12%) |
| 14 | CLA | s | 513 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.59 | 6 (11%) |
| 21 | SQD | V | 5216 | - | 45,46,54 | 1.01 | 5 (11%) | 54,57,65 | 1.69 | 11 (20%) |
| 14 | CLA | a | 511 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.71 | 9 (17%) |
| 14 | CLA | d | 507 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.69 | 9 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | d | 516 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.60 | 7 (13%) |
| 16 | SF4 | g | 3002 | 3 | 0,12,12 | - | - | - | | |
| 14 | CLA | B | 1221 | 23 | 62,70,73 | 1.50 | 8 (12%) | 72,109,113 | 1.69 | 11 (15%) |
| 14 | CLA | A | 1116 | 1 | 60,68,73 | 1.51 | 8 (13%) | 70,107,113 | 1.50 | 7 (10%) |
| 14 | CLA | G | 1011 | 1 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.73 | 14 (18%) |
| 14 | CLA | G | 1801 | 18 | 45,53,73 | 1.65 | 7 (15%) | 52,89,113 | 1.74 | 6 (11%) |
| 14 | CLA | 2 | 504 | - | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.63 | 8 (15%) |
| 17 | BCR | B | 4005 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.72 | 12 (21%) |
| 17 | BCR | e | 4007 | - | 41,41,41 | 0.87 | 0 | 56,56,56 | 2.10 | 19 (33%) |
| 14 | CLA | 4 | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.61 | 6 (11%) |
| 14 | CLA | G | 1108 | 1 | 54,62,73 | 1.57 | 8 (14%) | 62,99,113 | 1.57 | 8 (12%) |
| 18 | LHG | G | 5005 | - | 42,42,48 | 0.65 | 1 (2%) | 45,48,54 | 1.21 | 4 (8%) |
| 17 | BCR | b | 524 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 1.85 | 14 (25%) |
| 14 | CLA | Y | 504 | - | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.79 | 10 (19%) |
| 14 | CLA | A | 1022 | 23 | 65,73,73 | 1.54 | 11 (16%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | 2 | 507 | - | 45,53,73 | 1.72 | 8 (17%) | 52,89,113 | 1.71 | 10 (19%) |
| 14 | CLA | c | 507 | - | 45,53,73 | 1.74 | 6 (13%) | 52,89,113 | 1.71 | 9 (17%) |
| 21 | SQD | c | 822 | - | 25,26,54 | 1.29 | 4 (16%) | 34,37,65 | 1.95 | 11 (32%) |
| 17 | BCR | V | 4219 | - | 41,41,41 | 1.08 | 5 (12%) | 56,56,56 | 2.26 | 23 (41%) |
| 21 | SQD | L | 5216 | - | 45,46,54 | 1.01 | 5 (11%) | 54,57,65 | 1.69 | 11 (20%) |
| 14 | CLA | q | 509 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.66 | 9 (17%) |
| 17 | BCR | q | 524 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.85 | 17 (30%) |
| 18 | LHG | S | 5001 | - | 47,47,48 | 0.62 | 0 | 50,53,54 | 1.24 | 5 (10%) |
| 14 | CLA | e | 1110 | 1 | 53,61,73 | 1.60 | 8 (15%) | 61,98,113 | 1.57 | 8 (13%) |
| 14 | CLA | G | 1134 | 1 | 56,64,73 | 1.55 | 8 (14%) | 65,102,113 | 1.64 | 11 (16%) |
| 14 | CLA | B | 1201 | 2 | 60,68,73 | 1.49 | 7 (11%) | 70,107,113 | 1.66 | 9 (12%) |
| 14 | CLA | G | 1114 | 23 | 45,53,73 | 1.80 | 8 (17%) | 52,89,113 | 1.69 | 9 (17%) |
| 14 | CLA | G | 1101 | 1 | 65,73,73 | 1.50 | 9 (13%) | 76,113,113 | 1.62 | 13 (17%) |
| 21 | SQD | s | 822 | - | 27,28,54 | 1.29 | 5 (18%) | 36,39,65 | 1.80 | 10 (27%) |
| 14 | CLA | f | 1209 | 2 | 53,61,73 | 1.63 | 8 (15%) | 61,98,113 | 1.68 | 8 (13%) |
| 14 | CLA | f | 1234 | 2 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.65 | 10 (13%) |
| 14 | CLA | 3 | 503 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.64 | 8 (15%) |
| 17 | BCR | k | 4018 | - | 41,41,41 | 0.93 | 2 (4%) | 56,56,56 | 1.93 | 16 (28%) |
| 18 | LHG | G | 5006 | - | 39,39,48 | 0.67 | 1 (2%) | 42,45,54 | 1.22 | 5 (11%) |
| 14 | CLA | Y | 516 | 13 | 45,53,73 | 1.71 | 9 (20%) | 52,89,113 | 1.64 | 9 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | G | 1022 | 23 | 65,73,73 | 1.53 | 11 (16%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | 5 | 508 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.84 | 7 (13%) |
| 14 | CLA | a | 513 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.60 | 6 (11%) |
| 16 | SF4 | C | 3003 | 3 | 0,12,12 | - | - | - | | |
| 14 | CLA | G | 1113 | 1 | 45,53,73 | 1.67 | 7 (15%) | 52,89,113 | 1.80 | 7 (13%) |
| 21 | SQD | b | 822 | - | 25,26,54 | 1.32 | 4 (16%) | 34,37,65 | 1.97 | 9 (26%) |
| 14 | CLA | 6 | 505 | 13 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.45 | 8 (10%) |
| 14 | CLA | A | 1124 | 23 | 60,68,73 | 1.52 | 9 (15%) | 70,107,113 | 1.58 | 9 (12%) |
| 14 | CLA | 1 | 504 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.78 | 9 (17%) |
| 14 | CLA | e | 1135 | 1 | 55,63,73 | 1.50 | 10 (18%) | 64,101,113 | 1.76 | 11 (17%) |
| 17 | BCR | J | 4013 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.93 | 16 (28%) |
| 14 | CLA | Y | 512 | 13 | 45,53,73 | 1.74 | 8 (17%) | 52,89,113 | 1.49 | 5 (9%) |
| 14 | CLA | t | 510 | 13 | 45,53,73 | 1.73 | 6 (13%) | 52,89,113 | 1.67 | 6 (11%) |
| 14 | CLA | B | 1239 | 2 | 65,73,73 | 1.48 | 8 (12%) | 76,113,113 | 1.72 | 15 (19%) |
| 17 | BCR | c | 523 | - | 41,41,41 | 0.78 | 1 (2%) | 56,56,56 | 1.78 | 15 (26%) |
| 18 | LHG | V | 5221 | - | 48,48,48 | 0.62 | 0 | 51,54,54 | 1.28 | 7 (13%) |
| 19 | LMU | H | 1843 | - | 36,36,36 | 1.17 | 2 (5%) | 47,47,47 | 1.06 | 3 (6%) |
| 14 | CLA | 4 | 519 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.64 | 7 (13%) |
| 14 | CLA | e | 1112 | 1 | 50,58,73 | 1.62 | 10 (20%) | 58,95,113 | 1.67 | 8 (13%) |
| 14 | CLA | 3 | 509 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.77 | 7 (13%) |
| 14 | CLA | A | 1101 | 1 | 65,73,73 | 1.50 | 9 (13%) | 76,113,113 | 1.61 | 13 (17%) |
| 14 | CLA | H | 1202 | 2 | 65,73,73 | 1.41 | 7 (10%) | 76,113,113 | 1.58 | 8 (10%) |
| 14 | CLA | H | 1209 | 2 | 53,61,73 | 1.62 | 8 (15%) | 61,98,113 | 1.67 | 8 (13%) |
| 14 | CLA | u | 517 | - | 45,53,73 | 1.80 | 8 (17%) | 52,89,113 | 1.57 | 6 (11%) |
| 14 | CLA | 2 | 501 | 13 | 60,68,73 | 1.51 | 7 (11%) | 70,107,113 | 1.57 | 8 (11%) |
| 17 | BCR | s | 524 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.93 | 18 (32%) |
| 14 | CLA | 5 | 504 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.68 | 7 (13%) |
| 14 | CLA | A | 1113 | 1 | 45,53,73 | 1.67 | 7 (15%) | 52,89,113 | 1.81 | 7 (13%) |
| 14 | CLA | u | 509 | 13 | 65,73,73 | 1.43 | 7 (10%) | 76,113,113 | 1.50 | 7 (9%) |
| 17 | BCR | Z | 524 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.75 | 12 (21%) |
| 14 | CLA | f | 1220 | 2 | 55,63,73 | 1.58 | 10 (18%) | 64,101,113 | 1.63 | 10 (15%) |
| 14 | CLA | e | 1109 | 1 | 65,73,73 | 1.40 | 9 (13%) | 76,113,113 | 1.60 | 8 (10%) |
| 14 | CLA | 6 | 508 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.78 | 11 (21%) |
| 14 | CLA | 1 | 516 | 13 | 45,53,73 | 1.71 | 9 (20%) | 52,89,113 | 1.63 | 8 (15%) |
| 14 | CLA | s | 510 | 13 | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.64 | 7 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | Y | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.67 | 6 (11%) |
| 21 | SQD | 2 | 822 | - | 27,28,54 | 1.22 | 4 (14%) | 36,39,65 | 1.86 | 10 (27%) |
| 18 | LHG | G | 5002 | - | 42,42,48 | 0.76 | 1 (2%) | 45,48,54 | 1.23 | 4 (8%) |
| 14 | CLA | 1 | 512 | 13 | 45,53,73 | 1.74 | 8 (17%) | 52,89,113 | 1.49 | 5 (9%) |
| 14 | CLA | e | 1125 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.59 | 9 (11%) |
| 14 | CLA | e | 1130 | 1 | 56,64,73 | 1.52 | 8 (14%) | 65,102,113 | 1.73 | 9 (13%) |
| 14 | CLA | v | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.71 | 7 (13%) |
| 18 | LHG | A | 5008 | - | 34,34,48 | 0.70 | 1 (2%) | 37,40,54 | 1.25 | 4 (10%) |
| 14 | CLA | B | 1208 | 2 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.38 | 7 (9%) |
| 14 | CLA | A | 1110 | 1 | 53,61,73 | 1.59 | 8 (15%) | 61,98,113 | 1.57 | 8 (13%) |
| 14 | CLA | B | 1228 | 2 | 55,63,73 | 1.52 | 7 (12%) | 64,101,113 | 1.70 | 8 (12%) |
| 18 | LHG | e | 5004 | - | 34,34,48 | 0.67 | 0 | 37,40,54 | 1.28 | 4 (10%) |
| 17 | BCR | G | 4002 | - | 41,41,41 | 0.88 | 1 (2%) | 56,56,56 | 1.94 | 16 (28%) |
| 17 | BCR | j | 4016 | - | 41,41,41 | 0.82 | 0 | 56,56,56 | 1.91 | 11 (19%) |
| 17 | BCR | e | 4003 | - | 41,41,41 | 0.87 | 1 (2%) | 56,56,56 | 1.78 | 14 (25%) |
| 21 | SQD | 6 | 822 | - | 25,26,54 | 1.31 | 4 (16%) | 34,37,65 | 2.00 | 10 (29%) |
| 14 | CLA | Z | 505 | 13 | 65,73,73 | 1.42 | 6 (9%) | 76,113,113 | 1.47 | 8 (10%) |
| 14 | CLA | L | 1503 | 23 | 60,68,73 | 1.48 | 8 (13%) | 70,107,113 | 1.56 | 7 (10%) |
| 14 | CLA | b | 504 | - | 45,53,73 | 1.77 | 5 (11%) | 52,89,113 | 1.64 | 7 (13%) |
| 14 | CLA | e | 1134 | 1 | 56,64,73 | 1.56 | 8 (14%) | 65,102,113 | 1.64 | 11 (16%) |
| 14 | CLA | t | 519 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.64 | 7 (13%) |
| 17 | BCR | 3 | 524 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.93 | 18 (32%) |
| 21 | SQD | q | 822 | - | 31,32,54 | 1.20 | 5 (16%) | 40,43,65 | 2.05 | 13 (32%) |
| 14 | CLA | s | 503 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.64 | 8 (15%) |
| 14 | CLA | 2 | 517 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.65 | 7 (13%) |
| 16 | SF4 | G | 3001 | 1,2 | 0,12,12 | - | - | - | - | - |
| 14 | CLA | b | 506 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.66 | 6 (11%) |
| 14 | CLA | 1 | 503 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.66 | 7 (13%) |
| 14 | CLA | G | 1109 | 1 | 65,73,73 | 1.40 | 9 (13%) | 76,113,113 | 1.60 | 8 (10%) |
| 14 | CLA | v | 511 | 13 | 45,53,73 | 1.78 | 5 (11%) | 52,89,113 | 1.70 | 7 (13%) |
| 14 | CLA | 5 | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.71 | 8 (15%) |
| 14 | CLA | a | 501 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.67 | 9 (17%) |
| 14 | CLA | b | 503 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.70 | 8 (15%) |
| 14 | CLA | 6 | 512 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.59 | 6 (11%) |
| 14 | CLA | B | 1212 | 2 | 51,59,73 | 1.60 | 7 (13%) | 59,96,113 | 1.67 | 6 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 18 | LHG | A | 5006 | - | 39,39,48 | 0.67 | 1 (2%) | 42,45,54 | 1.22 | 5 (11%) |
| 14 | CLA | c | 508 | 13 | 45,53,73 | 1.79 | 9 (20%) | 52,89,113 | 1.84 | 7 (13%) |
| 17 | BCR | W | 4021 | - | 41,41,41 | 0.77 | 0 | 56,56,56 | 1.91 | 15 (26%) |
| 18 | LHG | V | 5218 | - | 36,36,48 | 0.76 | 2 (5%) | 39,42,54 | 1.20 | 4 (10%) |
| 14 | CLA | r | 510 | 13 | 45,53,73 | 1.71 | 7 (15%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | f | 1205 | 2 | 65,73,73 | 1.46 | 10 (15%) | 76,113,113 | 1.59 | 11 (14%) |
| 14 | CLA | Z | 510 | 13 | 45,53,73 | 1.72 | 7 (15%) | 52,89,113 | 1.62 | 6 (11%) |
| 17 | BCR | L | 4022 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.82 | 10 (17%) |
| 21 | SQD | t | 822 | - | 25,26,54 | 1.32 | 4 (16%) | 34,37,65 | 1.97 | 9 (26%) |
| 16 | SF4 | N | 3003 | 3 | 0,12,12 | - | - | - | - | - |
| 14 | CLA | 6 | 507 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.69 | 9 (17%) |
| 14 | CLA | f | 1206 | 2 | 65,73,73 | 1.49 | 11 (16%) | 76,113,113 | 1.61 | 10 (13%) |
| 14 | CLA | G | 1117 | 1 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.57 | 10 (13%) |
| 14 | CLA | q | 504 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.79 | 11 (21%) |
| 14 | CLA | a | 505 | 13 | 55,63,73 | 1.56 | 8 (14%) | 64,101,113 | 1.49 | 7 (10%) |
| 14 | CLA | d | 519 | 13 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.57 | 7 (13%) |
| 14 | CLA | H | 1207 | 2 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.39 | 6 (7%) |
| 14 | CLA | l | 502 | 13 | 45,53,73 | 1.75 | 8 (17%) | 52,89,113 | 1.66 | 8 (15%) |
| 17 | BCR | t | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.79 | 10 (17%) |
| 19 | LMU | l | 5105 | - | 22,22,36 | 1.21 | 1 (4%) | 27,27,47 | 1.43 | 5 (18%) |
| 14 | CLA | r | 504 | - | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.63 | 8 (15%) |
| 14 | CLA | 4 | 503 | 13 | 45,53,73 | 1.79 | 7 (15%) | 52,89,113 | 1.71 | 8 (15%) |
| 14 | CLA | H | 1232 | 23 | 55,63,73 | 1.54 | 8 (14%) | 64,101,113 | 1.70 | 7 (10%) |
| 14 | CLA | e | 1107 | 1 | 65,73,73 | 1.53 | 10 (15%) | 76,113,113 | 1.49 | 10 (13%) |
| 14 | CLA | G | 1104 | 1 | 65,73,73 | 1.43 | 9 (13%) | 76,113,113 | 1.60 | 13 (17%) |
| 17 | BCR | U | 4104 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.88 | 16 (28%) |
| 14 | CLA | R | 1302 | 6 | 45,53,73 | 1.77 | 9 (20%) | 52,89,113 | 1.59 | 8 (15%) |
| 17 | BCR | B | 4006 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 2.09 | 18 (32%) |
| 14 | CLA | r | 507 | - | 45,53,73 | 1.72 | 8 (17%) | 52,89,113 | 1.71 | 10 (19%) |
| 18 | LHG | n | 5218 | - | 36,36,48 | 0.76 | 2 (5%) | 39,42,54 | 1.20 | 4 (10%) |
| 14 | CLA | G | 1124 | 23 | 60,68,73 | 1.52 | 9 (15%) | 70,107,113 | 1.59 | 9 (12%) |
| 14 | CLA | 6 | 511 | 13 | 45,53,73 | 1.78 | 5 (11%) | 52,89,113 | 1.69 | 7 (13%) |
| 21 | SQD | u | 822 | - | 25,26,54 | 1.29 | 4 (16%) | 34,37,65 | 1.95 | 11 (32%) |
| 17 | BCR | 6 | 522 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.89 | 19 (33%) |
| 14 | CLA | 4 | 513 | 13 | 45,53,73 | 1.78 | 7 (15%) | 52,89,113 | 1.64 | 6 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | H | 1012 | 23 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.58 | 9 (11%) |
| 14 | CLA | 5 | 517 | - | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.56 | 6 (11%) |
| 19 | LMU | f | 1843 | - | 36,36,36 | 1.16 | 2 (5%) | 47,47,47 | 1.06 | 3 (6%) |
| 14 | CLA | e | 1119 | 23 | 65,73,73 | 1.50 | 11 (16%) | 76,113,113 | 1.67 | 13 (17%) |
| 14 | CLA | H | 1212 | 2 | 51,59,73 | 1.59 | 7 (13%) | 59,96,113 | 1.68 | 6 (10%) |
| 14 | CLA | q | 506 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.64 | 6 (11%) |
| 17 | BCR | t | 524 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.85 | 14 (25%) |
| 20 | LMG | H | 5002 | - | 53,53,55 | 0.86 | 3 (5%) | 61,61,63 | 1.51 | 12 (19%) |
| 14 | CLA | f | 1012 | 23 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.58 | 9 (11%) |
| 14 | CLA | b | 516 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.62 | 7 (13%) |
| 14 | CLA | B | 1213 | 2 | 61,69,73 | 1.47 | 7 (11%) | 71,108,113 | 1.60 | 9 (12%) |
| 14 | CLA | e | 1104 | 1 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.60 | 13 (17%) |
| 14 | CLA | f | 1212 | 2 | 51,59,73 | 1.60 | 7 (13%) | 59,96,113 | 1.67 | 6 (10%) |
| 14 | CLA | f | 1213 | 2 | 61,69,73 | 1.47 | 7 (11%) | 71,108,113 | 1.60 | 8 (11%) |
| 14 | CLA | A | 1130 | 1 | 56,64,73 | 1.52 | 8 (14%) | 65,102,113 | 1.73 | 9 (13%) |
| 17 | BCR | 4 | 521 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.79 | 11 (19%) |
| 14 | CLA | A | 1104 | 1 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.59 | 13 (17%) |
| 14 | CLA | T | 1302 | 8 | 55,63,73 | 1.55 | 9 (16%) | 64,101,113 | 1.56 | 9 (14%) |
| 14 | CLA | q | 512 | 13 | 45,53,73 | 1.74 | 8 (17%) | 52,89,113 | 1.48 | 5 (9%) |
| 20 | LMG | l | 5104 | - | 32,32,55 | 0.96 | 2 (6%) | 40,40,63 | 1.26 | 4 (10%) |
| 14 | CLA | d | 505 | 13 | 65,73,73 | 1.45 | 7 (10%) | 76,113,113 | 1.46 | 8 (10%) |
| 14 | CLA | H | 1238 | 23 | 65,73,73 | 1.40 | 7 (10%) | 76,113,113 | 1.64 | 11 (14%) |
| 14 | CLA | f | 1226 | 2 | 55,63,73 | 1.70 | 10 (18%) | 64,101,113 | 1.98 | 15 (23%) |
| 14 | CLA | A | 1103 | 1 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.73 | 11 (14%) |
| 14 | CLA | H | 1021 | 2 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.45 | 9 (11%) |
| 14 | CLA | a | 502 | 13 | 45,53,73 | 1.77 | 8 (17%) | 52,89,113 | 1.72 | 9 (17%) |
| 14 | CLA | B | 1210 | 2 | 65,73,73 | 1.43 | 9 (13%) | 76,113,113 | 1.48 | 9 (11%) |
| 14 | CLA | G | 1110 | 1 | 53,61,73 | 1.60 | 8 (15%) | 61,98,113 | 1.58 | 8 (13%) |
| 14 | CLA | V | 1503 | 23 | 60,68,73 | 1.47 | 8 (13%) | 70,107,113 | 1.56 | 7 (10%) |
| 18 | LHG | G | 5003 | 14 | 39,39,48 | 0.86 | 1 (2%) | 42,45,54 | 1.38 | 6 (14%) |
| 14 | CLA | q | 511 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 8 (15%) |
| 18 | LHG | e | 5007 | - | 46,46,48 | 0.61 | 0 | 49,52,54 | 1.20 | 4 (8%) |
| 14 | CLA | A | 1125 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.58 | 9 (11%) |
| 14 | CLA | F | 1301 | 23 | 45,53,73 | 1.73 | 9 (20%) | 52,89,113 | 1.60 | 6 (11%) |
| 14 | CLA | H | 1240 | 18 | 65,73,73 | 1.47 | 6 (9%) | 76,113,113 | 1.46 | 8 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | LMU | B | 1843 | - | 36,36,36 | 1.16 | 2 (5%) | 47,47,47 | 1.06 | 3 (6%) |
| 17 | BCR | F | 4016 | - | 41,41,41 | 0.82 | 0 | 56,56,56 | 1.91 | 11 (19%) |
| 14 | CLA | d | 502 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.67 | 8 (15%) |
| 14 | CLA | G | 1135 | 1 | 55,63,73 | 1.49 | 10 (18%) | 64,101,113 | 1.76 | 11 (17%) |
| 14 | CLA | G | 1129 | 1 | 53,61,73 | 1.63 | 10 (18%) | 61,98,113 | 1.60 | 9 (14%) |
| 14 | CLA | s | 501 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 9 (17%) |
| 17 | BCR | A | 4003 | - | 41,41,41 | 0.88 | 1 (2%) | 56,56,56 | 1.78 | 14 (25%) |
| 14 | CLA | H | 1235 | 2 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.51 | 8 (10%) |
| 14 | CLA | Z | 502 | 13 | 45,53,73 | 1.76 | 9 (20%) | 52,89,113 | 1.71 | 9 (17%) |
| 14 | CLA | G | 1120 | 1 | 50,58,73 | 1.57 | 8 (16%) | 58,95,113 | 1.73 | 10 (17%) |
| 14 | CLA | 1 | 519 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.56 | 6 (11%) |
| 14 | CLA | Y | 505 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.66 | 6 (11%) |
| 14 | CLA | 3 | 518 | 13 | 55,63,73 | 1.58 | 8 (14%) | 64,101,113 | 1.49 | 7 (10%) |
| 21 | SQD | 4 | 822 | - | 25,26,54 | 1.32 | 4 (16%) | 34,37,65 | 1.97 | 9 (26%) |
| 14 | CLA | B | 1021 | 2 | 65,73,73 | 1.47 | 9 (13%) | 76,113,113 | 1.45 | 9 (11%) |
| 18 | LHG | L | 5221 | - | 48,48,48 | 0.62 | 0 | 51,54,54 | 1.28 | 7 (13%) |
| 14 | CLA | A | 1119 | 23 | 65,73,73 | 1.50 | 11 (16%) | 76,113,113 | 1.67 | 13 (17%) |
| 14 | CLA | c | 518 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.56 | 8 (15%) |
| 14 | CLA | L | 1502 | 10 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.53 | 8 (10%) |
| 17 | BCR | c | 522 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.94 | 20 (35%) |
| 18 | LHG | A | 5009 | - | 41,41,48 | 0.67 | 0 | 44,47,54 | 1.22 | 5 (11%) |
| 14 | CLA | J | 1303 | 8 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.73 | 9 (17%) |
| 17 | BCR | v | 521 | - | 41,41,41 | 0.68 | 0 | 56,56,56 | 1.79 | 12 (21%) |
| 14 | CLA | A | 1115 | 1 | 60,68,73 | 1.51 | 9 (15%) | 70,107,113 | 1.59 | 7 (10%) |
| 14 | CLA | L | 1501 | 10 | 60,68,73 | 1.56 | 10 (16%) | 70,107,113 | 1.50 | 9 (12%) |
| 17 | BCR | A | 4007 | - | 41,41,41 | 0.87 | 0 | 56,56,56 | 2.10 | 20 (35%) |
| 14 | CLA | t | 504 | - | 45,53,73 | 1.79 | 6 (13%) | 52,89,113 | 1.64 | 7 (13%) |
| 14 | CLA | s | 511 | 13 | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.71 | 9 (17%) |
| 14 | CLA | Y | 517 | - | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.61 | 7 (13%) |
| 14 | CLA | u | 513 | 13 | 45,53,73 | 1.79 | 8 (17%) | 52,89,113 | 1.55 | 6 (11%) |
| 17 | BCR | G | 4007 | - | 41,41,41 | 0.87 | 0 | 56,56,56 | 2.11 | 20 (35%) |
| 14 | CLA | H | 1223 | 2 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.63 | 7 (9%) |
| 14 | CLA | B | 1207 | 2 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.38 | 6 (7%) |
| 14 | CLA | Z | 511 | 13 | 45,53,73 | 1.75 | 7 (15%) | 52,89,113 | 1.70 | 7 (13%) |
| 17 | BCR | 6 | 523 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.72 | 14 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 18 | LHG | G | 5007 | - | 46,46,48 | 0.60 | 0 | 49,52,54 | 1.20 | 4 (8%) |
| 14 | CLA | t | 507 | - | 45,53,73 | 1.73 | 6 (13%) | 52,89,113 | 1.73 | 8 (15%) |
| 14 | CLA | H | 1220 | 2 | 55,63,73 | 1.58 | 10 (18%) | 64,101,113 | 1.64 | 10 (15%) |
| 17 | BCR | n | 4020 | - | 41,41,41 | 0.98 | 2 (4%) | 56,56,56 | 1.67 | 14 (25%) |
| 17 | BCR | 4 | 524 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.85 | 14 (25%) |
| 14 | CLA | v | 517 | - | 45,53,73 | 1.74 | 8 (17%) | 52,89,113 | 1.61 | 7 (13%) |
| 14 | CLA | B | 1227 | 2 | 60,68,73 | 1.54 | 10 (16%) | 70,107,113 | 1.51 | 8 (11%) |
| 14 | CLA | b | 511 | 13 | 45,53,73 | 1.79 | 7 (15%) | 52,89,113 | 1.68 | 9 (17%) |
| 14 | CLA | l | 505 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.65 | 6 (11%) |
| 14 | CLA | e | 1132 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | 6 | 519 | 13 | 45,53,73 | 1.78 | 9 (20%) | 52,89,113 | 1.58 | 7 (13%) |
| 14 | CLA | B | 1211 | 2 | 55,63,73 | 1.52 | 8 (14%) | 64,101,113 | 1.68 | 8 (12%) |
| 14 | CLA | A | 1121 | 1 | 55,63,73 | 1.57 | 10 (18%) | 64,101,113 | 1.66 | 12 (18%) |
| 14 | CLA | G | 1103 | 1 | 65,73,73 | 1.46 | 9 (13%) | 76,113,113 | 1.73 | 11 (14%) |
| 14 | CLA | b | 517 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 8 (15%) |
| 14 | CLA | f | 1211 | 2 | 55,63,73 | 1.53 | 8 (14%) | 64,101,113 | 1.69 | 8 (12%) |
| 14 | CLA | A | 1102 | 1 | 55,63,73 | 1.56 | 9 (16%) | 64,101,113 | 1.62 | 7 (10%) |
| 14 | CLA | 4 | 504 | - | 45,53,73 | 1.78 | 6 (13%) | 52,89,113 | 1.65 | 7 (13%) |
| 17 | BCR | b | 522 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.91 | 19 (33%) |
| 18 | LHG | f | 1842 | 14 | 36,36,48 | 0.81 | 1 (2%) | 39,42,54 | 1.25 | 3 (7%) |
| 17 | BCR | I | 4018 | - | 41,41,41 | 0.93 | 2 (4%) | 56,56,56 | 1.93 | 17 (30%) |
| 14 | CLA | T | 1303 | 8 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.73 | 9 (17%) |
| 14 | CLA | G | 1121 | 1 | 55,63,73 | 1.57 | 10 (18%) | 64,101,113 | 1.66 | 12 (18%) |
| 14 | CLA | A | 1106 | 1 | 65,73,73 | 1.41 | 8 (12%) | 76,113,113 | 1.53 | 9 (11%) |
| 21 | SQD | Y | 822 | - | 31,32,54 | 1.20 | 5 (16%) | 40,43,65 | 2.05 | 13 (32%) |
| 20 | LMG | B | 5002 | - | 53,53,55 | 0.85 | 3 (5%) | 61,61,63 | 1.51 | 12 (19%) |
| 14 | CLA | t | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.61 | 6 (11%) |
| 14 | CLA | 5 | 505 | 13 | 45,53,73 | 1.73 | 7 (15%) | 52,89,113 | 1.61 | 6 (11%) |
| 15 | PQN | f | 2002 | - | 34,34,34 | 2.84 | 11 (32%) | 42,45,45 | 2.30 | 6 (14%) |
| 17 | BCR | G | 4001 | - | 41,41,41 | 0.79 | 0 | 56,56,56 | 1.68 | 11 (19%) |
| 14 | CLA | e | 1128 | 1 | 65,73,73 | 1.58 | 11 (16%) | 76,113,113 | 1.69 | 9 (11%) |
| 14 | CLA | s | 509 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.77 | 7 (13%) |
| 14 | CLA | s | 505 | 13 | 55,63,73 | 1.56 | 7 (12%) | 64,101,113 | 1.50 | 7 (10%) |
| 14 | CLA | s | 507 | - | 45,53,73 | 1.75 | 6 (13%) | 52,89,113 | 1.68 | 9 (17%) |
| 14 | CLA | e | 1138 | 1 | 65,73,73 | 1.45 | 9 (13%) | 76,113,113 | 1.54 | 7 (9%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 14 | CLA | 6 | 506 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 6 (11%) |
| 14 | CLA | f | 1235 | 2 | 65,73,73 | 1.48 | 10 (15%) | 76,113,113 | 1.52 | 8 (10%) |
| 14 | CLA | v | 507 | - | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.69 | 9 (17%) |
| 14 | CLA | G | 1115 | 1 | 60,68,73 | 1.50 | 9 (15%) | 70,107,113 | 1.59 | 7 (10%) |
| 14 | CLA | b | 509 | 13 | 45,53,73 | 1.77 | 7 (15%) | 52,89,113 | 1.75 | 8 (15%) |
| 14 | CLA | b | 505 | 13 | 45,53,73 | 1.76 | 8 (17%) | 52,89,113 | 1.54 | 6 (11%) |
| 17 | BCR | H | 4005 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.73 | 12 (21%) |
| 14 | CLA | 4 | 510 | 13 | 45,53,73 | 1.73 | 6 (13%) | 52,89,113 | 1.66 | 6 (11%) |
| 21 | SQD | a | 822 | - | 27,28,54 | 1.30 | 5 (18%) | 36,39,65 | 1.79 | 10 (27%) |
| 14 | CLA | A | 1129 | 1 | 53,61,73 | 1.62 | 10 (18%) | 61,98,113 | 1.60 | 9 (14%) |
| 14 | CLA | A | 1132 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.55 | 11 (14%) |
| 14 | CLA | G | 1125 | 1 | 65,73,73 | 1.42 | 10 (15%) | 76,113,113 | 1.58 | 9 (11%) |
| 14 | CLA | 5 | 519 | 13 | 45,53,73 | 1.78 | 6 (13%) | 52,89,113 | 1.61 | 7 (13%) |
| 17 | BCR | q | 522 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.91 | 20 (35%) |
| 14 | CLA | f | 1203 | 2 | 65,73,73 | 1.44 | 9 (13%) | 76,113,113 | 1.53 | 9 (11%) |
| 21 | SQD | Z | 822 | - | 27,28,54 | 1.22 | 4 (14%) | 36,39,65 | 1.86 | 10 (27%) |
| 14 | CLA | B | 1235 | 2 | 65,73,73 | 1.47 | 10 (15%) | 76,113,113 | 1.51 | 8 (10%) |
| 14 | CLA | u | 516 | 13 | 45,53,73 | 1.77 | 6 (13%) | 52,89,113 | 1.58 | 6 (11%) |
| 14 | CLA | A | 1123 | 23 | 65,73,73 | 1.42 | 8 (12%) | 76,113,113 | 1.53 | 8 (10%) |
| 14 | CLA | G | 1105 | 1 | 55,63,73 | 1.49 | 8 (14%) | 64,101,113 | 1.67 | 8 (12%) |
| 14 | CLA | G | 1116 | 1 | 60,68,73 | 1.51 | 8 (13%) | 70,107,113 | 1.51 | 7 (10%) |
| 17 | BCR | A | 4011 | - | 41,41,41 | 0.82 | 0 | 56,56,56 | 1.79 | 12 (21%) |
| 14 | CLA | 4 | 507 | - | 45,53,73 | 1.72 | 6 (13%) | 52,89,113 | 1.72 | 8 (15%) |
| 17 | BCR | s | 522 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 2.04 | 18 (32%) |
| 14 | CLA | 2 | 509 | 13 | 65,73,73 | 1.46 | 7 (10%) | 76,113,113 | 1.52 | 7 (9%) |
| 18 | LHG | A | 5001 | - | 48,48,48 | 0.80 | 1 (2%) | 51,54,54 | 1.30 | 7 (13%) |
| 14 | CLA | d | 506 | 13 | 45,53,73 | 1.76 | 7 (15%) | 52,89,113 | 1.67 | 6 (11%) |
| 14 | CLA | c | 509 | 13 | 65,73,73 | 1.44 | 7 (10%) | 76,113,113 | 1.49 | 7 (9%) |
| 14 | CLA | 5 | 518 | 13 | 45,53,73 | 1.76 | 6 (13%) | 52,89,113 | 1.56 | 8 (15%) |
| 14 | CLA | u | 512 | 13 | 45,53,73 | 1.74 | 7 (15%) | 52,89,113 | 1.57 | 6 (11%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | B | 1203 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | B | 1219 | 2 | 1/1/14/20 | 18/35/113/115 | - |
| 21 | SQD | n | 5216 | - | - | 17/41/61/69 | 0/1/1/1 |
| 14 | CLA | 3 | 501 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | b | 523 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1011 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 17 | BCR | l | 4013 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | Y | 508 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | 6 | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | G | 1136 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | e | 1122 | 1 | 1/1/14/20 | 12/31/109/115 | - |
| 14 | CLA | Z | 501 | 13 | 1/1/14/20 | 11/31/109/115 | - |
| 17 | BCR | 3 | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1206 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | Y | 506 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | 2 | 522 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | v | 506 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 16 | SF4 | C | 3002 | 3 | - | - | 0/6/5/5 |
| 14 | CLA | B | 1225 | 2 | 1/1/15/20 | 7/37/115/115 | - |
| 14 | CLA | A | 1126 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CLA | 6 | 513 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | f | 1240 | 18 | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | r | 518 | 13 | 1/1/13/20 | 14/25/103/115 | - |
| 14 | CLA | 3 | 511 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | q | 505 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | Y | 511 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | G | 1140 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | e | 1013 | - | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | B | 1216 | 23 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | a | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 4 | 512 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | Z | 522 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1108 | 1 | 1/1/12/20 | 14/24/102/115 | - |
| 17 | BCR | f | 4005 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | c | 516 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | G | 1137 | 1 | 1/1/14/20 | 18/31/109/115 | - |
| 14 | CLA | c | 517 | - | 1/1/11/20 | 10/13/91/115 | - |
| 14 | CLA | 3 | 517 | - | 1/1/11/20 | 7/13/91/115 | - |
| 18 | LHG | e | 5008 | - | - | 18/39/39/53 | - |
| 17 | BCR | q | 523 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | 1 | 506 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | H | 1219 | 2 | 1/1/14/20 | 18/35/113/115 | - |
| 14 | CLA | G | 1118 | 1 | 1/1/14/20 | 8/31/109/115 | - |
| 14 | CLA | t | 501 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | G | 1122 | 1 | 1/1/14/20 | 12/31/109/115 | - |
| 14 | CLA | t | 517 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | Z | 503 | 13 | 1/1/15/20 | 9/37/115/115 | - |
| 17 | BCR | s | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | u | 502 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | f | 1236 | 2 | 1/1/12/20 | 3/19/97/115 | - |
| 14 | CLA | t | 509 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | a | 509 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | v | 512 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | r | 501 | 13 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | c | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 22 | FMN | X | 170 | - | - | 0/18/18/18 | 0/3/3/3 |
| 14 | CLA | H | 1214 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | d | 512 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | 6 | 521 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | u | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | 3 | 505 | 13 | 1/1/13/20 | 11/25/103/115 | - |
| 16 | SF4 | e | 3001 | 1,2 | - | - | 0/6/5/5 |
| 14 | CLA | 1 | 511 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | A | 1138 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | e | 1123 | 23 | 1/1/15/20 | 11/37/115/115 | - |
| 14 | CLA | f | 1023 | - | 1/1/15/20 | 10/37/115/115 | - |
| 17 | BCR | 3 | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | 2 | 506 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | 1 | 510 | 13 | 1/1/11/20 | 4/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | 4 | 506 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | t | 511 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | H | 4004 | - | - | 8/29/63/63 | 0/2/2/2 |
| 14 | CLA | b | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 18 | LHG | e | 5003 | 14 | - | 17/44/44/53 | - |
| 14 | CLA | 2 | 512 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | t | 522 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | b | 518 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | o | 4021 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1134 | 1 | 1/1/13/20 | 9/27/105/115 | - |
| 14 | CLA | u | 505 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | d | 503 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | t | 523 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1131 | 1 | 1/1/15/20 | 6/37/115/115 | - |
| 20 | LMG | f | 5002 | - | - | 24/48/68/70 | 0/1/1/1 |
| 14 | CLA | 4 | 511 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 21 | SQD | v | 822 | - | - | 7/19/39/69 | 0/1/1/1 |
| 14 | CLA | e | 1120 | 1 | 1/1/12/20 | 11/19/97/115 | - |
| 17 | BCR | 6 | 524 | - | - | 5/29/63/63 | 0/2/2/2 |
| 17 | BCR | Y | 522 | - | - | 6/29/63/63 | 0/2/2/2 |
| 17 | BCR | r | 522 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | G | 1237 | 23 | 1/1/15/20 | 23/37/115/115 | - |
| 17 | BCR | B | 4004 | - | - | 8/29/63/63 | 0/2/2/2 |
| 14 | CLA | d | 513 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | K | 1103 | 9 | 1/1/11/20 | 8/17/95/115 | - |
| 14 | CLA | 3 | 519 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | b | 513 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | 2 | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | v | 503 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | Z | 523 | - | - | 6/29/63/63 | 0/2/2/2 |
| 15 | PQN | A | 2001 | - | - | 14/23/43/43 | 0/2/2/2 |
| 17 | BCR | r | 521 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1201 | 2 | 1/1/14/20 | 8/31/109/115 | - |
| 14 | CLA | 4 | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | B | 1230 | 2 | 1/1/14/20 | 10/31/109/115 | - |
| 14 | CLA | 6 | 510 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | G | 1128 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | B | 1012 | 23 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | G | 1123 | 23 | 1/1/15/20 | 11/37/115/115 | - |
| 14 | CLA | r | 519 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 15 | PQN | H | 2002 | - | - | 6/23/43/43 | 0/2/2/2 |
| 17 | BCR | r | 524 | - | - | 3/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1215 | 2 | 1/1/15/20 | 19/37/115/115 | - |
| 17 | BCR | m | 4104 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | B | 1220 | 2 | 1/1/13/20 | 9/25/103/115 | - |
| 18 | LHG | V | 5220 | - | - | 28/45/45/53 | - |
| 14 | CLA | c | 504 | - | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | A | 1109 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | 2 | 513 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | f | 1215 | 2 | 1/1/15/20 | 19/37/115/115 | - |
| 14 | CLA | r | 517 | - | - | 7/13/91/115 | - |
| 16 | SF4 | g | 3003 | 3 | - | - | 0/6/5/5 |
| 14 | CLA | 5 | 516 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | 5 | 506 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | 3 | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1225 | 2 | 1/1/15/20 | 7/37/115/115 | - |
| 14 | CLA | 4 | 505 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | e | 1137 | 1 | 1/1/14/20 | 18/31/109/115 | - |
| 14 | CLA | f | 1210 | 2 | 1/1/15/20 | 20/37/115/115 | - |
| 18 | LHG | G | 5004 | - | - | 18/39/39/53 | - |
| 20 | LMG | T | 5104 | - | - | 13/27/47/70 | 0/1/1/1 |
| 14 | CLA | B | 1202 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 19 | LMU | G | 1849 | - | - | 6/14/34/61 | 0/1/1/2 |
| 17 | BCR | T | 4015 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1117 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 15 | PQN | B | 2002 | - | - | 6/23/43/43 | 0/2/2/2 |
| 14 | CLA | f | 1225 | 2 | 1/1/15/20 | 7/37/115/115 | - |
| 14 | CLA | 2 | 511 | 13 | 1/1/11/20 | 4/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | 5 | 512 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | q | 508 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | H | 1222 | 23 | 1/1/12/20 | 2/19/97/115 | - |
| 14 | CLA | e | 1103 | 1 | 1/1/15/20 | 21/37/115/115 | - |
| 21 | SQD | d | 822 | - | - | 7/19/39/69 | 0/1/1/1 |
| 14 | CLA | f | 1222 | 23 | 1/1/12/20 | 2/19/97/115 | - |
| 14 | CLA | B | 1214 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | q | 513 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | A | 4002 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | R | 1301 | 23 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | B | 1023 | - | 1/1/15/20 | 10/37/115/115 | - |
| 19 | LMU | T | 5105 | - | - | 9/13/33/61 | 0/1/1/2 |
| 14 | CLA | v | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | a | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1124 | 23 | 1/1/14/20 | 11/31/109/115 | - |
| 19 | LMU | G | 1848 | - | - | 7/21/61/61 | 0/2/2/2 |
| 14 | CLA | e | 1136 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | e | 1114 | 23 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | 5 | 502 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | Z | 521 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | 4 | 509 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | r | 523 | - | - | 6/29/63/63 | 0/2/2/2 |
| 17 | BCR | u | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 17 | BCR | G | 4003 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | R | 4016 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | q | 510 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | B | 1229 | 2 | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | B | 1226 | 2 | 1/1/13/20 | 7/25/103/115 | - |
| 14 | CLA | u | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | c | 512 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 15 | PQN | G | 2001 | - | - | 14/23/43/43 | 0/2/2/2 |
| 17 | BCR | G | 4008 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | a | 510 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | 5 | 513 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | r | 509 | 13 | 1/1/15/20 | 4/37/115/115 | - |
| 14 | CLA | Y | 509 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | K | 4104 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1115 | 1 | 1/1/14/20 | 10/31/109/115 | - |
| 14 | CLA | e | 1116 | 1 | 1/1/14/20 | 9/31/109/115 | - |
| 18 | LHG | n | 5221 | - | - | 31/53/53/53 | - |
| 18 | LHG | A | 5003 | 14 | - | 17/44/44/53 | - |
| 14 | CLA | K | 1401 | - | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | f | 1021 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | d | 510 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | n | 1502 | 10 | 1/1/15/20 | 8/37/115/115 | - |
| 18 | LHG | A | 5004 | - | - | 18/39/39/53 | - |
| 14 | CLA | b | 510 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | b | 507 | - | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | 5 | 511 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | a | 507 | - | 1/1/11/20 | 5/13/91/115 | - |
| 19 | LMU | J | 5105 | - | - | 9/13/33/61 | 0/1/1/2 |
| 14 | CLA | 2 | 505 | 13 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | B | 1215 | 2 | 1/1/15/20 | 19/37/115/115 | - |
| 14 | CLA | e | 1102 | 1 | 1/1/13/20 | 7/25/103/115 | - |
| 14 | CLA | Z | 504 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | e | 1131 | 1 | 1/1/15/20 | 6/37/115/115 | - |
| 18 | LHG | e | 5002 | - | - | 22/47/47/53 | - |
| 21 | SQD | 1 | 822 | - | - | 10/27/47/69 | 0/1/1/1 |
| 17 | BCR | n | 4019 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | j | 1302 | 6 | 1/1/11/20 | 7/13/91/115 | - |
| 21 | SQD | r | 822 | - | - | 7/22/42/69 | 0/1/1/1 |
| 14 | CLA | 2 | 510 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | s | 506 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | c | 510 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | B | 1238 | 23 | 1/1/15/20 | 4/37/115/115 | - |
| 14 | CLA | Z | 507 | - | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | G | 1139 | 23 | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CLA | c | 513 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17 | BCR | Y | 523 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1210 | 2 | 1/1/15/20 | 20/37/115/115 | - |
| 17 | BCR | 2 | 523 | - | - | 6/29/63/63 | 0/2/2/2 |
| 17 | BCR | e | 4001 | - | - | 8/29/63/63 | 0/2/2/2 |
| 17 | BCR | s | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 17 | BCR | L | 4219 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | SQD | B | 1852 | - | - | 18/35/55/69 | 0/1/1/1 |
| 14 | CLA | 4 | 517 | - | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | f | 4010 | - | - | 7/29/63/63 | 0/2/2/2 |
| 17 | BCR | u | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | 4 | 501 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | n | 4219 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | SQD | f | 1852 | - | - | 18/35/55/69 | 0/1/1/1 |
| 14 | CLA | 2 | 519 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | B | 1231 | 23 | 1/1/15/20 | 8/37/115/115 | - |
| 14 | CLA | v | 516 | 13 | 1/1/11/20 | 9/13/91/115 | - |
| 18 | LHG | H | 1855 | - | - | 24/45/45/53 | - |
| 14 | CLA | r | 512 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | 3 | 504 | - | 1/1/11/20 | 5/13/91/115 | - |
| 18 | LHG | f | 1855 | - | - | 24/45/45/53 | - |
| 17 | BCR | J | 4015 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | 3 | 507 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | u | 504 | - | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | G | 1106 | 1 | 1/1/15/20 | 21/37/115/115 | - |
| 14 | CLA | 6 | 501 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | q | 516 | 13 | 1/1/11/20 | 12/13/91/115 | - |
| 17 | BCR | B | 4010 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1127 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | V | 1501 | 10 | 1/1/14/20 | 9/31/109/115 | - |
| 14 | CLA | t | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 16 | SF4 | N | 3002 | 3 | - | - | 0/6/5/5 |
| 14 | CLA | H | 1205 | 2 | 1/1/15/20 | 8/37/115/115 | - |
| 15 | PQN | e | 2001 | - | - | 14/23/43/43 | 0/2/2/2 |
| 14 | CLA | c | 502 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17 | BCR | 1 | 524 | - | - | 2/29/63/63 | 0/2/2/2 |
| 18 | LHG | e | 5005 | - | - | 28/47/47/53 | - |
| 14 | CLA | e | 1105 | 1 | 1/1/13/20 | 7/25/103/115 | - |
| 14 | CLA | Y | 518 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 18 | LHG | G | 5008 | - | - | 18/39/39/53 | - |
| 18 | LHG | k | 5001 | - | - | 25/52/52/53 | - |
| 21 | SQD | 3 | 822 | - | - | 9/23/43/69 | 0/1/1/1 |
| 14 | CLA | Y | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | 3 | 506 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 18 | LHG | e | 5001 | - | - | 23/53/53/53 | - |
| 14 | CLA | U | 1103 | 9 | 1/1/11/20 | 8/17/95/115 | - |
| 14 | CLA | A | 1111 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CLA | B | 1234 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | G | 1133 | 1 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | f | 1228 | 2 | 1/1/13/20 | 6/25/103/115 | - |
| 17 | BCR | 4 | 523 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1227 | 2 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | v | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | 1 | 508 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | Z | 506 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | e | 1118 | 1 | 1/1/14/20 | 8/31/109/115 | - |
| 14 | CLA | r | 506 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | l | 1302 | 8 | 1/1/13/20 | 12/25/103/115 | - |
| 17 | BCR | e | 4008 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | 2 | 518 | 13 | 1/1/13/20 | 14/25/103/115 | - |
| 14 | CLA | 5 | 510 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | s | 518 | 13 | 1/1/13/20 | 9/25/103/115 | - |
| 14 | CLA | f | 1227 | 2 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | H | 1230 | 2 | 1/1/14/20 | 10/31/109/115 | - |
| 14 | CLA | e | 1011 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | f | 1230 | 2 | 1/1/14/20 | 10/31/109/115 | - |
| 17 | BCR | A | 4001 | - | - | 8/29/63/63 | 0/2/2/2 |
| 14 | CLA | t | 516 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | Z | 516 | 13 | - | 6/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | H | 1229 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | A | 1128 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | H | 1203 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | r | 511 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | A | 1114 | 23 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | l | 518 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | c | 524 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | SQD | 5 | 822 | - | - | 3/19/39/69 | 0/1/1/1 |
| 17 | BCR | S | 4018 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | G | 1130 | 1 | 1/1/13/20 | 7/27/105/115 | - |
| 14 | CLA | t | 512 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 18 | LHG | A | 5007 | - | - | 23/51/51/53 | - |
| 14 | CLA | l | 513 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | H | 1208 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | u | 510 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | A | 1105 | 1 | 1/1/13/20 | 7/25/103/115 | - |
| 17 | BCR | v | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1140 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 18 | LHG | G | 5001 | - | - | 23/53/53/53 | - |
| 14 | CLA | 5 | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | n | 4022 | - | - | 3/29/63/63 | 0/2/2/2 |
| 14 | CLA | n | 1503 | 23 | 1/1/14/20 | 10/31/109/115 | - |
| 14 | CLA | e | 1139 | 23 | 1/1/15/20 | 18/37/115/115 | - |
| 18 | LHG | e | 5006 | - | - | 26/44/44/53 | - |
| 14 | CLA | Z | 512 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | l | 507 | - | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | e | 1113 | 1 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | s | 519 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | 4 | 522 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | r | 508 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | J | 1302 | 8 | 1/1/13/20 | 12/25/103/115 | - |
| 14 | CLA | t | 503 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | 3 | 516 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | T | 4012 | - | - | 9/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | Z | 508 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 17 | BCR | a | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | a | 518 | 13 | 1/1/13/20 | 9/25/103/115 | - |
| 14 | CLA | b | 519 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | 3 | 512 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | u | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | B | 1205 | 2 | 1/1/15/20 | 8/37/115/115 | - |
| 14 | CLA | v | 505 | 13 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | v | 509 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | G | 1111 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CLA | d | 518 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 4 | 516 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | G | 1132 | 1 | 1/1/15/20 | 16/37/115/115 | - |
| 14 | CLA | A | 1140 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 18 | LHG | H | 1842 | 14 | - | 19/41/41/53 | - |
| 14 | CLA | d | 511 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | H | 1211 | 2 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | f | 1202 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | 6 | 503 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | m | 1105 | 9 | 1/1/11/20 | 8/13/91/115 | - |
| 17 | BCR | L | 4019 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | Z | 513 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | B | 1222 | 23 | 1/1/12/20 | 2/19/97/115 | - |
| 17 | BCR | L | 4020 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | 3 | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | A | 1137 | 1 | 1/1/14/20 | 18/31/109/115 | - |
| 14 | CLA | B | 1223 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | t | 502 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 18 | LHG | A | 5005 | - | - | 28/47/47/53 | - |
| 14 | CLA | r | 516 | 13 | - | 6/13/91/115 | - |
| 17 | BCR | H | 4017 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1118 | 1 | 1/1/14/20 | 8/31/109/115 | - |
| 19 | LMU | e | 1848 | - | - | 7/21/61/61 | 0/2/2/2 |
| 14 | CLA | 3 | 508 | 13 | 1/1/11/20 | 2/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | H | 1231 | 23 | 1/1/15/20 | 8/37/115/115 | - |
| 17 | BCR | H | 4006 | - | - | 4/29/63/63 | 0/2/2/2 |
| 17 | BCR | H | 4009 | - | - | 1/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1208 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | a | 508 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | e | 1237 | 23 | 1/1/15/20 | 23/37/115/115 | - |
| 14 | CLA | H | 1224 | 2 | 1/1/14/20 | 7/31/109/115 | - |
| 17 | BCR | v | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | v | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 17 | BCR | f | 4006 | - | - | 4/29/63/63 | 0/2/2/2 |
| 18 | LHG | B | 1855 | - | - | 24/45/45/53 | - |
| 14 | CLA | 3 | 513 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | A | 1135 | 1 | 1/1/13/20 | 10/25/103/115 | - |
| 14 | CLA | f | 1224 | 2 | 1/1/14/20 | 7/31/109/115 | - |
| 14 | CLA | j | 1301 | 23 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | e | 1801 | 18 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | e | 1127 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | H | 1023 | - | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | A | 1112 | 1 | 1/1/12/20 | 2/19/97/115 | - |
| 14 | CLA | n | 1501 | 10 | 1/1/14/20 | 9/31/109/115 | - |
| 14 | CLA | b | 502 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | H | 1213 | 2 | 1/1/14/20 | 11/33/111/115 | - |
| 14 | CLA | d | 509 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | A | 1013 | - | 1/1/15/20 | 13/37/115/115 | - |
| 17 | BCR | V | 4020 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | c | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | Y | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | q | 518 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | B | 4009 | - | - | 1/29/63/63 | 0/2/2/2 |
| 14 | CLA | 1 | 501 | 13 | 1/1/11/20 | 9/13/91/115 | - |
| 14 | CLA | B | 1224 | 2 | 1/1/14/20 | 7/31/109/115 | - |
| 14 | CLA | B | 1209 | 2 | 1/1/12/20 | 9/23/101/115 | - |
| 14 | CLA | q | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | G | 4011 | - | - | 13/29/63/63 | 0/2/2/2 |
| 14 | CLA | G | 1013 | - | 1/1/15/20 | 14/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 18 | LHG | L | 5220 | - | - | 28/45/45/53 | - |
| 14 | CLA | H | 1236 | 2 | 1/1/12/20 | 3/19/97/115 | - |
| 14 | CLA | v | 518 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | V | 1502 | 10 | 1/1/15/20 | 8/37/115/115 | - |
| 17 | BCR | u | 524 | - | - | 2/29/63/63 | 0/2/2/2 |
| 18 | LHG | I | 5001 | - | - | 25/52/52/53 | - |
| 14 | CLA | e | 1101 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 19 | LMU | e | 1849 | - | - | 6/14/34/61 | 0/1/1/2 |
| 14 | CLA | G | 1112 | 1 | 1/1/12/20 | 2/19/97/115 | - |
| 14 | CLA | f | 1214 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | f | 1219 | 2 | 1/1/14/20 | 18/35/113/115 | - |
| 14 | CLA | q | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 2 | 516 | 13 | - | 6/13/91/115 | - |
| 14 | CLA | s | 516 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | A | 1237 | 23 | 1/1/15/20 | 22/37/115/115 | - |
| 17 | BCR | 5 | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 17 | BCR | d | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 16 | SF4 | A | 3001 | 1,2 | - | - | 0/6/5/5 |
| 14 | CLA | B | 1236 | 2 | 1/1/12/20 | 3/19/97/115 | - |
| 14 | CLA | a | 519 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | A | 1801 | 18 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | A | 1122 | 1 | 1/1/14/20 | 12/31/109/115 | - |
| 17 | BCR | a | 524 | - | - | 5/29/63/63 | 0/2/2/2 |
| 17 | BCR | e | 4002 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | Y | 502 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | b | 501 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | U | 1401 | - | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | H | 1218 | 2 | 1/1/14/20 | 7/31/109/115 | - |
| 14 | CLA | H | 1228 | 2 | 1/1/13/20 | 6/25/103/115 | - |
| 17 | BCR | f | 4017 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | c | 501 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | d | 524 | - | - | 5/29/63/63 | 0/2/2/2 |
| 20 | LMG | J | 5104 | - | - | 13/27/47/70 | 0/1/1/1 |
| 14 | CLA | Z | 519 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | f | 1231 | 23 | 1/1/15/20 | 8/37/115/115 | - |
| 14 | CLA | l | 517 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | Y | 507 | - | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | H | 1226 | 2 | 1/1/13/20 | 7/25/103/115 | - |
| 14 | CLA | c | 506 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | d | 501 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | s | 504 | - | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | u | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | l | 509 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 18 | LHG | n | 5220 | - | - | 28/45/45/53 | - |
| 14 | CLA | 6 | 518 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | Y | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | f | 1207 | 2 | 1/1/15/20 | 16/37/115/115 | - |
| 17 | BCR | B | 4017 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | B | 1206 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | 2 | 503 | 13 | 1/1/15/20 | 9/37/115/115 | - |
| 17 | BCR | c | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | G | 1126 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 19 | LMU | A | 1849 | - | - | 6/14/34/61 | 0/1/1/2 |
| 14 | CLA | B | 1218 | 2 | 1/1/14/20 | 7/31/109/115 | - |
| 18 | LHG | A | 5002 | - | - | 22/47/47/53 | - |
| 14 | CLA | t | 505 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | 2 | 521 | - | - | 4/29/63/63 | 0/2/2/2 |
| 17 | BCR | b | 521 | - | - | 10/29/63/63 | 0/2/2/2 |
| 14 | CLA | c | 511 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | Y | 513 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | 3 | 510 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | A | 1120 | 1 | 1/1/12/20 | 11/19/97/115 | - |
| 17 | BCR | a | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1139 | 23 | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CLA | r | 505 | 13 | 1/1/15/20 | 14/37/115/115 | - |
| 18 | LHG | e | 5009 | - | - | 28/46/46/53 | - |
| 14 | CLA | f | 1232 | 23 | 1/1/13/20 | 6/25/103/115 | - |
| 14 | CLA | v | 513 | 13 | 1/1/11/20 | 3/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22 | FMN | P | 170 | - | - | 0/18/18/18 | 0/3/3/3 |
| 14 | CLA | e | 1129 | 1 | 1/1/12/20 | 8/23/101/115 | - |
| 19 | LMU | A | 1848 | - | - | 7/21/61/61 | 0/2/2/2 |
| 17 | BCR | d | 521 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | 6 | 517 | - | 1/1/11/20 | 10/13/91/115 | - |
| 17 | BCR | 1 | 522 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | a | 517 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | m | 1401 | - | 1/1/13/20 | 8/25/103/115 | - |
| 17 | BCR | 1 | 523 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | 6 | 509 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | r | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | A | 1107 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 17 | BCR | d | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 17 | BCR | f | 4009 | - | - | 1/29/63/63 | 0/2/2/2 |
| 17 | BCR | V | 4019 | - | - | 6/29/63/63 | 0/2/2/2 |
| 17 | BCR | J | 4012 | - | - | 9/29/63/63 | 0/2/2/2 |
| 17 | BCR | Y | 524 | - | - | 2/29/63/63 | 0/2/2/2 |
| 17 | BCR | l | 4012 | - | - | 9/29/63/63 | 0/2/2/2 |
| 18 | LHG | G | 5009 | - | - | 28/46/46/53 | - |
| 14 | CLA | q | 501 | 13 | 1/1/11/20 | 9/13/91/115 | - |
| 14 | CLA | A | 1117 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | d | 517 | - | 1/1/11/20 | 10/13/91/115 | - |
| 14 | CLA | H | 1216 | 23 | 1/1/14/20 | 11/31/109/115 | - |
| 17 | BCR | 5 | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | b | 512 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | 2 | 508 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | 6 | 504 | - | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | e | 1121 | 1 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | F | 1302 | 6 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | s | 508 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | Z | 517 | - | - | 7/13/91/115 | - |
| 17 | BCR | l | 4015 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | U | 1105 | 9 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | G | 1119 | 23 | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | Z | 509 | 13 | 1/1/15/20 | 3/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | e | 1106 | 1 | 1/1/15/20 | 21/37/115/115 | - |
| 14 | CLA | u | 518 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | A | 4008 | - | - | 7/29/63/63 | 0/2/2/2 |
| 17 | BCR | 1 | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1221 | 23 | 1/1/14/20 | 14/34/112/115 | - |
| 21 | SQD | H | 1852 | - | - | 18/35/55/69 | 0/1/1/1 |
| 17 | BCR | f | 4004 | - | - | 8/29/63/63 | 0/2/2/2 |
| 14 | CLA | G | 1102 | 1 | 1/1/13/20 | 7/25/103/115 | - |
| 17 | BCR | 2 | 524 | - | - | 3/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1126 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 17 | BCR | q | 521 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1223 | 2 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | B | 1240 | 18 | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | 5 | 509 | 13 | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | B | 1232 | 23 | 1/1/13/20 | 6/25/103/115 | - |
| 14 | CLA | 5 | 507 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | r | 503 | 13 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | e | 1133 | 1 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | 4 | 502 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | H | 4010 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | Y | 510 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | l | 1303 | 8 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | m | 1103 | 9 | 1/1/11/20 | 8/17/95/115 | - |
| 14 | CLA | G | 1127 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 17 | BCR | H | 4014 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | q | 517 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 6 | 516 | 13 | 1/1/11/20 | 9/13/91/115 | - |
| 14 | CLA | H | 1204 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | H | 1217 | 2 | 1/1/14/20 | 12/31/109/115 | - |
| 14 | CLA | H | 1201 | 2 | 1/1/14/20 | 8/31/109/115 | - |
| 14 | CLA | K | 1105 | 9 | 1/1/11/20 | 8/13/91/115 | - |
| 17 | BCR | f | 4014 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1204 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | f | 1217 | 2 | 1/1/14/20 | 12/31/109/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | a | 504 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | s | 512 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | u | 501 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | T | 4013 | - | - | 4/29/63/63 | 0/2/2/2 |
| 17 | BCR | e | 4011 | - | - | 13/29/63/63 | 0/2/2/2 |
| 17 | BCR | v | 524 | - | - | 5/29/63/63 | 0/2/2/2 |
| 17 | BCR | M | 4021 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | G | 1107 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 22 | FMN | p | 170 | - | - | 0/18/18/18 | 0/3/3/3 |
| 14 | CLA | v | 504 | - | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | u | 506 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 18 | LHG | B | 1842 | 14 | - | 19/41/41/53 | - |
| 17 | BCR | B | 4014 | - | - | 7/29/63/63 | 0/2/2/2 |
| 14 | CLA | d | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | v | 510 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | B | 1204 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | B | 1217 | 2 | 1/1/14/20 | 12/31/109/115 | - |
| 14 | CLA | H | 1239 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | G | 1138 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | H | 1234 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | f | 1216 | 23 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | q | 502 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | c | 505 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | u | 507 | - | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | 5 | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1022 | 23 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | f | 1238 | 23 | 1/1/15/20 | 4/37/115/115 | - |
| 14 | CLA | G | 1131 | 1 | 1/1/15/20 | 6/37/115/115 | - |
| 14 | CLA | s | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | t | 506 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | Z | 518 | 13 | 1/1/13/20 | 14/25/103/115 | - |
| 14 | CLA | a | 506 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | a | 516 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | f | 1239 | 2 | 1/1/15/20 | 14/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | q | 507 | - | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | s | 517 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | t | 513 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | A | 1133 | 1 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | A | 1136 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | u | 511 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | f | 1218 | 2 | 1/1/14/20 | 7/31/109/115 | - |
| 17 | BCR | 5 | 524 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1111 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 17 | BCR | V | 4022 | - | - | 3/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1229 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | a | 512 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | d | 504 | - | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | f | 1221 | 23 | 1/1/14/20 | 14/34/112/115 | - |
| 18 | LHG | L | 5218 | - | - | 19/41/41/53 | - |
| 14 | CLA | r | 513 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | e | 1108 | 1 | 1/1/12/20 | 14/24/102/115 | - |
| 14 | CLA | s | 513 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 21 | SQD | V | 5216 | - | - | 17/41/61/69 | 0/1/1/1 |
| 14 | CLA | a | 511 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | d | 507 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | d | 516 | 13 | 1/1/11/20 | 9/13/91/115 | - |
| 16 | SF4 | g | 3002 | 3 | - | - | 0/6/5/5 |
| 14 | CLA | B | 1221 | 23 | 1/1/14/20 | 14/34/112/115 | - |
| 14 | CLA | A | 1116 | 1 | 1/1/14/20 | 9/31/109/115 | - |
| 14 | CLA | G | 1011 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | G | 1801 | 18 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 2 | 504 | - | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | B | 4005 | - | - | 6/29/63/63 | 0/2/2/2 |
| 17 | BCR | e | 4007 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | 4 | 518 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | G | 1108 | 1 | 1/1/12/20 | 14/24/102/115 | - |
| 18 | LHG | G | 5005 | - | - | 28/47/47/53 | - |
| 17 | BCR | b | 524 | - | - | 4/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | Y | 504 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | A | 1022 | 23 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | 2 | 507 | - | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | c | 507 | - | 1/1/11/20 | 7/13/91/115 | - |
| 21 | SQD | c | 822 | - | - | 3/19/39/69 | 0/1/1/1 |
| 17 | BCR | V | 4219 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | SQD | L | 5216 | - | - | 17/41/61/69 | 0/1/1/1 |
| 14 | CLA | q | 509 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | q | 524 | - | - | 2/29/63/63 | 0/2/2/2 |
| 18 | LHG | S | 5001 | - | - | 25/52/52/53 | - |
| 14 | CLA | e | 1110 | 1 | 1/1/12/20 | 10/23/101/115 | - |
| 14 | CLA | G | 1134 | 1 | 1/1/13/20 | 9/27/105/115 | - |
| 14 | CLA | B | 1201 | 2 | 1/1/14/20 | 8/31/109/115 | - |
| 14 | CLA | G | 1114 | 23 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | G | 1101 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 21 | SQD | s | 822 | - | - | 9/23/43/69 | 0/1/1/1 |
| 14 | CLA | f | 1209 | 2 | 1/1/12/20 | 9/23/101/115 | - |
| 14 | CLA | f | 1234 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | 3 | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | k | 4018 | - | - | 0/29/63/63 | 0/2/2/2 |
| 18 | LHG | G | 5006 | - | - | 26/44/44/53 | - |
| 14 | CLA | Y | 516 | 13 | 1/1/11/20 | 12/13/91/115 | - |
| 14 | CLA | G | 1022 | 23 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | 5 | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | a | 513 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 16 | SF4 | C | 3003 | 3 | - | - | 0/6/5/5 |
| 14 | CLA | G | 1113 | 1 | 1/1/11/20 | 6/13/91/115 | - |
| 21 | SQD | b | 822 | - | - | 10/19/39/69 | 0/1/1/1 |
| 14 | CLA | 6 | 505 | 13 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | A | 1124 | 23 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | 1 | 504 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | e | 1135 | 1 | 1/1/13/20 | 10/25/103/115 | - |
| 17 | BCR | J | 4013 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | Y | 512 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | t | 510 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | B | 1239 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 17 | BCR | c | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 18 | LHG | V | 5221 | - | - | 31/53/53/53 | - |
| 19 | LMU | H | 1843 | - | - | 12/21/61/61 | 0/2/2/2 |
| 14 | CLA | 4 | 519 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 14 | CLA | e | 1112 | 1 | 1/1/12/20 | 2/19/97/115 | - |
| 14 | CLA | 3 | 509 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | A | 1101 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 14 | CLA | H | 1202 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | H | 1209 | 2 | 1/1/12/20 | 9/23/101/115 | - |
| 14 | CLA | u | 517 | - | 1/1/11/20 | 10/13/91/115 | - |
| 14 | CLA | 2 | 501 | 13 | 1/1/14/20 | 11/31/109/115 | - |
| 17 | BCR | s | 524 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | 5 | 504 | - | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | A | 1113 | 1 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | u | 509 | 13 | 1/1/15/20 | 13/37/115/115 | - |
| 17 | BCR | Z | 524 | - | - | 3/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1220 | 2 | 1/1/13/20 | 9/25/103/115 | - |
| 14 | CLA | e | 1109 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | 6 | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | 1 | 516 | 13 | 1/1/11/20 | 12/13/91/115 | - |
| 14 | CLA | s | 510 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | Y | 501 | 13 | 1/1/11/20 | 9/13/91/115 | - |
| 21 | SQD | 2 | 822 | - | - | 7/22/42/69 | 0/1/1/1 |
| 18 | LHG | G | 5002 | - | - | 22/47/47/53 | - |
| 14 | CLA | 1 | 512 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | e | 1125 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | e | 1130 | 1 | 1/1/13/20 | 7/27/105/115 | - |
| 14 | CLA | v | 501 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 18 | LHG | A | 5008 | - | - | 18/39/39/53 | - |
| 14 | CLA | B | 1208 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | A | 1110 | 1 | 1/1/12/20 | 10/23/101/115 | - |
| 14 | CLA | B | 1228 | 2 | 1/1/13/20 | 6/25/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 18 | LHG | e | 5004 | - | - | 18/39/39/53 | - |
| 17 | BCR | G | 4002 | - | - | 0/29/63/63 | 0/2/2/2 |
| 17 | BCR | j | 4016 | - | - | 2/29/63/63 | 0/2/2/2 |
| 17 | BCR | e | 4003 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | SQD | 6 | 822 | - | - | 7/19/39/69 | 0/1/1/1 |
| 14 | CLA | Z | 505 | 13 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | L | 1503 | 23 | 1/1/14/20 | 10/31/109/115 | - |
| 14 | CLA | b | 504 | - | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | e | 1134 | 1 | 1/1/13/20 | 9/27/105/115 | - |
| 14 | CLA | t | 519 | 13 | 1/1/11/20 | 8/13/91/115 | - |
| 17 | BCR | 3 | 524 | - | - | 5/29/63/63 | 0/2/2/2 |
| 21 | SQD | q | 822 | - | - | 10/27/47/69 | 0/1/1/1 |
| 14 | CLA | s | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 2 | 517 | - | - | 7/13/91/115 | - |
| 16 | SF4 | G | 3001 | 1,2 | - | - | 0/6/5/5 |
| 14 | CLA | b | 506 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | 1 | 503 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | G | 1109 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | v | 511 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | 5 | 501 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | a | 501 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | b | 503 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | 6 | 512 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | B | 1212 | 2 | 1/1/12/20 | 8/21/99/115 | - |
| 18 | LHG | A | 5006 | - | - | 26/44/44/53 | - |
| 14 | CLA | c | 508 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | W | 4021 | - | - | 6/29/63/63 | 0/2/2/2 |
| 18 | LHG | V | 5218 | - | - | 19/41/41/53 | - |
| 14 | CLA | r | 510 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | f | 1205 | 2 | 1/1/15/20 | 8/37/115/115 | - |
| 14 | CLA | Z | 510 | 13 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | L | 4022 | - | - | 3/29/63/63 | 0/2/2/2 |
| 21 | SQD | t | 822 | - | - | 10/19/39/69 | 0/1/1/1 |
| 16 | SF4 | N | 3003 | 3 | - | - | 0/6/5/5 |
| 14 | CLA | 6 | 507 | - | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | f | 1206 | 2 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | G | 1117 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | q | 504 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | a | 505 | 13 | 1/1/13/20 | 11/25/103/115 | - |
| 14 | CLA | d | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | H | 1207 | 2 | 1/1/15/20 | 16/37/115/115 | - |
| 14 | CLA | l | 502 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 17 | BCR | t | 521 | - | - | 10/29/63/63 | 0/2/2/2 |
| 19 | LMU | l | 5105 | - | - | 9/13/33/61 | 0/1/1/2 |
| 14 | CLA | r | 504 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | 4 | 503 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | H | 1232 | 23 | 1/1/13/20 | 6/25/103/115 | - |
| 14 | CLA | e | 1107 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | G | 1104 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 17 | BCR | U | 4104 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | R | 1302 | 6 | 1/1/11/20 | 7/13/91/115 | - |
| 17 | BCR | B | 4006 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | r | 507 | - | 1/1/11/20 | 8/13/91/115 | - |
| 18 | LHG | n | 5218 | - | - | 19/41/41/53 | - |
| 14 | CLA | G | 1124 | 23 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | 6 | 511 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 21 | SQD | u | 822 | - | - | 3/19/39/69 | 0/1/1/1 |
| 17 | BCR | 6 | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | 4 | 513 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | H | 1012 | 23 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | 5 | 517 | - | 1/1/11/20 | 10/13/91/115 | - |
| 19 | LMU | f | 1843 | - | - | 12/21/61/61 | 0/2/2/2 |
| 14 | CLA | e | 1119 | 23 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | H | 1212 | 2 | 1/1/12/20 | 8/21/99/115 | - |
| 14 | CLA | q | 506 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | t | 524 | - | - | 4/29/63/63 | 0/2/2/2 |
| 20 | LMG | H | 5002 | - | - | 24/48/68/70 | 0/1/1/1 |
| 14 | CLA | f | 1012 | 23 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | b | 516 | 13 | 1/1/11/20 | 7/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | B | 1213 | 2 | 1/1/14/20 | 11/33/111/115 | - |
| 14 | CLA | e | 1104 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | f | 1212 | 2 | 1/1/12/20 | 8/21/99/115 | - |
| 14 | CLA | f | 1213 | 2 | 1/1/14/20 | 11/33/111/115 | - |
| 14 | CLA | A | 1130 | 1 | 1/1/13/20 | 7/27/105/115 | - |
| 17 | BCR | 4 | 521 | - | - | 10/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1104 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | T | 1302 | 8 | 1/1/13/20 | 12/25/103/115 | - |
| 14 | CLA | q | 512 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 20 | LMG | l | 5104 | - | - | 13/27/47/70 | 0/1/1/1 |
| 14 | CLA | d | 505 | 13 | 1/1/15/20 | 15/37/115/115 | - |
| 14 | CLA | H | 1238 | 23 | 1/1/15/20 | 4/37/115/115 | - |
| 14 | CLA | f | 1226 | 2 | 1/1/13/20 | 7/25/103/115 | - |
| 14 | CLA | A | 1103 | 1 | 1/1/15/20 | 21/37/115/115 | - |
| 14 | CLA | H | 1021 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | a | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | B | 1210 | 2 | 1/1/15/20 | 20/37/115/115 | - |
| 14 | CLA | G | 1110 | 1 | 1/1/12/20 | 10/23/101/115 | - |
| 14 | CLA | V | 1503 | 23 | 1/1/14/20 | 10/31/109/115 | - |
| 18 | LHG | G | 5003 | 14 | - | 17/44/44/53 | - |
| 14 | CLA | q | 511 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 18 | LHG | e | 5007 | - | - | 23/51/51/53 | - |
| 14 | CLA | A | 1125 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | F | 1301 | 23 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | H | 1240 | 18 | 1/1/15/20 | 13/37/115/115 | - |
| 19 | LMU | B | 1843 | - | - | 12/21/61/61 | 0/2/2/2 |
| 17 | BCR | F | 4016 | - | - | 2/29/63/63 | 0/2/2/2 |
| 14 | CLA | d | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | G | 1135 | 1 | 1/1/13/20 | 10/25/103/115 | - |
| 14 | CLA | G | 1129 | 1 | 1/1/12/20 | 8/23/101/115 | - |
| 14 | CLA | s | 501 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | A | 4003 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1235 | 2 | 1/1/15/20 | 7/37/115/115 | - |
| 14 | CLA | Z | 502 | 13 | 1/1/11/20 | 1/13/91/115 | - |
| 14 | CLA | G | 1120 | 1 | 1/1/12/20 | 11/19/97/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | 1 | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | Y | 505 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | 3 | 518 | 13 | 1/1/13/20 | 9/25/103/115 | - |
| 21 | SQD | 4 | 822 | - | - | 10/19/39/69 | 0/1/1/1 |
| 14 | CLA | B | 1021 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 18 | LHG | L | 5221 | - | - | 31/53/53/53 | - |
| 14 | CLA | A | 1119 | 23 | 1/1/15/20 | 14/37/115/115 | - |
| 14 | CLA | c | 518 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | L | 1502 | 10 | 1/1/15/20 | 8/37/115/115 | - |
| 17 | BCR | c | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 18 | LHG | A | 5009 | - | - | 28/46/46/53 | - |
| 14 | CLA | J | 1303 | 8 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | v | 521 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | A | 1115 | 1 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | L | 1501 | 10 | 1/1/14/20 | 9/31/109/115 | - |
| 17 | BCR | A | 4007 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | t | 504 | - | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | s | 511 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | Y | 517 | - | 1/1/11/20 | 7/13/91/115 | - |
| 14 | CLA | u | 513 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 17 | BCR | G | 4007 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | H | 1223 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 14 | CLA | B | 1207 | 2 | 1/1/15/20 | 16/37/115/115 | - |
| 14 | CLA | Z | 511 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | 6 | 523 | - | - | 4/29/63/63 | 0/2/2/2 |
| 18 | LHG | G | 5007 | - | - | 23/51/51/53 | - |
| 14 | CLA | t | 507 | - | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | H | 1220 | 2 | 1/1/13/20 | 9/25/103/115 | - |
| 17 | BCR | n | 4020 | - | - | 4/29/63/63 | 0/2/2/2 |
| 17 | BCR | 4 | 524 | - | - | 4/29/63/63 | 0/2/2/2 |
| 14 | CLA | v | 517 | - | 1/1/11/20 | 10/13/91/115 | - |
| 14 | CLA | B | 1227 | 2 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | b | 511 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | 1 | 505 | 13 | 1/1/11/20 | 6/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14 | CLA | e | 1132 | 1 | 1/1/15/20 | 16/37/115/115 | - |
| 14 | CLA | 6 | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | B | 1211 | 2 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | A | 1121 | 1 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | G | 1103 | 1 | 1/1/15/20 | 21/37/115/115 | - |
| 14 | CLA | b | 517 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | f | 1211 | 2 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | A | 1102 | 1 | 1/1/13/20 | 7/25/103/115 | - |
| 14 | CLA | 4 | 504 | - | 1/1/11/20 | 4/13/91/115 | - |
| 17 | BCR | b | 522 | - | - | 4/29/63/63 | 0/2/2/2 |
| 18 | LHG | f | 1842 | 14 | - | 19/41/41/53 | - |
| 17 | BCR | I | 4018 | - | - | 0/29/63/63 | 0/2/2/2 |
| 14 | CLA | T | 1303 | 8 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | G | 1121 | 1 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | A | 1106 | 1 | 1/1/15/20 | 21/37/115/115 | - |
| 21 | SQD | Y | 822 | - | - | 10/27/47/69 | 0/1/1/1 |
| 20 | LMG | B | 5002 | - | - | 24/48/68/70 | 0/1/1/1 |
| 14 | CLA | t | 518 | 13 | 1/1/11/20 | 4/13/91/115 | - |
| 14 | CLA | 5 | 505 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 15 | PQN | f | 2002 | - | - | 6/23/43/43 | 0/2/2/2 |
| 17 | BCR | G | 4001 | - | - | 8/29/63/63 | 0/2/2/2 |
| 14 | CLA | e | 1128 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 14 | CLA | s | 509 | 13 | 1/1/11/20 | 2/13/91/115 | - |
| 14 | CLA | s | 505 | 13 | 1/1/13/20 | 11/25/103/115 | - |
| 14 | CLA | s | 507 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | e | 1138 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | 6 | 506 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | f | 1235 | 2 | 1/1/15/20 | 7/37/115/115 | - |
| 14 | CLA | v | 507 | - | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | G | 1115 | 1 | 1/1/14/20 | 11/31/109/115 | - |
| 14 | CLA | b | 509 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | b | 505 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 17 | BCR | H | 4005 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | 4 | 510 | 13 | 1/1/11/20 | 5/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 21 | SQD | a | 822 | - | - | 9/23/43/69 | 0/1/1/1 |
| 14 | CLA | A | 1129 | 1 | 1/1/12/20 | 8/23/101/115 | - |
| 14 | CLA | A | 1132 | 1 | 1/1/15/20 | 16/37/115/115 | - |
| 14 | CLA | G | 1125 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 14 | CLA | 5 | 519 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | q | 522 | - | - | 6/29/63/63 | 0/2/2/2 |
| 14 | CLA | f | 1203 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 21 | SQD | Z | 822 | - | - | 7/22/42/69 | 0/1/1/1 |
| 14 | CLA | B | 1235 | 2 | 1/1/15/20 | 7/37/115/115 | - |
| 14 | CLA | u | 516 | 13 | 1/1/11/20 | 5/13/91/115 | - |
| 14 | CLA | A | 1123 | 23 | 1/1/15/20 | 11/37/115/115 | - |
| 14 | CLA | G | 1105 | 1 | 1/1/13/20 | 8/25/103/115 | - |
| 14 | CLA | G | 1116 | 1 | 1/1/14/20 | 9/31/109/115 | - |
| 17 | BCR | A | 4011 | - | - | 13/29/63/63 | 0/2/2/2 |
| 14 | CLA | 4 | 507 | - | 1/1/11/20 | 6/13/91/115 | - |
| 17 | BCR | s | 522 | - | - | 5/29/63/63 | 0/2/2/2 |
| 14 | CLA | 2 | 509 | 13 | 1/1/15/20 | 3/37/115/115 | - |
| 18 | LHG | A | 5001 | - | - | 23/53/53/53 | - |
| 14 | CLA | d | 506 | 13 | 1/1/11/20 | 6/13/91/115 | - |
| 14 | CLA | c | 509 | 13 | 1/1/15/20 | 13/37/115/115 | - |
| 14 | CLA | 5 | 518 | 13 | 1/1/11/20 | 3/13/91/115 | - |
| 14 | CLA | u | 512 | 13 | 1/1/11/20 | 5/13/91/115 | - |

All (5009) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 15 | G | 2001 | PQN | C12-C13 | 8.46 | 1.53 | 1.33 |
| 15 | A | 2001 | PQN | C12-C13 | 8.44 | 1.53 | 1.33 |
| 15 | e | 2001 | PQN | C12-C13 | 8.44 | 1.53 | 1.33 |
| 15 | B | 2002 | PQN | C12-C13 | 8.38 | 1.53 | 1.33 |
| 15 | H | 2002 | PQN | C12-C13 | 8.38 | 1.53 | 1.33 |
| 15 | f | 2002 | PQN | C12-C13 | 8.37 | 1.53 | 1.33 |
| 15 | f | 2002 | PQN | O1-C1 | 7.94 | 1.40 | 1.23 |
| 15 | H | 2002 | PQN | O1-C1 | 7.93 | 1.40 | 1.23 |
| 15 | B | 2002 | PQN | O1-C1 | 7.93 | 1.40 | 1.23 |
| 14 | t | 504 | CLA | C4B-NB | 7.59 | 1.42 | 1.35 |
| 14 | t | 501 | CLA | C4B-NB | 7.56 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 15 | G | 2001 | PQN | O1-C1 | 7.55 | 1.39 | 1.23 |
| 15 | A | 2001 | PQN | O1-C1 | 7.55 | 1.39 | 1.23 |
| 14 | v | 513 | CLA | C4B-NB | 7.54 | 1.41 | 1.35 |
| 14 | b | 501 | CLA | C4B-NB | 7.54 | 1.41 | 1.35 |
| 15 | e | 2001 | PQN | O1-C1 | 7.53 | 1.39 | 1.23 |
| 14 | a | 517 | CLA | C4B-NB | 7.52 | 1.41 | 1.35 |
| 14 | G | 1101 | CLA | C4B-NB | 7.50 | 1.41 | 1.35 |
| 14 | 4 | 504 | CLA | C4B-NB | 7.49 | 1.41 | 1.35 |
| 14 | 4 | 501 | CLA | C4B-NB | 7.49 | 1.41 | 1.35 |
| 14 | e | 1101 | CLA | C4B-NB | 7.49 | 1.41 | 1.35 |
| 14 | t | 509 | CLA | C4B-NB | 7.46 | 1.41 | 1.35 |
| 14 | u | 517 | CLA | C4B-NB | 7.46 | 1.41 | 1.35 |
| 14 | 6 | 513 | CLA | C4B-NB | 7.45 | 1.41 | 1.35 |
| 14 | A | 1101 | CLA | C4B-NB | 7.44 | 1.41 | 1.35 |
| 14 | b | 513 | CLA | C4B-NB | 7.44 | 1.41 | 1.35 |
| 14 | 5 | 513 | CLA | C4B-NB | 7.43 | 1.41 | 1.35 |
| 14 | d | 513 | CLA | C4B-NB | 7.43 | 1.41 | 1.35 |
| 14 | s | 512 | CLA | C4B-NB | 7.43 | 1.41 | 1.35 |
| 14 | c | 517 | CLA | C4B-NB | 7.42 | 1.41 | 1.35 |
| 14 | s | 506 | CLA | C4B-NB | 7.41 | 1.41 | 1.35 |
| 14 | s | 517 | CLA | C4B-NB | 7.41 | 1.41 | 1.35 |
| 14 | 4 | 509 | CLA | C4B-NB | 7.41 | 1.41 | 1.35 |
| 14 | b | 504 | CLA | C4B-NB | 7.41 | 1.41 | 1.35 |
| 14 | l | 1303 | CLA | C4B-NB | 7.41 | 1.41 | 1.35 |
| 14 | b | 509 | CLA | C4B-NB | 7.40 | 1.41 | 1.35 |
| 14 | 3 | 506 | CLA | C4B-NB | 7.40 | 1.41 | 1.35 |
| 14 | u | 513 | CLA | C4B-NB | 7.40 | 1.41 | 1.35 |
| 14 | 3 | 517 | CLA | C4B-NB | 7.40 | 1.41 | 1.35 |
| 14 | b | 502 | CLA | C4B-NB | 7.40 | 1.41 | 1.35 |
| 14 | c | 513 | CLA | C4B-NB | 7.39 | 1.41 | 1.35 |
| 14 | m | 1105 | CLA | C4B-NB | 7.38 | 1.41 | 1.35 |
| 14 | 4 | 502 | CLA | C4B-NB | 7.38 | 1.41 | 1.35 |
| 14 | b | 506 | CLA | C4B-NB | 7.37 | 1.41 | 1.35 |
| 14 | 4 | 513 | CLA | C4B-NB | 7.36 | 1.41 | 1.35 |
| 14 | v | 511 | CLA | C4B-NB | 7.36 | 1.41 | 1.35 |
| 14 | a | 513 | CLA | C4B-NB | 7.36 | 1.41 | 1.35 |
| 14 | T | 1303 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 14 | 3 | 512 | CLA | C4B-NB | 7.35 | 1.41 | 1.35 |
| 14 | c | 516 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 14 | q | 506 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 14 | 5 | 517 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 14 | 4 | 506 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | 6 | 512 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 14 | a | 512 | CLA | C4B-NB | 7.34 | 1.41 | 1.35 |
| 14 | A | 1114 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 14 | t | 513 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 14 | s | 513 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 14 | u | 516 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 14 | G | 1114 | CLA | C4B-NB | 7.33 | 1.41 | 1.35 |
| 14 | e | 1114 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | K | 1105 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | t | 502 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | 2 | 512 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | d | 516 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | s | 504 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | Y | 506 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | 5 | 516 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | v | 516 | CLA | C4B-NB | 7.32 | 1.41 | 1.35 |
| 14 | a | 506 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 14 | u | 503 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 14 | J | 1303 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 14 | H | 1219 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 14 | u | 519 | CLA | C4B-NB | 7.31 | 1.41 | 1.35 |
| 14 | B | 1219 | CLA | C4B-NB | 7.30 | 1.41 | 1.35 |
| 14 | 6 | 516 | CLA | C4B-NB | 7.30 | 1.41 | 1.35 |
| 14 | Z | 512 | CLA | C4B-NB | 7.30 | 1.41 | 1.35 |
| 14 | U | 1105 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | d | 512 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | H | 1217 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | t | 506 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | u | 502 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | 1 | 506 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | Y | 504 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | 1 | 504 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | 2 | 504 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | 6 | 510 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | t | 503 | CLA | C4B-NB | 7.29 | 1.41 | 1.35 |
| 14 | 2 | 513 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | b | 511 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | 5 | 503 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | B | 1217 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | b | 517 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | v | 512 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | 6 | 511 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | q | 504 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | r | 504 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | r | 512 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | t | 516 | CLA | C4B-NB | 7.28 | 1.41 | 1.35 |
| 14 | 3 | 513 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 14 | v | 509 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 14 | H | 1236 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 14 | t | 511 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 14 | 6 | 509 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 14 | u | 504 | CLA | C4B-NB | 7.27 | 1.41 | 1.35 |
| 14 | f | 1219 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 14 | 1 | 513 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 14 | Y | 513 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 14 | 4 | 516 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 14 | c | 503 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 14 | f | 1217 | CLA | C4B-NB | 7.26 | 1.41 | 1.35 |
| 14 | Z | 506 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | Z | 513 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | b | 516 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | B | 1236 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 15 | A | 2001 | PQN | O4-C4 | 7.25 | 1.38 | 1.23 |
| 14 | a | 504 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | q | 510 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | 2 | 506 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | 3 | 504 | CLA | C4B-NB | 7.25 | 1.41 | 1.35 |
| 14 | r | 517 | CLA | C4B-NB | 7.24 | 1.41 | 1.35 |
| 15 | e | 2001 | PQN | O4-C4 | 7.24 | 1.38 | 1.23 |
| 14 | v | 510 | CLA | C4B-NB | 7.24 | 1.41 | 1.35 |
| 14 | 3 | 501 | CLA | C4B-NB | 7.24 | 1.41 | 1.35 |
| 15 | G | 2001 | PQN | O4-C4 | 7.24 | 1.38 | 1.23 |
| 14 | d | 509 | CLA | C4B-NB | 7.24 | 1.41 | 1.35 |
| 14 | 5 | 502 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | 5 | 519 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | Y | 518 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | c | 502 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | r | 513 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | s | 501 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | Z | 504 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | Y | 519 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | q | 519 | CLA | C4B-NB | 7.23 | 1.41 | 1.35 |
| 14 | d | 511 | CLA | C4B-NB | 7.22 | 1.41 | 1.35 |
| 14 | r | 516 | CLA | C4B-NB | 7.22 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | 2 | 516 | CLA | C4B-NB | 7.22 | 1.41 | 1.35 |
| 14 | 6 | 508 | CLA | C4B-NB | 7.21 | 1.41 | 1.35 |
| 14 | q | 513 | CLA | C4B-NB | 7.21 | 1.41 | 1.35 |
| 14 | c | 519 | CLA | C4B-NB | 7.21 | 1.41 | 1.35 |
| 14 | 4 | 517 | CLA | C4B-NB | 7.21 | 1.41 | 1.35 |
| 14 | Z | 516 | CLA | C4B-NB | 7.20 | 1.41 | 1.35 |
| 14 | 5 | 504 | CLA | C4B-NB | 7.20 | 1.41 | 1.35 |
| 14 | 4 | 503 | CLA | C4B-NB | 7.20 | 1.41 | 1.35 |
| 14 | d | 510 | CLA | C4B-NB | 7.20 | 1.41 | 1.35 |
| 14 | q | 501 | CLA | C4B-NB | 7.20 | 1.41 | 1.35 |
| 14 | 1 | 519 | CLA | C4B-NB | 7.19 | 1.41 | 1.35 |
| 14 | 4 | 511 | CLA | C4B-NB | 7.19 | 1.41 | 1.35 |
| 14 | q | 507 | CLA | C4B-NB | 7.19 | 1.41 | 1.35 |
| 14 | 6 | 501 | CLA | C4B-NB | 7.19 | 1.41 | 1.35 |
| 14 | d | 506 | CLA | C4B-NB | 7.19 | 1.41 | 1.35 |
| 14 | 6 | 506 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | c | 504 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | t | 512 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | 1 | 510 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | 1 | 518 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | v | 504 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | 3 | 509 | CLA | C4B-NB | 7.18 | 1.41 | 1.35 |
| 14 | a | 509 | CLA | C4B-NB | 7.17 | 1.41 | 1.35 |
| 14 | f | 1236 | CLA | C4B-NB | 7.17 | 1.41 | 1.35 |
| 14 | a | 502 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | t | 517 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | s | 511 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | Y | 517 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | q | 518 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | b | 512 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | Y | 501 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | b | 503 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | v | 506 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | r | 506 | CLA | C4B-NB | 7.16 | 1.41 | 1.35 |
| 14 | b | 519 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 14 | v | 501 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 14 | d | 501 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 14 | 1 | 507 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 14 | 1 | 501 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 14 | u | 518 | CLA | C4B-NB | 7.15 | 1.41 | 1.35 |
| 14 | 4 | 512 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |
| 14 | 6 | 507 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | 2 | 517 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |
| 14 | Y | 510 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |
| 14 | s | 509 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |
| 14 | 5 | 511 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |
| 14 | v | 519 | CLA | C4B-NB | 7.14 | 1.41 | 1.35 |
| 14 | t | 508 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 14 | Y | 512 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 14 | 4 | 519 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 14 | a | 501 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 14 | d | 508 | CLA | C4B-NB | 7.13 | 1.41 | 1.35 |
| 14 | Y | 503 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | Y | 507 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | 3 | 502 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | 4 | 505 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | c | 511 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | 1 | 512 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | u | 511 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | v | 508 | CLA | C4B-NB | 7.12 | 1.41 | 1.35 |
| 14 | V | 1501 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 14 | b | 505 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 14 | r | 519 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 14 | v | 507 | CLA | C4B-NB | 7.11 | 1.41 | 1.35 |
| 14 | 6 | 519 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | 1 | 503 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | q | 512 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | 1 | 517 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | 3 | 511 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | d | 502 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | 2 | 519 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | t | 505 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | 6 | 504 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | 6 | 518 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | Z | 517 | CLA | C4B-NB | 7.10 | 1.41 | 1.35 |
| 14 | t | 519 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | 5 | 518 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | s | 502 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | b | 508 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | d | 519 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | s | 508 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | s | 507 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | 3 | 508 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | 4 | 508 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | u | 501 | CLA | C4B-NB | 7.09 | 1.41 | 1.35 |
| 14 | f | 1209 | CLA | C4B-NB | 7.08 | 1.41 | 1.35 |
| 14 | s | 516 | CLA | C4B-NB | 7.08 | 1.41 | 1.35 |
| 14 | u | 508 | CLA | C4B-NB | 7.08 | 1.41 | 1.35 |
| 14 | a | 508 | CLA | C4B-NB | 7.08 | 1.41 | 1.35 |
| 14 | H | 1209 | CLA | C4B-NB | 7.07 | 1.41 | 1.35 |
| 14 | Y | 502 | CLA | C4B-NB | 7.07 | 1.41 | 1.35 |
| 14 | t | 518 | CLA | C4B-NB | 7.07 | 1.41 | 1.35 |
| 14 | H | 1216 | CLA | C4B-NB | 7.07 | 1.41 | 1.35 |
| 14 | 3 | 516 | CLA | C4B-NB | 7.07 | 1.41 | 1.35 |
| 14 | q | 517 | CLA | C4B-NB | 7.07 | 1.41 | 1.35 |
| 14 | 6 | 503 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | d | 504 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | B | 1209 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | c | 508 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | c | 518 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | q | 502 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | q | 509 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | B | 1216 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | a | 511 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | v | 518 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | 5 | 501 | CLA | C4B-NB | 7.06 | 1.41 | 1.35 |
| 14 | 4 | 518 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | 5 | 508 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | 3 | 503 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | a | 516 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | q | 503 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | r | 502 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | 2 | 511 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | c | 509 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | v | 502 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | Z | 519 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | n | 1501 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | B | 1240 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | 2 | 502 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | Z | 511 | CLA | C4B-NB | 7.05 | 1.41 | 1.35 |
| 14 | d | 507 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 14 | f | 1240 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 14 | Z | 509 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 14 | f | 1216 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 14 | b | 518 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 14 | L | 1501 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | d | 503 | CLA | C4B-NB | 7.04 | 1.41 | 1.35 |
| 14 | d | 518 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 14 | v | 517 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 14 | 1 | 502 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 14 | 5 | 509 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 14 | r | 508 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 14 | R | 1302 | CLA | C4B-NB | 7.03 | 1.41 | 1.35 |
| 14 | 5 | 512 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | 2 | 501 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | G | 1128 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | s | 510 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | u | 507 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | c | 512 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | Z | 508 | CLA | C4B-NB | 7.02 | 1.41 | 1.35 |
| 14 | 2 | 509 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | Z | 502 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | c | 501 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | 2 | 508 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | 6 | 502 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | u | 509 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | r | 501 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | r | 511 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | 5 | 506 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | v | 503 | CLA | C4B-NB | 7.01 | 1.41 | 1.35 |
| 14 | 1 | 509 | CLA | C4B-NB | 7.00 | 1.41 | 1.35 |
| 14 | a | 503 | CLA | C4B-NB | 7.00 | 1.41 | 1.35 |
| 14 | 5 | 507 | CLA | C4B-NB | 7.00 | 1.41 | 1.35 |
| 14 | 3 | 507 | CLA | C4B-NB | 7.00 | 1.41 | 1.35 |
| 14 | 5 | 505 | CLA | C4B-NB | 7.00 | 1.41 | 1.35 |
| 14 | H | 1218 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | s | 503 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | Y | 505 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | a | 519 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | c | 507 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | q | 511 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | u | 512 | CLA | C4B-NB | 6.99 | 1.41 | 1.35 |
| 14 | a | 507 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | c | 505 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | Z | 510 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | c | 506 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | J | 1302 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | c | 510 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | 1 | 505 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | H | 1240 | CLA | C4B-NB | 6.98 | 1.41 | 1.35 |
| 14 | 2 | 510 | CLA | C4B-NB | 6.97 | 1.41 | 1.35 |
| 14 | q | 505 | CLA | C4B-NB | 6.97 | 1.41 | 1.35 |
| 14 | u | 505 | CLA | C4B-NB | 6.97 | 1.41 | 1.35 |
| 14 | 3 | 510 | CLA | C4B-NB | 6.97 | 1.41 | 1.35 |
| 14 | e | 1128 | CLA | C4B-NB | 6.97 | 1.41 | 1.35 |
| 14 | a | 510 | CLA | C4B-NB | 6.96 | 1.41 | 1.35 |
| 14 | u | 510 | CLA | C4B-NB | 6.96 | 1.41 | 1.35 |
| 14 | B | 1226 | CLA | C4B-NB | 6.96 | 1.41 | 1.35 |
| 14 | Y | 509 | CLA | C4B-NB | 6.96 | 1.41 | 1.35 |
| 14 | f | 1230 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 14 | 6 | 517 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 15 | B | 2002 | PQN | O4-C4 | 6.95 | 1.37 | 1.23 |
| 14 | u | 506 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 14 | Z | 501 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 14 | r | 509 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 14 | B | 1218 | CLA | C4B-NB | 6.95 | 1.41 | 1.35 |
| 14 | f | 1213 | CLA | C4B-NB | 6.94 | 1.41 | 1.35 |
| 14 | F | 1302 | CLA | C4B-NB | 6.94 | 1.41 | 1.35 |
| 15 | H | 2002 | PQN | O4-C4 | 6.94 | 1.37 | 1.23 |
| 14 | q | 508 | CLA | C4B-NB | 6.94 | 1.41 | 1.35 |
| 14 | 5 | 510 | CLA | C4B-NB | 6.94 | 1.41 | 1.35 |
| 14 | 6 | 505 | CLA | C4B-NB | 6.94 | 1.41 | 1.35 |
| 14 | 1 | 508 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | f | 1201 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | T | 1302 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | e | 1116 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 15 | f | 2002 | PQN | O4-C4 | 6.93 | 1.37 | 1.23 |
| 14 | G | 1108 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | A | 1134 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | 1 | 511 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | l | 1302 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | v | 505 | CLA | C4B-NB | 6.93 | 1.41 | 1.35 |
| 14 | d | 505 | CLA | C4B-NB | 6.92 | 1.41 | 1.35 |
| 14 | a | 518 | CLA | C4B-NB | 6.92 | 1.41 | 1.35 |
| 14 | e | 1134 | CLA | C4B-NB | 6.92 | 1.41 | 1.35 |
| 14 | A | 1128 | CLA | C4B-NB | 6.92 | 1.41 | 1.35 |
| 14 | Y | 508 | CLA | C4B-NB | 6.92 | 1.41 | 1.35 |
| 14 | s | 518 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |
| 14 | 4 | 510 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |
| 14 | r | 503 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | f | 1218 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |
| 14 | H | 1201 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |
| 14 | Y | 511 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |
| 14 | 3 | 518 | CLA | C4B-NB | 6.91 | 1.41 | 1.35 |
| 14 | d | 517 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | A | 1108 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | 3 | 519 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | H | 1230 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | B | 1213 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | B | 1201 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | Z | 518 | CLA | C4B-NB | 6.90 | 1.41 | 1.35 |
| 14 | H | 1214 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 14 | m | 1401 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 14 | B | 1214 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 14 | G | 1116 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 14 | e | 1108 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 14 | s | 519 | CLA | C4B-NB | 6.89 | 1.41 | 1.35 |
| 14 | r | 510 | CLA | C4B-NB | 6.88 | 1.41 | 1.35 |
| 14 | B | 1208 | CLA | C4B-NB | 6.88 | 1.41 | 1.35 |
| 14 | 2 | 503 | CLA | C4B-NB | 6.88 | 1.41 | 1.35 |
| 14 | H | 1213 | CLA | C4B-NB | 6.87 | 1.41 | 1.35 |
| 14 | G | 1134 | CLA | C4B-NB | 6.87 | 1.41 | 1.35 |
| 14 | Z | 503 | CLA | C4B-NB | 6.87 | 1.41 | 1.35 |
| 14 | f | 1208 | CLA | C4B-NB | 6.87 | 1.41 | 1.35 |
| 14 | f | 1226 | CLA | C4B-NB | 6.87 | 1.41 | 1.35 |
| 14 | A | 1116 | CLA | C4B-NB | 6.87 | 1.41 | 1.35 |
| 14 | 2 | 518 | CLA | C4B-NB | 6.86 | 1.41 | 1.35 |
| 14 | j | 1302 | CLA | C4B-NB | 6.86 | 1.41 | 1.35 |
| 14 | B | 1230 | CLA | C4B-NB | 6.86 | 1.41 | 1.35 |
| 14 | H | 1208 | CLA | C4B-NB | 6.86 | 1.41 | 1.35 |
| 14 | K | 1401 | CLA | C4B-NB | 6.86 | 1.41 | 1.35 |
| 14 | q | 516 | CLA | C4B-NB | 6.85 | 1.41 | 1.35 |
| 14 | H | 1226 | CLA | C4B-NB | 6.85 | 1.41 | 1.35 |
| 14 | e | 1139 | CLA | C4B-NB | 6.85 | 1.41 | 1.35 |
| 14 | l | 516 | CLA | C4B-NB | 6.84 | 1.41 | 1.35 |
| 14 | b | 510 | CLA | C4B-NB | 6.84 | 1.41 | 1.35 |
| 14 | t | 510 | CLA | C4B-NB | 6.84 | 1.41 | 1.35 |
| 14 | t | 507 | CLA | C4B-NB | 6.84 | 1.41 | 1.35 |
| 14 | G | 1102 | CLA | C4B-NB | 6.83 | 1.41 | 1.35 |
| 14 | r | 518 | CLA | C4B-NB | 6.83 | 1.41 | 1.35 |
| 14 | 4 | 507 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |
| 14 | U | 1401 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | e | 1102 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |
| 14 | Y | 516 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |
| 14 | A | 1102 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |
| 14 | A | 1140 | CLA | C4B-NB | 6.82 | 1.41 | 1.35 |
| 14 | H | 1224 | CLA | C4B-NB | 6.81 | 1.41 | 1.35 |
| 14 | A | 1139 | CLA | C4B-NB | 6.81 | 1.41 | 1.35 |
| 14 | f | 1214 | CLA | C4B-NB | 6.81 | 1.41 | 1.35 |
| 14 | 2 | 507 | CLA | C4B-NB | 6.81 | 1.41 | 1.35 |
| 14 | H | 1235 | CLA | C4B-NB | 6.80 | 1.41 | 1.35 |
| 14 | B | 1224 | CLA | C4B-NB | 6.80 | 1.41 | 1.35 |
| 14 | G | 1139 | CLA | C4B-NB | 6.79 | 1.41 | 1.35 |
| 14 | G | 1140 | CLA | C4B-NB | 6.79 | 1.41 | 1.35 |
| 14 | b | 507 | CLA | C4B-NB | 6.78 | 1.41 | 1.35 |
| 14 | Z | 507 | CLA | C4B-NB | 6.77 | 1.41 | 1.35 |
| 14 | r | 507 | CLA | C4B-NB | 6.77 | 1.41 | 1.35 |
| 14 | e | 1110 | CLA | C4B-NB | 6.77 | 1.41 | 1.35 |
| 14 | e | 1140 | CLA | C4B-NB | 6.76 | 1.41 | 1.35 |
| 14 | f | 1232 | CLA | C4B-NB | 6.75 | 1.41 | 1.35 |
| 14 | B | 1235 | CLA | C4B-NB | 6.75 | 1.41 | 1.35 |
| 14 | f | 1224 | CLA | C4B-NB | 6.75 | 1.41 | 1.35 |
| 14 | e | 1138 | CLA | C4B-NB | 6.74 | 1.41 | 1.35 |
| 14 | f | 1227 | CLA | C4B-NB | 6.73 | 1.41 | 1.35 |
| 14 | a | 505 | CLA | C4B-NB | 6.73 | 1.41 | 1.35 |
| 14 | s | 505 | CLA | C4B-NB | 6.73 | 1.41 | 1.35 |
| 14 | 3 | 505 | CLA | C4B-NB | 6.73 | 1.41 | 1.35 |
| 14 | B | 1206 | CLA | C4B-NB | 6.71 | 1.41 | 1.35 |
| 14 | f | 1235 | CLA | C4B-NB | 6.70 | 1.41 | 1.35 |
| 14 | e | 1123 | CLA | C4B-NB | 6.70 | 1.41 | 1.35 |
| 14 | H | 1232 | CLA | C4B-NB | 6.70 | 1.41 | 1.35 |
| 14 | A | 1115 | CLA | C4B-NB | 6.70 | 1.41 | 1.35 |
| 14 | B | 1239 | CLA | C4B-NB | 6.69 | 1.41 | 1.35 |
| 14 | f | 1206 | CLA | C4B-NB | 6.69 | 1.41 | 1.35 |
| 14 | H | 1227 | CLA | C4B-NB | 6.69 | 1.41 | 1.35 |
| 14 | F | 1301 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 14 | H | 1239 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 14 | B | 1227 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 14 | B | 1232 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 14 | B | 1229 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 14 | B | 1221 | CLA | C4B-NB | 6.68 | 1.41 | 1.35 |
| 14 | H | 1229 | CLA | C4B-NB | 6.67 | 1.41 | 1.35 |
| 14 | e | 1115 | CLA | C4B-NB | 6.67 | 1.41 | 1.35 |
| 14 | e | 1107 | CLA | C4B-NB | 6.67 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | A | 1107 | CLA | C4B-NB | 6.67 | 1.41 | 1.35 |
| 14 | G | 1115 | CLA | C4B-NB | 6.67 | 1.41 | 1.35 |
| 14 | A | 1110 | CLA | C4B-NB | 6.66 | 1.41 | 1.35 |
| 14 | G | 1107 | CLA | C4B-NB | 6.66 | 1.41 | 1.35 |
| 14 | H | 1206 | CLA | C4B-NB | 6.66 | 1.41 | 1.35 |
| 14 | f | 1202 | CLA | C4B-NB | 6.66 | 1.41 | 1.35 |
| 14 | Z | 505 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | A | 1123 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | 2 | 505 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | U | 1103 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | f | 1021 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | B | 1202 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | B | 1215 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | B | 1228 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | G | 1123 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | H | 1228 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | n | 1502 | CLA | C4B-NB | 6.65 | 1.41 | 1.35 |
| 14 | r | 505 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | K | 1103 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | f | 1228 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | B | 1207 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | G | 1110 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | G | 1138 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | H | 1221 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | A | 1138 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | f | 1221 | CLA | C4B-NB | 6.64 | 1.41 | 1.35 |
| 14 | L | 1502 | CLA | C4B-NB | 6.63 | 1.41 | 1.35 |
| 14 | m | 1103 | CLA | C4B-NB | 6.63 | 1.41 | 1.35 |
| 14 | j | 1301 | CLA | C4B-NB | 6.63 | 1.41 | 1.35 |
| 14 | H | 1202 | CLA | C4B-NB | 6.63 | 1.41 | 1.35 |
| 14 | f | 1239 | CLA | C4B-NB | 6.63 | 1.41 | 1.35 |
| 14 | e | 1104 | CLA | C4B-NB | 6.63 | 1.41 | 1.35 |
| 14 | f | 1229 | CLA | C4B-NB | 6.62 | 1.41 | 1.35 |
| 14 | B | 1021 | CLA | C4B-NB | 6.62 | 1.41 | 1.35 |
| 14 | H | 1215 | CLA | C4B-NB | 6.61 | 1.41 | 1.35 |
| 14 | R | 1301 | CLA | C4B-NB | 6.61 | 1.41 | 1.35 |
| 14 | V | 1502 | CLA | C4B-NB | 6.61 | 1.41 | 1.35 |
| 14 | G | 1106 | CLA | C4B-NB | 6.61 | 1.41 | 1.35 |
| 14 | f | 1207 | CLA | C4B-NB | 6.60 | 1.41 | 1.35 |
| 14 | e | 1106 | CLA | C4B-NB | 6.60 | 1.41 | 1.35 |
| 14 | f | 1215 | CLA | C4B-NB | 6.59 | 1.41 | 1.35 |
| 14 | A | 1104 | CLA | C4B-NB | 6.59 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | A | 1106 | CLA | C4B-NB | 6.59 | 1.41 | 1.35 |
| 14 | G | 1104 | CLA | C4B-NB | 6.57 | 1.41 | 1.35 |
| 14 | L | 1503 | CLA | C4B-NB | 6.57 | 1.41 | 1.35 |
| 14 | H | 1207 | CLA | C4B-NB | 6.57 | 1.41 | 1.35 |
| 14 | n | 1503 | CLA | C4B-NB | 6.56 | 1.41 | 1.35 |
| 14 | H | 1220 | CLA | C4B-NB | 6.55 | 1.41 | 1.35 |
| 14 | H | 1021 | CLA | C4B-NB | 6.54 | 1.41 | 1.35 |
| 14 | H | 1205 | CLA | C4B-NB | 6.53 | 1.41 | 1.35 |
| 14 | V | 1503 | CLA | C4B-NB | 6.53 | 1.41 | 1.35 |
| 14 | A | 1137 | CLA | C4B-NB | 6.53 | 1.41 | 1.35 |
| 14 | f | 1212 | CLA | C4B-NB | 6.52 | 1.41 | 1.35 |
| 14 | e | 1137 | CLA | C4B-NB | 6.52 | 1.41 | 1.35 |
| 14 | B | 1205 | CLA | C4B-NB | 6.51 | 1.41 | 1.35 |
| 14 | A | 1117 | CLA | C4B-NB | 6.51 | 1.41 | 1.35 |
| 14 | G | 1117 | CLA | C4B-NB | 6.50 | 1.41 | 1.35 |
| 14 | f | 1205 | CLA | C4B-NB | 6.50 | 1.41 | 1.35 |
| 14 | B | 1220 | CLA | C4B-NB | 6.49 | 1.41 | 1.35 |
| 14 | f | 1220 | CLA | C4B-NB | 6.49 | 1.41 | 1.35 |
| 14 | e | 1117 | CLA | C4B-NB | 6.46 | 1.41 | 1.35 |
| 14 | G | 1136 | CLA | C4B-NB | 6.46 | 1.41 | 1.35 |
| 14 | A | 1136 | CLA | C4B-NB | 6.46 | 1.41 | 1.35 |
| 14 | e | 1131 | CLA | C4B-NB | 6.45 | 1.41 | 1.35 |
| 14 | G | 1137 | CLA | C4B-NB | 6.44 | 1.41 | 1.35 |
| 14 | A | 1124 | CLA | C4B-NB | 6.42 | 1.40 | 1.35 |
| 14 | H | 1212 | CLA | C4B-NB | 6.42 | 1.40 | 1.35 |
| 14 | A | 1120 | CLA | C4B-NB | 6.42 | 1.40 | 1.35 |
| 14 | B | 1212 | CLA | C4B-NB | 6.42 | 1.40 | 1.35 |
| 14 | e | 1120 | CLA | C4B-NB | 6.41 | 1.40 | 1.35 |
| 14 | G | 1130 | CLA | C4B-NB | 6.41 | 1.40 | 1.35 |
| 14 | H | 1204 | CLA | C4B-NB | 6.41 | 1.40 | 1.35 |
| 14 | e | 1124 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | e | 1130 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | A | 1103 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | e | 1136 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | A | 1131 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | B | 1222 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | G | 1131 | CLA | C4B-NB | 6.40 | 1.40 | 1.35 |
| 14 | G | 1124 | CLA | C4B-NB | 6.39 | 1.40 | 1.35 |
| 14 | G | 1103 | CLA | C4B-NB | 6.39 | 1.40 | 1.35 |
| 14 | A | 1130 | CLA | C4B-NB | 6.37 | 1.40 | 1.35 |
| 14 | H | 1222 | CLA | C4B-NB | 6.36 | 1.40 | 1.35 |
| 14 | G | 1121 | CLA | C4B-NB | 6.36 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | A | 1121 | CLA | C4B-NB | 6.35 | 1.40 | 1.35 |
| 14 | e | 1022 | CLA | C4B-NB | 6.34 | 1.40 | 1.35 |
| 14 | G | 1120 | CLA | C4B-NB | 6.34 | 1.40 | 1.35 |
| 14 | B | 1204 | CLA | C4B-NB | 6.33 | 1.40 | 1.35 |
| 14 | A | 1112 | CLA | C4B-NB | 6.32 | 1.40 | 1.35 |
| 14 | f | 1012 | CLA | C4B-NB | 6.32 | 1.40 | 1.35 |
| 14 | e | 1103 | CLA | C4B-NB | 6.32 | 1.40 | 1.35 |
| 14 | e | 1122 | CLA | C4B-NB | 6.31 | 1.40 | 1.35 |
| 14 | G | 1237 | CLA | C4B-NB | 6.31 | 1.40 | 1.35 |
| 14 | G | 1022 | CLA | C4B-NB | 6.31 | 1.40 | 1.35 |
| 14 | A | 1118 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | e | 1119 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | f | 1204 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | f | 1222 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | G | 1118 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | H | 1234 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | f | 1223 | CLA | C4B-NB | 6.30 | 1.40 | 1.35 |
| 14 | A | 1113 | CLA | C4B-NB | 6.29 | 1.40 | 1.35 |
| 14 | G | 1801 | CLA | C4B-NB | 6.29 | 1.40 | 1.35 |
| 14 | H | 1231 | CLA | C4B-NB | 6.29 | 1.40 | 1.35 |
| 14 | A | 1022 | CLA | C4B-NB | 6.29 | 1.40 | 1.35 |
| 14 | e | 1113 | CLA | C4B-NB | 6.29 | 1.40 | 1.35 |
| 14 | G | 1112 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | H | 1223 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | e | 1112 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | B | 1223 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | G | 1113 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | A | 1801 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | e | 1111 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | G | 1122 | CLA | C4B-NB | 6.28 | 1.40 | 1.35 |
| 14 | A | 1119 | CLA | C4B-NB | 6.27 | 1.40 | 1.35 |
| 14 | H | 1210 | CLA | C4B-NB | 6.27 | 1.40 | 1.35 |
| 14 | f | 1238 | CLA | C4B-NB | 6.27 | 1.40 | 1.35 |
| 14 | G | 1119 | CLA | C4B-NB | 6.26 | 1.40 | 1.35 |
| 14 | e | 1121 | CLA | C4B-NB | 6.26 | 1.40 | 1.35 |
| 14 | B | 1210 | CLA | C4B-NB | 6.25 | 1.40 | 1.35 |
| 14 | A | 1237 | CLA | C4B-NB | 6.25 | 1.40 | 1.35 |
| 14 | A | 1122 | CLA | C4B-NB | 6.25 | 1.40 | 1.35 |
| 14 | B | 1231 | CLA | C4B-NB | 6.24 | 1.40 | 1.35 |
| 14 | f | 1210 | CLA | C4B-NB | 6.24 | 1.40 | 1.35 |
| 14 | e | 1801 | CLA | C4B-NB | 6.23 | 1.40 | 1.35 |
| 14 | B | 1234 | CLA | C4B-NB | 6.23 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14 | e | 1118 | CLA | C4B-NB | 6.23 | 1.40 | 1.35 |
| 14 | B | 1238 | CLA | C4B-NB | 6.22 | 1.40 | 1.35 |
| 14 | f | 1234 | CLA | C4B-NB | 6.22 | 1.40 | 1.35 |
| 14 | G | 1133 | CLA | C4B-NB | 6.22 | 1.40 | 1.35 |
| 14 | G | 1111 | CLA | C4B-NB | 6.21 | 1.40 | 1.35 |
| 14 | A | 1111 | CLA | C4B-NB | 6.21 | 1.40 | 1.35 |
| 14 | B | 1012 | CLA | C4B-NB | 6.21 | 1.40 | 1.35 |
| 14 | e | 1013 | CLA | C4B-NB | 6.20 | 1.40 | 1.35 |
| 14 | H | 1238 | CLA | C4B-NB | 6.19 | 1.40 | 1.35 |
| 14 | e | 1237 | CLA | C4B-NB | 6.19 | 1.40 | 1.35 |
| 14 | H | 1211 | CLA | C4B-NB | 6.17 | 1.40 | 1.35 |
| 14 | A | 1013 | CLA | C4B-NB | 6.17 | 1.40 | 1.35 |
| 14 | H | 1012 | CLA | C4B-NB | 6.16 | 1.40 | 1.35 |
| 14 | A | 1011 | CLA | C4B-NB | 6.16 | 1.40 | 1.35 |
| 14 | f | 1231 | CLA | C4B-NB | 6.16 | 1.40 | 1.35 |
| 14 | A | 1133 | CLA | C4B-NB | 6.16 | 1.40 | 1.35 |
| 14 | G | 1013 | CLA | C4B-NB | 6.14 | 1.40 | 1.35 |
| 14 | G | 1011 | CLA | C4B-NB | 6.14 | 1.40 | 1.35 |
| 14 | H | 1203 | CLA | C4B-NB | 6.12 | 1.40 | 1.35 |
| 14 | e | 1133 | CLA | C4B-NB | 6.10 | 1.40 | 1.35 |
| 14 | B | 1211 | CLA | C4B-NB | 6.10 | 1.40 | 1.35 |
| 14 | A | 1127 | CLA | C4B-NB | 6.10 | 1.40 | 1.35 |
| 14 | e | 1127 | CLA | C4B-NB | 6.10 | 1.40 | 1.35 |
| 14 | f | 1211 | CLA | C4B-NB | 6.09 | 1.40 | 1.35 |
| 14 | A | 1105 | CLA | C4B-NB | 6.08 | 1.40 | 1.35 |
| 14 | G | 1127 | CLA | C4B-NB | 6.08 | 1.40 | 1.35 |
| 14 | B | 1203 | CLA | C4B-NB | 6.06 | 1.40 | 1.35 |
| 14 | H | 1225 | CLA | C4B-NB | 6.06 | 1.40 | 1.35 |
| 14 | e | 1105 | CLA | C4B-NB | 6.05 | 1.40 | 1.35 |
| 14 | f | 1203 | CLA | C4B-NB | 6.05 | 1.40 | 1.35 |
| 14 | e | 1011 | CLA | C4B-NB | 6.04 | 1.40 | 1.35 |
| 14 | f | 1225 | CLA | C4B-NB | 6.04 | 1.40 | 1.35 |
| 14 | B | 1225 | CLA | C4B-NB | 6.03 | 1.40 | 1.35 |
| 14 | G | 1105 | CLA | C4B-NB | 6.03 | 1.40 | 1.35 |
| 14 | G | 1129 | CLA | C4B-NB | 5.97 | 1.40 | 1.35 |
| 14 | A | 1109 | CLA | C4B-NB | 5.94 | 1.40 | 1.35 |
| 14 | f | 1023 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | A | 1126 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | e | 1109 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | H | 1023 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | G | 1125 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | e | 1126 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1129 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | e | 1129 | CLA | C4B-NB | 5.92 | 1.40 | 1.35 |
| 14 | B | 1023 | CLA | C4B-NB | 5.91 | 1.40 | 1.35 |
| 14 | G | 1126 | CLA | C4B-NB | 5.90 | 1.40 | 1.35 |
| 14 | G | 1109 | CLA | C4B-NB | 5.89 | 1.40 | 1.35 |
| 14 | e | 1125 | CLA | C4B-NB | 5.86 | 1.40 | 1.35 |
| 14 | A | 1125 | CLA | C4B-NB | 5.85 | 1.40 | 1.35 |
| 14 | e | 1132 | CLA | C4B-NB | 5.71 | 1.40 | 1.35 |
| 14 | A | 1132 | CLA | C4B-NB | 5.70 | 1.40 | 1.35 |
| 14 | G | 1132 | CLA | C4B-NB | 5.68 | 1.40 | 1.35 |
| 14 | e | 1135 | CLA | C4B-NB | 5.23 | 1.39 | 1.35 |
| 14 | G | 1135 | CLA | C4B-NB | 5.20 | 1.39 | 1.35 |
| 14 | A | 1135 | CLA | C4B-NB | 5.20 | 1.39 | 1.35 |
| 15 | B | 2002 | PQN | C2-C1 | -5.02 | 1.37 | 1.48 |
| 15 | f | 2002 | PQN | C2-C1 | -5.00 | 1.37 | 1.48 |
| 15 | H | 2002 | PQN | C2-C1 | -5.00 | 1.37 | 1.48 |
| 15 | G | 2001 | PQN | C2-C1 | -4.83 | 1.37 | 1.48 |
| 15 | e | 2001 | PQN | C2-C1 | -4.82 | 1.37 | 1.48 |
| 15 | A | 2001 | PQN | C2-C1 | -4.82 | 1.37 | 1.48 |
| 14 | A | 1128 | CLA | CMB-C2B | -4.53 | 1.42 | 1.51 |
| 14 | e | 1128 | CLA | CMB-C2B | -4.51 | 1.42 | 1.51 |
| 14 | G | 1128 | CLA | CMB-C2B | -4.50 | 1.42 | 1.51 |
| 14 | f | 1226 | CLA | CMB-C2B | -4.44 | 1.42 | 1.51 |
| 14 | B | 1226 | CLA | CMB-C2B | -4.43 | 1.42 | 1.51 |
| 14 | H | 1226 | CLA | CMB-C2B | -4.39 | 1.42 | 1.51 |
| 14 | H | 1229 | CLA | C4D-ND | -4.03 | 1.32 | 1.37 |
| 14 | B | 1023 | CLA | C4D-ND | -4.03 | 1.32 | 1.37 |
| 14 | B | 1229 | CLA | C4D-ND | -4.02 | 1.32 | 1.37 |
| 14 | H | 1023 | CLA | C4D-ND | -4.02 | 1.32 | 1.37 |
| 19 | l | 5105 | LMU | O5'-C1' | 4.01 | 1.52 | 1.41 |
| 14 | f | 1023 | CLA | C4D-ND | -4.01 | 1.32 | 1.37 |
| 19 | T | 5105 | LMU | O5'-C1' | 4.01 | 1.52 | 1.41 |
| 19 | J | 5105 | LMU | O5'-C1' | 3.99 | 1.52 | 1.41 |
| 14 | f | 1229 | CLA | C4D-ND | -3.98 | 1.32 | 1.37 |
| 14 | B | 1234 | CLA | C4D-ND | -3.97 | 1.32 | 1.37 |
| 14 | t | 503 | CLA | C1D-ND | 3.97 | 1.42 | 1.37 |
| 14 | f | 1234 | CLA | C4D-ND | -3.96 | 1.32 | 1.37 |
| 14 | H | 1226 | CLA | CMD-C2D | -3.95 | 1.42 | 1.50 |
| 14 | B | 1226 | CLA | CMD-C2D | -3.94 | 1.42 | 1.50 |
| 14 | s | 503 | CLA | C1D-ND | 3.94 | 1.42 | 1.37 |
| 14 | 3 | 503 | CLA | C1D-ND | 3.94 | 1.42 | 1.37 |
| 22 | P | 170 | FMN | C4A-N5 | 3.93 | 1.38 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | X | 170 | FMN | C4A-N5 | 3.92 | 1.38 | 1.30 |
| 14 | e | 1109 | CLA | C4D-ND | -3.92 | 1.32 | 1.37 |
| 14 | H | 1234 | CLA | C4D-ND | -3.92 | 1.32 | 1.37 |
| 14 | n | 1502 | CLA | C4D-ND | -3.92 | 1.32 | 1.37 |
| 14 | f | 1226 | CLA | CMD-C2D | -3.92 | 1.42 | 1.50 |
| 14 | V | 1502 | CLA | C4D-ND | -3.91 | 1.32 | 1.37 |
| 14 | 4 | 503 | CLA | C1D-ND | 3.91 | 1.42 | 1.37 |
| 14 | G | 1109 | CLA | C4D-ND | -3.91 | 1.32 | 1.37 |
| 22 | p | 170 | FMN | C4A-N5 | 3.91 | 1.38 | 1.30 |
| 14 | A | 1109 | CLA | C4D-ND | -3.91 | 1.32 | 1.37 |
| 14 | L | 1502 | CLA | C4D-ND | -3.90 | 1.32 | 1.37 |
| 14 | a | 503 | CLA | C1D-ND | 3.89 | 1.42 | 1.37 |
| 14 | A | 1022 | CLA | C4D-ND | -3.89 | 1.32 | 1.37 |
| 14 | G | 1122 | CLA | C4D-ND | -3.87 | 1.32 | 1.37 |
| 14 | e | 1022 | CLA | C4D-ND | -3.87 | 1.32 | 1.37 |
| 14 | G | 1022 | CLA | C4D-ND | -3.87 | 1.32 | 1.37 |
| 14 | e | 1135 | CLA | C4D-ND | -3.87 | 1.32 | 1.37 |
| 14 | A | 1122 | CLA | C4D-ND | -3.86 | 1.32 | 1.37 |
| 14 | A | 1132 | CLA | C4D-ND | -3.86 | 1.32 | 1.37 |
| 14 | b | 503 | CLA | C1D-ND | 3.86 | 1.42 | 1.37 |
| 14 | G | 1135 | CLA | C4D-ND | -3.85 | 1.32 | 1.37 |
| 14 | e | 1122 | CLA | C4D-ND | -3.85 | 1.32 | 1.37 |
| 14 | A | 1135 | CLA | C4D-ND | -3.84 | 1.32 | 1.37 |
| 14 | e | 1132 | CLA | C4D-ND | -3.83 | 1.32 | 1.37 |
| 14 | t | 516 | CLA | C1D-ND | 3.83 | 1.42 | 1.37 |
| 14 | t | 507 | CLA | C1D-ND | 3.82 | 1.42 | 1.37 |
| 14 | A | 1128 | CLA | C4D-ND | -3.82 | 1.32 | 1.37 |
| 14 | m | 1105 | CLA | C1D-ND | 3.82 | 1.42 | 1.37 |
| 14 | G | 1128 | CLA | C4D-ND | -3.82 | 1.32 | 1.37 |
| 14 | b | 516 | CLA | C1D-ND | 3.82 | 1.42 | 1.37 |
| 14 | f | 1204 | CLA | C4D-ND | -3.81 | 1.32 | 1.37 |
| 14 | G | 1132 | CLA | C4D-ND | -3.81 | 1.32 | 1.37 |
| 14 | u | 511 | CLA | C1D-ND | 3.81 | 1.42 | 1.37 |
| 14 | e | 1125 | CLA | C4D-ND | -3.80 | 1.32 | 1.37 |
| 14 | K | 1105 | CLA | C1D-ND | 3.80 | 1.42 | 1.37 |
| 14 | e | 1115 | CLA | C4D-ND | -3.80 | 1.32 | 1.37 |
| 14 | f | 1203 | CLA | C4D-ND | -3.79 | 1.32 | 1.37 |
| 14 | v | 503 | CLA | C1D-ND | 3.79 | 1.42 | 1.37 |
| 14 | H | 1204 | CLA | C4D-ND | -3.79 | 1.32 | 1.37 |
| 14 | B | 1204 | CLA | C4D-ND | -3.79 | 1.32 | 1.37 |
| 14 | 6 | 503 | CLA | C1D-ND | 3.78 | 1.42 | 1.37 |
| 14 | 4 | 516 | CLA | C1D-ND | 3.78 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1115 | CLA | C4D-ND | -3.78 | 1.32 | 1.37 |
| 14 | e | 1128 | CLA | C4D-ND | -3.78 | 1.32 | 1.37 |
| 14 | v | 511 | CLA | C1D-ND | 3.78 | 1.42 | 1.37 |
| 14 | G | 1115 | CLA | C4D-ND | -3.78 | 1.32 | 1.37 |
| 14 | e | 1129 | CLA | C4D-ND | -3.78 | 1.32 | 1.37 |
| 14 | G | 1137 | CLA | C4D-ND | -3.78 | 1.32 | 1.37 |
| 14 | d | 503 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 14 | 4 | 507 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 14 | A | 1129 | CLA | C4D-ND | -3.77 | 1.32 | 1.37 |
| 14 | 3 | 513 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 14 | G | 1140 | CLA | C4D-ND | -3.77 | 1.32 | 1.37 |
| 14 | 6 | 511 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 14 | a | 513 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 14 | A | 1119 | CLA | C4D-ND | -3.76 | 1.32 | 1.37 |
| 14 | e | 1119 | CLA | C4D-ND | -3.76 | 1.32 | 1.37 |
| 14 | H | 1206 | CLA | CMB-C2B | -3.76 | 1.43 | 1.51 |
| 14 | 5 | 511 | CLA | C1D-ND | 3.76 | 1.42 | 1.37 |
| 14 | B | 1203 | CLA | C4D-ND | -3.76 | 1.32 | 1.37 |
| 14 | Z | 516 | CLA | C1D-ND | 3.76 | 1.42 | 1.37 |
| 14 | r | 516 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 14 | A | 1111 | CLA | C4D-ND | -3.75 | 1.32 | 1.37 |
| 14 | G | 1129 | CLA | C4D-ND | -3.75 | 1.32 | 1.37 |
| 14 | s | 513 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 14 | H | 1203 | CLA | C4D-ND | -3.75 | 1.32 | 1.37 |
| 14 | Z | 503 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 14 | t | 502 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 14 | b | 502 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 14 | B | 1206 | CLA | CMB-C2B | -3.75 | 1.43 | 1.51 |
| 14 | A | 1137 | CLA | C4D-ND | -3.75 | 1.32 | 1.37 |
| 14 | 4 | 502 | CLA | C1D-ND | 3.74 | 1.42 | 1.37 |
| 14 | U | 1105 | CLA | C1D-ND | 3.74 | 1.42 | 1.37 |
| 14 | f | 1235 | CLA | C4D-ND | -3.74 | 1.32 | 1.37 |
| 14 | r | 517 | CLA | C1D-ND | 3.74 | 1.42 | 1.37 |
| 14 | v | 506 | CLA | C1D-ND | 3.74 | 1.42 | 1.37 |
| 14 | b | 506 | CLA | C1D-ND | 3.74 | 1.42 | 1.37 |
| 14 | u | 517 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 14 | A | 1125 | CLA | C4D-ND | -3.73 | 1.32 | 1.37 |
| 14 | 6 | 506 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 14 | e | 1124 | CLA | C4D-ND | -3.73 | 1.32 | 1.37 |
| 14 | f | 1206 | CLA | CMB-C2B | -3.73 | 1.43 | 1.51 |
| 14 | s | 507 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | t | 506 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 14 | b | 507 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | c | 511 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | t | 517 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | Z | 517 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | 2 | 516 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | s | 506 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | t | 504 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | e | 1137 | CLA | C4D-ND | -3.72 | 1.32 | 1.37 |
| 14 | d | 511 | CLA | C1D-ND | 3.72 | 1.42 | 1.37 |
| 14 | G | 1111 | CLA | C4D-ND | -3.71 | 1.32 | 1.37 |
| 14 | 2 | 517 | CLA | C1D-ND | 3.71 | 1.42 | 1.37 |
| 14 | G | 1124 | CLA | C4D-ND | -3.71 | 1.32 | 1.37 |
| 14 | s | 519 | CLA | C1D-ND | 3.71 | 1.42 | 1.37 |
| 14 | G | 1119 | CLA | C4D-ND | -3.71 | 1.32 | 1.37 |
| 14 | H | 1012 | CLA | C4D-ND | -3.71 | 1.32 | 1.37 |
| 14 | A | 1103 | CLA | C4D-ND | -3.70 | 1.32 | 1.37 |
| 14 | A | 1140 | CLA | C4D-ND | -3.70 | 1.32 | 1.37 |
| 14 | 3 | 519 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | 4 | 504 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | a | 518 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | e | 1136 | CLA | C4D-ND | -3.70 | 1.32 | 1.37 |
| 14 | f | 1236 | CLA | C4D-ND | -3.70 | 1.32 | 1.37 |
| 14 | d | 506 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | B | 1235 | CLA | C4D-ND | -3.70 | 1.32 | 1.37 |
| 14 | 2 | 503 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | u | 508 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | r | 503 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 14 | G | 1125 | CLA | C4D-ND | -3.69 | 1.32 | 1.37 |
| 14 | 4 | 506 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | Y | 519 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | H | 1235 | CLA | C4D-ND | -3.69 | 1.32 | 1.37 |
| 14 | 1 | 506 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | a | 506 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | q | 519 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | A | 1124 | CLA | C4D-ND | -3.69 | 1.32 | 1.37 |
| 14 | b | 504 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | u | 503 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | Y | 506 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | e | 1111 | CLA | C4D-ND | -3.69 | 1.32 | 1.37 |
| 14 | 1 | 519 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 14 | e | 1140 | CLA | C4D-ND | -3.69 | 1.32 | 1.37 |
| 14 | G | 1136 | CLA | C4D-ND | -3.68 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 5 | 517 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | A | 1136 | CLA | C4D-ND | -3.68 | 1.32 | 1.37 |
| 14 | 3 | 507 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 15 | H | 2002 | PQN | C3-C4 | -3.68 | 1.37 | 1.47 |
| 14 | 3 | 506 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | 5 | 503 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | 3 | 518 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | r | 507 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | v | 519 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | t | 511 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | e | 1131 | CLA | C4D-ND | -3.68 | 1.32 | 1.37 |
| 14 | s | 517 | CLA | C1D-ND | 3.68 | 1.42 | 1.37 |
| 14 | G | 1103 | CLA | C4D-ND | -3.68 | 1.32 | 1.37 |
| 14 | q | 508 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 14 | e | 1103 | CLA | C4D-ND | -3.67 | 1.32 | 1.37 |
| 14 | B | 1236 | CLA | C4D-ND | -3.67 | 1.32 | 1.37 |
| 14 | q | 511 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 15 | B | 2002 | PQN | C3-C4 | -3.67 | 1.38 | 1.47 |
| 14 | 4 | 517 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 14 | 6 | 519 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 14 | G | 1117 | CLA | C4D-ND | -3.67 | 1.32 | 1.37 |
| 14 | B | 1012 | CLA | C4D-ND | -3.67 | 1.32 | 1.37 |
| 14 | A | 1127 | CLA | C4D-ND | -3.67 | 1.32 | 1.37 |
| 14 | 3 | 517 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 14 | v | 507 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 14 | e | 1139 | CLA | C4D-ND | -3.66 | 1.32 | 1.37 |
| 14 | c | 519 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | l | 508 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | c | 508 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | t | 510 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | G | 1127 | CLA | C4D-ND | -3.66 | 1.32 | 1.37 |
| 14 | 5 | 519 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | b | 511 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | a | 507 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | e | 1127 | CLA | C4D-ND | -3.66 | 1.32 | 1.37 |
| 14 | Y | 511 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | T | 1303 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 19 | G | 1849 | LMU | O5'-C1' | 3.66 | 1.51 | 1.41 |
| 14 | 4 | 513 | CLA | C1D-ND | 3.66 | 1.42 | 1.37 |
| 14 | A | 1131 | CLA | C4D-ND | -3.65 | 1.32 | 1.37 |
| 14 | b | 517 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | q | 513 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | q | 506 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | Y | 513 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | b | 508 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | 1 | 513 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | Y | 503 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | c | 517 | CLA | C1D-ND | 3.65 | 1.42 | 1.37 |
| 14 | e | 1117 | CLA | C4D-ND | -3.64 | 1.32 | 1.37 |
| 14 | G | 1131 | CLA | C4D-ND | -3.64 | 1.32 | 1.37 |
| 14 | 2 | 507 | CLA | C1D-ND | 3.64 | 1.42 | 1.37 |
| 15 | f | 2002 | PQN | C3-C4 | -3.64 | 1.38 | 1.47 |
| 14 | 4 | 511 | CLA | C1D-ND | 3.64 | 1.42 | 1.37 |
| 14 | Y | 508 | CLA | C1D-ND | 3.64 | 1.42 | 1.37 |
| 14 | H | 1236 | CLA | C4D-ND | -3.63 | 1.32 | 1.37 |
| 14 | b | 513 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 14 | t | 513 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 14 | s | 518 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 14 | r | 511 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 14 | G | 1139 | CLA | C4D-ND | -3.63 | 1.32 | 1.37 |
| 14 | c | 503 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 14 | A | 1139 | CLA | C4D-ND | -3.63 | 1.32 | 1.37 |
| 14 | 1 | 511 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 19 | A | 1849 | LMU | O5'-C1' | 3.63 | 1.51 | 1.41 |
| 14 | u | 507 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 14 | d | 519 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | b | 518 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | 5 | 508 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | Y | 505 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | 1 | 518 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | Z | 507 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | b | 510 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | u | 502 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | d | 501 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | q | 509 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | e | 1105 | CLA | C4D-ND | -3.62 | 1.32 | 1.37 |
| 14 | 4 | 510 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | n | 1503 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | a | 517 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | J | 1303 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | 4 | 508 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | a | 519 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | u | 519 | CLA | C1D-ND | 3.62 | 1.42 | 1.37 |
| 14 | G | 1011 | CLA | C4D-ND | -3.62 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | f | 1209 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | v | 501 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 19 | e | 1849 | LMU | O5'-C1' | 3.61 | 1.51 | 1.41 |
| 14 | A | 1133 | CLA | C4D-ND | -3.61 | 1.32 | 1.37 |
| 14 | H | 1225 | CLA | C4D-ND | -3.61 | 1.32 | 1.37 |
| 14 | a | 501 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | b | 501 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | Y | 509 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | 6 | 507 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | Y | 517 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | Z | 504 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | q | 505 | CLA | C1D-ND | 3.61 | 1.42 | 1.37 |
| 14 | q | 503 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | A | 1117 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | u | 501 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | A | 1011 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | B | 1217 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | 5 | 501 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | Y | 518 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | f | 1012 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | Y | 507 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | e | 1011 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | 2 | 511 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | d | 507 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | c | 501 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | q | 518 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | V | 1503 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | e | 1133 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | 1 | 507 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | 6 | 501 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 14 | G | 1105 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | G | 1237 | CLA | C4D-ND | -3.60 | 1.32 | 1.37 |
| 14 | f | 1216 | CLA | CMB-C2B | -3.60 | 1.44 | 1.51 |
| 14 | A | 1105 | CLA | C4D-ND | -3.59 | 1.32 | 1.37 |
| 14 | 3 | 511 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | q | 517 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | B | 1209 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | 4 | 518 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | H | 1217 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | t | 501 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | f | 1217 | CLA | C1D-ND | 3.59 | 1.42 | 1.37 |
| 14 | H | 1216 | CLA | CMB-C2B | -3.59 | 1.44 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 6 | 513 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | e | 1104 | CLA | C4D-ND | -3.58 | 1.32 | 1.37 |
| 14 | e | 1107 | CLA | CMB-C2B | -3.58 | 1.44 | 1.51 |
| 14 | j | 1301 | CLA | C4D-ND | -3.58 | 1.32 | 1.37 |
| 14 | r | 509 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | v | 510 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | G | 1102 | CLA | C4D-ND | -3.58 | 1.32 | 1.37 |
| 14 | r | 504 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | t | 519 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | A | 1107 | CLA | CMB-C2B | -3.58 | 1.44 | 1.51 |
| 14 | L | 1503 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | G | 1133 | CLA | C4D-ND | -3.58 | 1.32 | 1.37 |
| 14 | 4 | 501 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | b | 519 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 14 | A | 1013 | CLA | C4D-ND | -3.58 | 1.32 | 1.37 |
| 14 | B | 1216 | CLA | CMB-C2B | -3.57 | 1.44 | 1.51 |
| 14 | 1 | 503 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | f | 1225 | CLA | C4D-ND | -3.57 | 1.32 | 1.37 |
| 14 | 2 | 504 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | d | 513 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 15 | e | 2001 | PQN | C3-C4 | -3.57 | 1.38 | 1.47 |
| 14 | c | 502 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | 1 | 509 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | 5 | 502 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | c | 507 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | d | 516 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | e | 1113 | CLA | C4D-ND | -3.57 | 1.32 | 1.37 |
| 14 | 5 | 507 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | A | 1237 | CLA | C4D-ND | -3.57 | 1.32 | 1.37 |
| 14 | q | 507 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | 1 | 505 | CLA | C1D-ND | 3.57 | 1.42 | 1.37 |
| 14 | Z | 511 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | d | 504 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | t | 509 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | 5 | 518 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | 3 | 501 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | u | 518 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | a | 511 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | l | 1303 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | B | 1212 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | s | 511 | CLA | C1D-ND | 3.56 | 1.42 | 1.37 |
| 14 | B | 1225 | CLA | C4D-ND | -3.55 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 1 | 517 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 14 | A | 1104 | CLA | C4D-ND | -3.55 | 1.32 | 1.37 |
| 14 | Y | 510 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 14 | r | 513 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 14 | G | 1013 | CLA | C4D-ND | -3.55 | 1.32 | 1.37 |
| 14 | 6 | 504 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 14 | t | 508 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 14 | e | 1237 | CLA | CMB-C2B | -3.55 | 1.44 | 1.51 |
| 14 | d | 509 | CLA | C1D-ND | 3.55 | 1.42 | 1.37 |
| 14 | G | 1104 | CLA | C4D-ND | -3.55 | 1.32 | 1.37 |
| 14 | G | 1113 | CLA | C4D-ND | -3.55 | 1.32 | 1.37 |
| 15 | A | 2001 | PQN | C3-C4 | -3.55 | 1.38 | 1.47 |
| 14 | c | 504 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | f | 1212 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | 6 | 510 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | G | 1130 | CLA | C4D-ND | -3.54 | 1.32 | 1.37 |
| 14 | H | 1212 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | e | 1013 | CLA | C4D-ND | -3.54 | 1.32 | 1.37 |
| 14 | 6 | 502 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | G | 1107 | CLA | CMB-C2B | -3.54 | 1.44 | 1.51 |
| 14 | A | 1130 | CLA | C4D-ND | -3.54 | 1.32 | 1.37 |
| 14 | F | 1301 | CLA | C4D-ND | -3.54 | 1.32 | 1.37 |
| 14 | t | 518 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | v | 513 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | 6 | 516 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | c | 513 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | 5 | 513 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | f | 1224 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 14 | A | 1113 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | B | 1223 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | f | 1202 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | 4 | 519 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 15 | G | 2001 | PQN | C3-C4 | -3.53 | 1.38 | 1.47 |
| 14 | G | 1120 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | s | 502 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | v | 509 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | v | 517 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | a | 508 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | H | 1223 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | G | 1237 | CLA | CMB-C2B | -3.53 | 1.44 | 1.51 |
| 14 | c | 518 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | e | 1237 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1120 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | f | 1223 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | 6 | 508 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | H | 1210 | CLA | C4D-ND | -3.53 | 1.32 | 1.37 |
| 14 | v | 516 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | d | 508 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | A | 1237 | CLA | CMB-C2B | -3.53 | 1.44 | 1.51 |
| 14 | H | 1209 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | b | 509 | CLA | C1D-ND | 3.53 | 1.42 | 1.37 |
| 14 | A | 1102 | CLA | C4D-ND | -3.52 | 1.32 | 1.37 |
| 14 | f | 1239 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | 6 | 509 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | v | 502 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | 2 | 513 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | c | 516 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | 2 | 509 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | 5 | 516 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | H | 1224 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | v | 518 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | u | 504 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 14 | 4 | 509 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | v | 504 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | q | 510 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | d | 505 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | e | 1102 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 14 | e | 1120 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 14 | f | 1215 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 19 | H | 1843 | LMU | O5'-C1' | 3.51 | 1.50 | 1.41 |
| 14 | G | 1107 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 14 | e | 1130 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 14 | Y | 501 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | e | 1107 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 14 | 6 | 518 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | B | 1210 | CLA | C4D-ND | -3.51 | 1.32 | 1.37 |
| 14 | f | 1223 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | u | 509 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | B | 1224 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | 5 | 504 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | a | 502 | CLA | C1D-ND | 3.51 | 1.42 | 1.37 |
| 14 | s | 501 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | u | 513 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | B | 1202 | CLA | C4D-ND | -3.50 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 2 | 501 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | 3 | 509 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | G | 1121 | CLA | C4D-ND | -3.50 | 1.32 | 1.37 |
| 14 | 1 | 510 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | 2 | 506 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | s | 504 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | u | 516 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | R | 1301 | CLA | C4D-ND | -3.50 | 1.32 | 1.37 |
| 14 | Z | 508 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | Z | 501 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | 6 | 505 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | c | 509 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | d | 510 | CLA | C1D-ND | 3.50 | 1.42 | 1.37 |
| 14 | 1 | 501 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | H | 1215 | CLA | C4D-ND | -3.49 | 1.32 | 1.37 |
| 14 | v | 508 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | 3 | 508 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | U | 1103 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | B | 1215 | CLA | C4D-ND | -3.49 | 1.32 | 1.37 |
| 14 | 3 | 504 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | r | 501 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | 5 | 509 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | e | 1116 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | e | 1121 | CLA | C4D-ND | -3.49 | 1.32 | 1.37 |
| 14 | t | 512 | CLA | C1D-ND | 3.49 | 1.42 | 1.37 |
| 14 | A | 1106 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 14 | B | 1239 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 14 | a | 510 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 14 | e | 1119 | CLA | CMB-C2B | -3.48 | 1.44 | 1.51 |
| 19 | B | 1843 | LMU | O5'-C1' | 3.48 | 1.50 | 1.41 |
| 14 | A | 1107 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 14 | Z | 506 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 14 | H | 1216 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 14 | f | 1214 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 14 | s | 508 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 14 | H | 1207 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 14 | f | 1222 | CLA | C4D-ND | -3.48 | 1.32 | 1.37 |
| 14 | 3 | 502 | CLA | C1D-ND | 3.48 | 1.42 | 1.37 |
| 14 | q | 501 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | A | 1116 | CLA | C4D-ND | -3.47 | 1.32 | 1.37 |
| 14 | H | 1202 | CLA | C4D-ND | -3.47 | 1.32 | 1.37 |
| 14 | B | 1207 | CLA | C4D-ND | -3.47 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | c | 510 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | d | 502 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | f | 1240 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | e | 1118 | CLA | C4D-ND | -3.47 | 1.32 | 1.37 |
| 14 | A | 1116 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | B | 1223 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | B | 1240 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | 2 | 508 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | u | 510 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | G | 1106 | CLA | C4D-ND | -3.47 | 1.32 | 1.37 |
| 14 | H | 1223 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | B | 1231 | CLA | C4D-ND | -3.47 | 1.32 | 1.37 |
| 14 | r | 508 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | Y | 504 | CLA | C1D-ND | 3.47 | 1.42 | 1.37 |
| 14 | f | 1216 | CLA | C4D-ND | -3.46 | 1.32 | 1.37 |
| 14 | Z | 513 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 19 | f | 1843 | LMU | O5'-C1' | 3.46 | 1.50 | 1.41 |
| 14 | G | 1011 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 14 | f | 1210 | CLA | C4D-ND | -3.46 | 1.32 | 1.37 |
| 14 | B | 1214 | CLA | C4D-ND | -3.46 | 1.32 | 1.37 |
| 14 | H | 1239 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 15 | f | 2002 | PQN | C10-C1 | -3.46 | 1.41 | 1.48 |
| 14 | H | 1214 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 14 | e | 1116 | CLA | C4D-ND | -3.46 | 1.32 | 1.37 |
| 14 | f | 1207 | CLA | C4D-ND | -3.46 | 1.32 | 1.37 |
| 14 | 3 | 510 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 14 | d | 517 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 14 | d | 518 | CLA | C1D-ND | 3.46 | 1.42 | 1.37 |
| 14 | 6 | 517 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | Z | 509 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | A | 1119 | CLA | CMB-C2B | -3.45 | 1.44 | 1.51 |
| 14 | H | 1231 | CLA | C4D-ND | -3.45 | 1.32 | 1.37 |
| 14 | v | 505 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | a | 509 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | a | 504 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | Z | 519 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | f | 1214 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | G | 1116 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | f | 1203 | CLA | C1D-ND | 3.45 | 1.42 | 1.37 |
| 14 | 5 | 510 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 14 | H | 1222 | CLA | C4D-ND | -3.44 | 1.33 | 1.37 |
| 14 | B | 1216 | CLA | C4D-ND | -3.44 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 2 | 519 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 14 | 4 | 512 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 14 | A | 1121 | CLA | C4D-ND | -3.44 | 1.33 | 1.37 |
| 14 | e | 1112 | CLA | C4D-ND | -3.44 | 1.33 | 1.37 |
| 14 | q | 502 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 14 | u | 506 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 14 | e | 1106 | CLA | C4D-ND | -3.44 | 1.33 | 1.37 |
| 14 | 5 | 506 | CLA | C1D-ND | 3.44 | 1.42 | 1.37 |
| 14 | B | 1214 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 14 | G | 1116 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | G | 1119 | CLA | CMB-C2B | -3.43 | 1.44 | 1.51 |
| 14 | f | 1231 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | K | 1401 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | H | 1240 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 14 | r | 506 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 14 | Y | 516 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | q | 516 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | m | 1103 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 14 | n | 1501 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | B | 1222 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | K | 1103 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 14 | a | 505 | CLA | C1D-ND | 3.43 | 1.42 | 1.37 |
| 14 | B | 1238 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | l | 516 | CLA | C4D-ND | -3.43 | 1.33 | 1.37 |
| 14 | r | 519 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 14 | s | 510 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 15 | B | 2002 | PQN | C10-C1 | -3.42 | 1.41 | 1.48 |
| 14 | b | 512 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 14 | A | 1122 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 14 | H | 1203 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 14 | A | 1118 | CLA | C4D-ND | -3.42 | 1.33 | 1.37 |
| 14 | U | 1401 | CLA | C4D-ND | -3.42 | 1.33 | 1.37 |
| 14 | s | 509 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 14 | e | 1122 | CLA | C1D-ND | 3.42 | 1.42 | 1.37 |
| 14 | r | 518 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 14 | G | 1118 | CLA | C4D-ND | -3.41 | 1.33 | 1.37 |
| 14 | B | 1203 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 14 | c | 506 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 14 | L | 1501 | CLA | C4D-ND | -3.41 | 1.33 | 1.37 |
| 14 | s | 505 | CLA | C1D-ND | 3.41 | 1.42 | 1.37 |
| 14 | H | 1214 | CLA | C4D-ND | -3.41 | 1.33 | 1.37 |
| 14 | G | 1122 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | u | 505 | CLA | C1D-ND | 3.40 | 1.42 | 1.37 |
| 14 | f | 1238 | CLA | C4D-ND | -3.40 | 1.33 | 1.37 |
| 14 | m | 1401 | CLA | C4D-ND | -3.40 | 1.33 | 1.37 |
| 14 | f | 1218 | CLA | C4D-ND | -3.40 | 1.33 | 1.37 |
| 14 | f | 1220 | CLA | C4D-ND | -3.40 | 1.33 | 1.37 |
| 15 | H | 2002 | PQN | C10-C1 | -3.40 | 1.41 | 1.48 |
| 14 | H | 1218 | CLA | C4D-ND | -3.40 | 1.33 | 1.37 |
| 14 | B | 1218 | CLA | C4D-ND | -3.39 | 1.33 | 1.37 |
| 14 | B | 1220 | CLA | C4D-ND | -3.39 | 1.33 | 1.37 |
| 14 | 3 | 505 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 14 | H | 1238 | CLA | C4D-ND | -3.39 | 1.33 | 1.37 |
| 14 | 1 | 504 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 14 | c | 505 | CLA | C1D-ND | 3.39 | 1.42 | 1.37 |
| 14 | G | 1102 | CLA | CHC-C1C | 3.39 | 1.43 | 1.35 |
| 14 | 5 | 505 | CLA | C1D-ND | 3.39 | 1.41 | 1.37 |
| 14 | H | 1012 | CLA | CHC-C1C | 3.39 | 1.43 | 1.35 |
| 14 | H | 1212 | CLA | C4D-ND | -3.39 | 1.33 | 1.37 |
| 14 | f | 1221 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | B | 1206 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | 2 | 518 | CLA | C1D-ND | 3.38 | 1.41 | 1.37 |
| 14 | B | 1221 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | G | 1126 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | e | 1102 | CLA | CHC-C1C | 3.38 | 1.43 | 1.35 |
| 14 | A | 1112 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | 1 | 502 | CLA | C1D-ND | 3.38 | 1.41 | 1.37 |
| 14 | V | 1501 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | B | 1212 | CLA | C4D-ND | -3.38 | 1.33 | 1.37 |
| 14 | H | 1211 | CLA | C4D-ND | -3.37 | 1.33 | 1.37 |
| 14 | H | 1226 | CLA | C4D-ND | -3.37 | 1.33 | 1.37 |
| 19 | e | 1848 | LMU | O5'-C1' | 3.37 | 1.50 | 1.41 |
| 14 | A | 1011 | CLA | C1D-ND | 3.37 | 1.41 | 1.37 |
| 14 | B | 1012 | CLA | CHC-C1C | 3.37 | 1.43 | 1.35 |
| 14 | A | 1126 | CLA | C4D-ND | -3.37 | 1.33 | 1.37 |
| 14 | q | 504 | CLA | C1D-ND | 3.37 | 1.41 | 1.37 |
| 14 | B | 1021 | CLA | C4D-ND | -3.37 | 1.33 | 1.37 |
| 14 | f | 1226 | CLA | C4D-ND | -3.37 | 1.33 | 1.37 |
| 19 | G | 1848 | LMU | O5'-C1' | 3.37 | 1.50 | 1.41 |
| 14 | H | 1220 | CLA | C4D-ND | -3.37 | 1.33 | 1.37 |
| 14 | 2 | 502 | CLA | C1D-ND | 3.37 | 1.41 | 1.37 |
| 19 | A | 1848 | LMU | O5'-C1' | 3.36 | 1.50 | 1.41 |
| 14 | A | 1102 | CLA | CHC-C1C | 3.36 | 1.43 | 1.35 |
| 14 | f | 1012 | CLA | CHC-C1C | 3.36 | 1.43 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | m | 1401 | CLA | C1D-ND | 3.36 | 1.41 | 1.37 |
| 19 | G | 1848 | LMU | O5B-C1B | 3.36 | 1.50 | 1.41 |
| 14 | H | 1227 | CLA | C4D-ND | -3.36 | 1.33 | 1.37 |
| 14 | f | 1206 | CLA | C4D-ND | -3.36 | 1.33 | 1.37 |
| 14 | B | 1239 | CLA | CMB-C2B | -3.36 | 1.44 | 1.51 |
| 14 | e | 1011 | CLA | C1D-ND | 3.36 | 1.41 | 1.37 |
| 14 | H | 1239 | CLA | CMB-C2B | -3.36 | 1.44 | 1.51 |
| 14 | b | 508 | CLA | CMB-C2B | -3.36 | 1.44 | 1.51 |
| 14 | f | 1212 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 14 | G | 1114 | CLA | C1D-ND | 3.35 | 1.41 | 1.37 |
| 14 | e | 1126 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 14 | H | 1206 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 14 | Z | 502 | CLA | C1D-ND | 3.35 | 1.41 | 1.37 |
| 14 | Z | 518 | CLA | C1D-ND | 3.35 | 1.41 | 1.37 |
| 14 | e | 1129 | CLA | CMB-C2B | -3.35 | 1.44 | 1.51 |
| 14 | f | 1021 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 14 | A | 1129 | CLA | CMB-C2B | -3.35 | 1.44 | 1.51 |
| 14 | L | 1501 | CLA | CMB-C2B | -3.35 | 1.44 | 1.51 |
| 14 | B | 1226 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 14 | H | 1221 | CLA | C4D-ND | -3.35 | 1.33 | 1.37 |
| 14 | G | 1022 | CLA | CMB-C2B | -3.34 | 1.44 | 1.51 |
| 14 | G | 1112 | CLA | C4D-ND | -3.34 | 1.33 | 1.37 |
| 14 | f | 1239 | CLA | CMB-C2B | -3.34 | 1.44 | 1.51 |
| 14 | V | 1501 | CLA | CMB-C2B | -3.34 | 1.44 | 1.51 |
| 19 | e | 1848 | LMU | O5B-C1B | 3.34 | 1.50 | 1.41 |
| 14 | A | 1022 | CLA | CMB-C2B | -3.34 | 1.44 | 1.51 |
| 14 | 4 | 508 | CLA | CMB-C2B | -3.34 | 1.44 | 1.51 |
| 14 | A | 1134 | CLA | C4D-ND | -3.34 | 1.33 | 1.37 |
| 14 | B | 1232 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 14 | U | 1103 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 19 | A | 1848 | LMU | O5B-C1B | 3.33 | 1.50 | 1.41 |
| 14 | H | 1021 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 14 | f | 1235 | CLA | C1D-ND | 3.33 | 1.41 | 1.37 |
| 14 | e | 1022 | CLA | CMB-C2B | -3.33 | 1.44 | 1.51 |
| 14 | f | 1211 | CLA | C1D-ND | 3.33 | 1.41 | 1.37 |
| 14 | e | 1134 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 19 | H | 1843 | LMU | O5B-C1B | 3.33 | 1.50 | 1.41 |
| 21 | t | 822 | SQD | O47-C7 | 3.33 | 1.42 | 1.35 |
| 14 | n | 1503 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 14 | R | 1302 | CLA | C1D-ND | 3.33 | 1.41 | 1.37 |
| 14 | f | 1211 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 14 | f | 1232 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | K | 1401 | CLA | C1D-ND | 3.33 | 1.41 | 1.37 |
| 14 | B | 1211 | CLA | C4D-ND | -3.33 | 1.33 | 1.37 |
| 14 | B | 1227 | CLA | C4D-ND | -3.32 | 1.33 | 1.37 |
| 14 | f | 1224 | CLA | C4D-ND | -3.32 | 1.33 | 1.37 |
| 14 | H | 1216 | CLA | C3B-C2B | -3.32 | 1.35 | 1.40 |
| 14 | e | 1114 | CLA | C1D-ND | 3.32 | 1.41 | 1.37 |
| 14 | n | 1501 | CLA | CMB-C2B | -3.32 | 1.44 | 1.51 |
| 14 | r | 502 | CLA | C1D-ND | 3.32 | 1.41 | 1.37 |
| 14 | t | 508 | CLA | CMB-C2B | -3.32 | 1.44 | 1.51 |
| 21 | 4 | 822 | SQD | O47-C7 | 3.32 | 1.42 | 1.35 |
| 14 | 3 | 516 | CLA | C1D-ND | 3.32 | 1.41 | 1.37 |
| 21 | b | 822 | SQD | O47-C7 | 3.32 | 1.42 | 1.35 |
| 19 | B | 1843 | LMU | O5B-C1B | 3.32 | 1.50 | 1.41 |
| 14 | G | 1129 | CLA | CMB-C2B | -3.32 | 1.44 | 1.51 |
| 14 | L | 1503 | CLA | C4D-ND | -3.32 | 1.33 | 1.37 |
| 14 | r | 510 | CLA | C1D-ND | 3.32 | 1.41 | 1.37 |
| 14 | V | 1503 | CLA | C4D-ND | -3.32 | 1.33 | 1.37 |
| 14 | A | 1114 | CLA | C1D-ND | 3.31 | 1.41 | 1.37 |
| 14 | f | 1208 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 14 | G | 1134 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 14 | e | 1110 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 14 | A | 1110 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 14 | H | 1230 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 14 | s | 501 | CLA | C4D-ND | -3.31 | 1.33 | 1.37 |
| 14 | Z | 510 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | 2 | 510 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | H | 1218 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | B | 1224 | CLA | C4D-ND | -3.30 | 1.33 | 1.37 |
| 19 | f | 1843 | LMU | O5B-C1B | 3.30 | 1.50 | 1.41 |
| 14 | B | 1207 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | U | 1401 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | e | 1134 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | J | 1302 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | s | 516 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | H | 1211 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | e | 1138 | CLA | C4D-ND | -3.30 | 1.33 | 1.37 |
| 14 | 3 | 501 | CLA | C4D-ND | -3.30 | 1.33 | 1.37 |
| 14 | s | 506 | CLA | C4D-ND | -3.30 | 1.33 | 1.37 |
| 14 | Y | 502 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | j | 1302 | CLA | C1D-ND | 3.30 | 1.41 | 1.37 |
| 14 | B | 1218 | CLA | C1D-ND | 3.29 | 1.41 | 1.37 |
| 14 | 2 | 506 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | a | 501 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | F | 1302 | CLA | C1D-ND | 3.29 | 1.41 | 1.37 |
| 14 | Z | 508 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | b | 519 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | v | 505 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | B | 1222 | CLA | C1D-ND | 3.29 | 1.41 | 1.37 |
| 14 | H | 1207 | CLA | C1D-ND | 3.29 | 1.41 | 1.37 |
| 14 | B | 1230 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | v | 510 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | Z | 506 | CLA | C4D-ND | -3.29 | 1.33 | 1.37 |
| 14 | f | 1222 | CLA | C1D-ND | 3.29 | 1.41 | 1.37 |
| 14 | a | 516 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | e | 1801 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | d | 512 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | 2 | 508 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | f | 1227 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | f | 1208 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | f | 1218 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | e | 1114 | CLA | CMB-C2B | -3.28 | 1.44 | 1.51 |
| 14 | A | 1801 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | c | 501 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 21 | c | 822 | SQD | O47-C7 | 3.28 | 1.42 | 1.35 |
| 14 | G | 1138 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | r | 508 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | n | 1501 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | A | 1134 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | f | 1207 | CLA | C1D-ND | 3.28 | 1.41 | 1.37 |
| 14 | B | 1216 | CLA | C3B-C2B | -3.28 | 1.35 | 1.40 |
| 14 | 5 | 506 | CLA | C4D-ND | -3.28 | 1.33 | 1.37 |
| 14 | A | 1114 | CLA | CMB-C2B | -3.27 | 1.44 | 1.51 |
| 14 | H | 1232 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | u | 506 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | r | 505 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | K | 1103 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | f | 1216 | CLA | C3B-C2B | -3.27 | 1.35 | 1.40 |
| 14 | m | 1103 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 21 | 5 | 822 | SQD | O47-C7 | 3.27 | 1.42 | 1.35 |
| 14 | l | 1302 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | r | 519 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | B | 1235 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | G | 1801 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | B | 1208 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 5 | 501 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | H | 1208 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 14 | H | 1224 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 21 | u | 822 | SQD | O47-C7 | 3.27 | 1.42 | 1.35 |
| 14 | l | 512 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | Y | 509 | CLA | C4D-ND | -3.27 | 1.33 | 1.37 |
| 21 | d | 822 | SQD | O47-C7 | 3.27 | 1.42 | 1.35 |
| 14 | Y | 512 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 21 | 6 | 822 | SQD | O47-C7 | 3.27 | 1.42 | 1.35 |
| 14 | G | 1134 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | f | 1210 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | b | 505 | CLA | C1D-ND | 3.27 | 1.41 | 1.37 |
| 14 | A | 1138 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | T | 1302 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | c | 506 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | 6 | 512 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | 6 | 505 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | B | 1211 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | H | 1228 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | f | 1230 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | q | 501 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | d | 505 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | f | 1240 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | G | 1114 | CLA | CMB-C2B | -3.26 | 1.44 | 1.51 |
| 14 | f | 1239 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | B | 1228 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | r | 506 | CLA | C4D-ND | -3.26 | 1.33 | 1.37 |
| 14 | L | 1501 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | 2 | 505 | CLA | C1D-ND | 3.26 | 1.41 | 1.37 |
| 14 | Y | 501 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 21 | v | 822 | SQD | O47-C7 | 3.25 | 1.42 | 1.35 |
| 14 | 2 | 509 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | q | 512 | CLA | C1D-ND | 3.25 | 1.41 | 1.37 |
| 14 | 6 | 501 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | G | 1110 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | q | 509 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | v | 501 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | l | 502 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | u | 501 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | B | 1208 | CLA | C1D-ND | 3.25 | 1.41 | 1.37 |
| 14 | l | 509 | CLA | C4D-ND | -3.25 | 1.33 | 1.37 |
| 14 | Y | 503 | CLA | C4D-ND | -3.24 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | V | 1501 | CLA | C1D-ND | 3.24 | 1.41 | 1.37 |
| 14 | 1 | 519 | CLA | C4D-ND | -3.24 | 1.33 | 1.37 |
| 14 | a | 508 | CLA | CMB-C2B | -3.24 | 1.44 | 1.51 |
| 14 | 3 | 506 | CLA | C4D-ND | -3.24 | 1.33 | 1.37 |
| 14 | Z | 503 | CLA | C4D-ND | -3.24 | 1.33 | 1.37 |
| 14 | 6 | 508 | CLA | C4D-ND | -3.24 | 1.33 | 1.37 |
| 14 | Z | 505 | CLA | C1D-ND | 3.24 | 1.41 | 1.37 |
| 14 | f | 1228 | CLA | C1D-ND | 3.24 | 1.41 | 1.37 |
| 14 | v | 512 | CLA | C1D-ND | 3.24 | 1.41 | 1.37 |
| 14 | 1 | 501 | CLA | C4D-ND | -3.24 | 1.33 | 1.37 |
| 14 | f | 1202 | CLA | C1D-ND | 3.24 | 1.41 | 1.37 |
| 14 | H | 1208 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | d | 501 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | r | 509 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | A | 1101 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | 4 | 505 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | s | 512 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | t | 505 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | f | 1238 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | B | 1213 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | 3 | 512 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | H | 1222 | CLA | C1D-ND | 3.23 | 1.41 | 1.37 |
| 14 | 6 | 510 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | G | 1114 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | Y | 519 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | d | 508 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | 4 | 519 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | 3 | 518 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | u | 508 | CLA | C4D-ND | -3.23 | 1.33 | 1.37 |
| 14 | j | 1301 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | H | 1239 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | a | 508 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | f | 1228 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | A | 1114 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | 2 | 519 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | H | 1213 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | q | 502 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | H | 1219 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | a | 512 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | 1 | 508 | CLA | CMB-C2B | -3.22 | 1.44 | 1.51 |
| 14 | Y | 508 | CLA | CMB-C2B | -3.22 | 1.44 | 1.51 |
| 14 | G | 1132 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1239 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | B | 1240 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | s | 518 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | q | 503 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | G | 1117 | CLA | CMB-C2B | -3.22 | 1.44 | 1.51 |
| 14 | 3 | 508 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | v | 508 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | G | 1113 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | H | 1235 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | H | 1238 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | e | 1108 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | c | 512 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | A | 1108 | CLA | C4D-ND | -3.22 | 1.33 | 1.37 |
| 14 | e | 1110 | CLA | C1D-ND | 3.22 | 1.41 | 1.37 |
| 14 | a | 506 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | r | 518 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | f | 1234 | CLA | C1D-ND | 3.21 | 1.41 | 1.37 |
| 14 | e | 1114 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | q | 519 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | 3 | 508 | CLA | CMB-C2B | -3.21 | 1.45 | 1.51 |
| 14 | s | 508 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | q | 508 | CLA | CMB-C2B | -3.21 | 1.45 | 1.51 |
| 14 | u | 510 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | G | 1133 | CLA | CMB-C2B | -3.21 | 1.45 | 1.51 |
| 14 | H | 1228 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | B | 1228 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | 1 | 504 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | Z | 509 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | f | 1213 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | B | 1201 | CLA | C1D-ND | 3.21 | 1.41 | 1.37 |
| 14 | e | 1101 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | Z | 519 | CLA | C4D-ND | -3.21 | 1.33 | 1.37 |
| 14 | Y | 502 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | 3 | 519 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | e | 1133 | CLA | CMB-C2B | -3.20 | 1.45 | 1.51 |
| 14 | q | 504 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | A | 1110 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 14 | 5 | 512 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 14 | H | 1210 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 14 | t | 517 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | B | 1222 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 14 | a | 518 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1110 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 14 | 2 | 503 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | H | 1222 | CLA | CHC-C1C | 3.20 | 1.43 | 1.35 |
| 14 | 1 | 503 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | B | 1238 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 14 | d | 510 | CLA | C4D-ND | -3.20 | 1.33 | 1.37 |
| 14 | B | 1210 | CLA | C1D-ND | 3.20 | 1.41 | 1.37 |
| 14 | f | 1222 | CLA | CHC-C1C | 3.19 | 1.43 | 1.35 |
| 14 | A | 1136 | CLA | C1D-ND | 3.19 | 1.41 | 1.37 |
| 14 | e | 1107 | CLA | CMD-C2D | -3.19 | 1.44 | 1.50 |
| 14 | H | 1240 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | c | 510 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | t | 519 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | G | 1107 | CLA | CMD-C2D | -3.19 | 1.44 | 1.50 |
| 14 | 5 | 517 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | G | 1108 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | B | 1219 | CLA | C1D-ND | 3.19 | 1.41 | 1.37 |
| 14 | 2 | 518 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | F | 1301 | CLA | C1D-ND | 3.19 | 1.41 | 1.37 |
| 14 | 5 | 510 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | Y | 505 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | b | 508 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | s | 508 | CLA | CMB-C2B | -3.19 | 1.45 | 1.51 |
| 14 | e | 1136 | CLA | C1D-ND | 3.19 | 1.41 | 1.37 |
| 14 | B | 1202 | CLA | C1D-ND | 3.19 | 1.41 | 1.37 |
| 14 | Z | 505 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | R | 1301 | CLA | C1D-ND | 3.19 | 1.41 | 1.37 |
| 14 | 3 | 509 | CLA | C4D-ND | -3.19 | 1.33 | 1.37 |
| 14 | 1 | 518 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | A | 1107 | CLA | CMD-C2D | -3.18 | 1.44 | 1.50 |
| 14 | f | 1215 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |
| 14 | G | 1101 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | s | 509 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | f | 1201 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |
| 14 | s | 519 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | H | 1232 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |
| 14 | f | 1232 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |
| 14 | 5 | 508 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | A | 1133 | CLA | CMB-C2B | -3.18 | 1.45 | 1.51 |
| 14 | 4 | 508 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | d | 509 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | A | 1132 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1215 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |
| 14 | 5 | 509 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | B | 1232 | CLA | C1D-ND | 3.18 | 1.41 | 1.37 |
| 14 | u | 517 | CLA | C4D-ND | -3.18 | 1.33 | 1.37 |
| 14 | A | 1117 | CLA | CMB-C2B | -3.17 | 1.45 | 1.51 |
| 14 | H | 1201 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | v | 509 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | 2 | 508 | CLA | CMB-C2B | -3.17 | 1.45 | 1.51 |
| 14 | F | 1302 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | u | 512 | CLA | C1D-ND | 3.17 | 1.41 | 1.37 |
| 14 | Y | 508 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | 6 | 509 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | d | 511 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | t | 508 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | u | 505 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | Z | 508 | CLA | CMB-C2B | -3.17 | 1.45 | 1.51 |
| 14 | v | 502 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 21 | a | 822 | SQD | O48-C23 | 3.17 | 1.42 | 1.33 |
| 14 | s | 517 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | H | 1201 | CLA | C1D-ND | 3.17 | 1.41 | 1.37 |
| 14 | B | 1201 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 14 | l | 506 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | f | 1215 | CLA | CMB-C2B | -3.17 | 1.45 | 1.51 |
| 14 | c | 508 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | K | 1401 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 14 | f | 1219 | CLA | C1D-ND | 3.17 | 1.41 | 1.37 |
| 14 | c | 509 | CLA | C4D-ND | -3.17 | 1.33 | 1.37 |
| 14 | f | 1201 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 14 | f | 1234 | CLA | CHC-C1C | 3.17 | 1.43 | 1.35 |
| 14 | l | 508 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | R | 1302 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | q | 508 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | B | 1234 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | 6 | 516 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | e | 1125 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | Z | 518 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | A | 1113 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | Y | 504 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | B | 1201 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | q | 518 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | t | 505 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | d | 516 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1234 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 14 | G | 1123 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | G | 1138 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | B | 1234 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 14 | Y | 519 | CLA | CHC-C1C | 3.16 | 1.43 | 1.35 |
| 14 | H | 1205 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | G | 1136 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | H | 1216 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | e | 1132 | CLA | C1D-ND | 3.16 | 1.41 | 1.37 |
| 14 | a | 509 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | v | 516 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | b | 517 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | v | 511 | CLA | C4D-ND | -3.16 | 1.33 | 1.37 |
| 14 | q | 506 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 14 | H | 1215 | CLA | C1D-ND | 3.15 | 1.41 | 1.37 |
| 14 | 2 | 513 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | q | 511 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | 4 | 517 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | u | 504 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | H | 1201 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 14 | G | 1119 | CLA | C1D-ND | 3.15 | 1.41 | 1.37 |
| 14 | 3 | 516 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | 6 | 502 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | a | 516 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | Z | 513 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | r | 513 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | m | 1401 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 14 | 5 | 505 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | Y | 510 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | s | 516 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 21 | 3 | 822 | SQD | O48-C23 | 3.15 | 1.42 | 1.33 |
| 14 | r | 501 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | r | 503 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | G | 1137 | CLA | C1D-ND | 3.15 | 1.41 | 1.37 |
| 14 | e | 1113 | CLA | C1D-ND | 3.15 | 1.41 | 1.37 |
| 14 | U | 1401 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |
| 14 | e | 1117 | CLA | CMB-C2B | -3.15 | 1.45 | 1.51 |
| 21 | Y | 822 | SQD | O48-C23 | 3.15 | 1.42 | 1.33 |
| 14 | B | 1215 | CLA | CMB-C2B | -3.15 | 1.45 | 1.51 |
| 14 | H | 1215 | CLA | CMB-C2B | -3.15 | 1.45 | 1.51 |
| 14 | 6 | 511 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | q | 519 | CLA | CHC-C1C | 3.15 | 1.43 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | Z | 510 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | c | 505 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | c | 517 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 14 | s | 503 | CLA | C4D-ND | -3.15 | 1.33 | 1.37 |
| 21 | 1 | 822 | SQD | O48-C23 | 3.15 | 1.42 | 1.33 |
| 14 | H | 1225 | CLA | CMD-C2D | -3.15 | 1.44 | 1.50 |
| 14 | H | 1240 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | B | 1240 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | 5 | 503 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | f | 1201 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 21 | q | 822 | SQD | O48-C23 | 3.14 | 1.42 | 1.33 |
| 14 | H | 1234 | CLA | C1D-ND | 3.14 | 1.41 | 1.37 |
| 14 | e | 1123 | CLA | C1D-ND | 3.14 | 1.41 | 1.37 |
| 14 | 2 | 505 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | H | 1231 | CLA | C1D-ND | 3.14 | 1.41 | 1.37 |
| 14 | 2 | 510 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | Y | 506 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | 1 | 505 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | Z | 501 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | a | 505 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | r | 507 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | r | 508 | CLA | CMB-C2B | -3.14 | 1.45 | 1.51 |
| 14 | H | 1228 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | f | 1240 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 21 | s | 822 | SQD | O48-C23 | 3.14 | 1.42 | 1.33 |
| 14 | 4 | 505 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | j | 1302 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | r | 505 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | v | 517 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | f | 1228 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | 2 | 501 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | q | 505 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | e | 1116 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | f | 1225 | CLA | CMD-C2D | -3.14 | 1.44 | 1.50 |
| 14 | q | 506 | CLA | C4D-ND | -3.14 | 1.33 | 1.37 |
| 14 | b | 519 | CLA | CHC-C1C | 3.14 | 1.43 | 1.35 |
| 14 | Y | 506 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | c | 503 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | 1 | 506 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 14 | A | 1119 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | e | 1138 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | B | 1236 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 3 | 507 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | Z | 517 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | a | 507 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | A | 1125 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | e | 1119 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | B | 1219 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | c | 519 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | A | 1137 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | B | 1231 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | G | 1112 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 14 | c | 504 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | 4 | 519 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 14 | B | 1225 | CLA | CMD-C2D | -3.13 | 1.44 | 1.50 |
| 14 | Y | 517 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | 1 | 519 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 14 | s | 510 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | e | 1137 | CLA | C1D-ND | 3.13 | 1.41 | 1.37 |
| 14 | G | 1121 | CLA | CMB-C2B | -3.13 | 1.45 | 1.51 |
| 14 | H | 1023 | CLA | CHC-C1C | 3.13 | 1.43 | 1.35 |
| 14 | d | 502 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 14 | 2 | 517 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | 1 | 511 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | Y | 511 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | d | 503 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | B | 1205 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | a | 519 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | b | 501 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 14 | b | 505 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | t | 519 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 14 | A | 1123 | CLA | C1D-ND | 3.12 | 1.41 | 1.37 |
| 14 | G | 1118 | CLA | C1D-ND | 3.12 | 1.41 | 1.37 |
| 14 | G | 1140 | CLA | C1D-ND | 3.12 | 1.41 | 1.37 |
| 14 | t | 501 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 14 | 3 | 517 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | 5 | 519 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | Y | 518 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | 6 | 517 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | s | 512 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | B | 1229 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 14 | a | 503 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | e | 1123 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | v | 506 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1121 | CLA | CMB-C2B | -3.12 | 1.45 | 1.51 |
| 14 | A | 1116 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 14 | 5 | 504 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | 6 | 503 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | G | 1123 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | v | 503 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | 4 | 501 | CLA | CHC-C1C | 3.12 | 1.43 | 1.35 |
| 14 | 2 | 507 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | Z | 502 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | u | 509 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | A | 1118 | CLA | C1D-ND | 3.12 | 1.41 | 1.37 |
| 14 | f | 1205 | CLA | C4D-ND | -3.12 | 1.33 | 1.37 |
| 14 | Z | 507 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | v | 519 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | A | 1138 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 14 | t | 518 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | e | 1112 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 14 | B | 1023 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | A | 1121 | CLA | CMB-C2B | -3.11 | 1.45 | 1.51 |
| 14 | A | 1123 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | 6 | 519 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | Z | 516 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | B | 1216 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 14 | u | 513 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | 1 | 517 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | 3 | 503 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | a | 510 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | r | 510 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | a | 501 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | e | 1112 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | B | 1228 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | G | 1125 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 14 | a | 517 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | r | 511 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | G | 1116 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | v | 509 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | f | 1231 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 21 | B | 1852 | SQD | O48-C23 | 3.11 | 1.42 | 1.33 |
| 14 | u | 519 | CLA | C4D-ND | -3.11 | 1.33 | 1.37 |
| 14 | f | 1023 | CLA | CHC-C1C | 3.11 | 1.42 | 1.35 |
| 14 | f | 1236 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 14 | 1 | 510 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | b | 509 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | A | 1112 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | B | 1227 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 14 | 3 | 501 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | Z | 504 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | s | 501 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | Z | 512 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 14 | B | 1207 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | 6 | 510 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | b | 518 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | Y | 513 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | u | 518 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | 6 | 506 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | t | 513 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | f | 1216 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 14 | H | 1229 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | 2 | 516 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | a | 502 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | u | 502 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | H | 1202 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 14 | r | 516 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | f | 1229 | CLA | CHC-C1C | 3.10 | 1.42 | 1.35 |
| 14 | 3 | 510 | CLA | C4D-ND | -3.10 | 1.33 | 1.37 |
| 14 | e | 1801 | CLA | C1D-ND | 3.09 | 1.41 | 1.37 |
| 14 | 5 | 513 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | H | 1207 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | l | 513 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | c | 511 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | s | 507 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | H | 1236 | CLA | C1D-ND | 3.09 | 1.41 | 1.37 |
| 14 | u | 508 | CLA | CMB-C2B | -3.09 | 1.45 | 1.51 |
| 14 | 6 | 512 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | B | 1213 | CLA | C1D-ND | 3.09 | 1.41 | 1.37 |
| 14 | r | 512 | CLA | C1D-ND | 3.09 | 1.41 | 1.37 |
| 21 | H | 1852 | SQD | O48-C23 | 3.09 | 1.42 | 1.33 |
| 14 | b | 501 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | f | 1207 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 21 | f | 1852 | SQD | O48-C23 | 3.09 | 1.42 | 1.33 |
| 14 | d | 506 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | u | 518 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | c | 513 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | 6 | 518 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1219 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | c | 508 | CLA | CMB-C2B | -3.09 | 1.45 | 1.51 |
| 14 | 2 | 502 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | d | 512 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | v | 518 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | c | 517 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | u | 511 | CLA | C4D-ND | -3.09 | 1.33 | 1.37 |
| 14 | t | 513 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | r | 513 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | d | 509 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | 6 | 504 | CLA | CHC-C1C | 3.09 | 1.42 | 1.35 |
| 14 | A | 1112 | CLA | C1D-ND | 3.09 | 1.41 | 1.37 |
| 14 | q | 513 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | T | 1303 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | d | 504 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | q | 517 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | H | 1227 | CLA | CMB-C2B | -3.08 | 1.45 | 1.51 |
| 14 | d | 517 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | e | 1118 | CLA | C1D-ND | 3.08 | 1.41 | 1.37 |
| 14 | 5 | 508 | CLA | CMB-C2B | -3.08 | 1.45 | 1.51 |
| 14 | c | 518 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | 5 | 518 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | H | 1213 | CLA | C1D-ND | 3.08 | 1.41 | 1.37 |
| 14 | B | 1202 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | 5 | 518 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | v | 510 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | b | 502 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | q | 510 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | f | 1202 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | r | 517 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | H | 1202 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | d | 518 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | f | 1221 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | B | 1221 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | 5 | 511 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | t | 509 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | d | 510 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | A | 1801 | CLA | C1D-ND | 3.08 | 1.41 | 1.37 |
| 14 | G | 1138 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | f | 1021 | CLA | CMD-C2D | -3.08 | 1.44 | 1.50 |
| 14 | 3 | 502 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | 4 | 513 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1221 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | B | 1209 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | 4 | 509 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | f | 1227 | CLA | C1D-ND | 3.08 | 1.41 | 1.37 |
| 14 | l | 1303 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | J | 1303 | CLA | C4D-ND | -3.08 | 1.33 | 1.37 |
| 14 | 3 | 503 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | d | 506 | CLA | CHC-C1C | 3.08 | 1.42 | 1.35 |
| 14 | c | 502 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | t | 511 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | e | 1139 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | G | 1112 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | H | 1209 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | 2 | 512 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | 6 | 504 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | f | 1219 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | A | 1140 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | v | 504 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | 3 | 512 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | H | 1209 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | s | 505 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | u | 503 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | G | 1801 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | 6 | 509 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | t | 501 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | 2 | 512 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | f | 1209 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | f | 1213 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | v | 508 | CLA | CMB-C2B | -3.07 | 1.45 | 1.51 |
| 14 | f | 1209 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | b | 513 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | 3 | 505 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | 4 | 518 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | H | 1227 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | d | 519 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |
| 14 | 5 | 517 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | B | 1209 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | A | 1108 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | e | 1117 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | f | 1213 | CLA | C1D-ND | 3.07 | 1.41 | 1.37 |
| 14 | 6 | 506 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | 2 | 511 | CLA | C4D-ND | -3.07 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1139 | CLA | CHC-C1C | 3.07 | 1.42 | 1.35 |
| 14 | 6 | 508 | CLA | CMB-C2B | -3.06 | 1.45 | 1.51 |
| 14 | c | 518 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | s | 503 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | 2 | 504 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | r | 512 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | 4 | 501 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | q | 513 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | G | 1109 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 14 | B | 1205 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 14 | A | 1139 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | A | 1138 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | A | 1013 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | 2 | 513 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | r | 504 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | Z | 512 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | Z | 513 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | e | 1138 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | e | 1139 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 14 | e | 1104 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 14 | e | 1121 | CLA | C1D-ND | 3.06 | 1.41 | 1.37 |
| 14 | B | 1227 | CLA | CMB-C2B | -3.06 | 1.45 | 1.51 |
| 14 | c | 513 | CLA | C4D-ND | -3.06 | 1.33 | 1.37 |
| 14 | 4 | 513 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | t | 509 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | H | 1213 | CLA | CHC-C1C | 3.06 | 1.42 | 1.35 |
| 14 | c | 516 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | u | 516 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | t | 511 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | 5 | 516 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | B | 1213 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | G | 1108 | CLA | C1D-ND | 3.05 | 1.41 | 1.37 |
| 14 | B | 1021 | CLA | CMD-C2D | -3.05 | 1.44 | 1.50 |
| 14 | v | 516 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | e | 1108 | CLA | C1D-ND | 3.05 | 1.41 | 1.37 |
| 14 | d | 508 | CLA | CMB-C2B | -3.05 | 1.45 | 1.51 |
| 14 | a | 504 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | G | 1135 | CLA | CMD-C2D | -3.05 | 1.44 | 1.50 |
| 14 | G | 1130 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | Z | 511 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | a | 503 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | 1 | 512 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | c | 506 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | f | 1217 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | Y | 510 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | d | 511 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | s | 511 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | 5 | 502 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | 5 | 513 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | a | 512 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | r | 502 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | A | 1135 | CLA | CMD-C2D | -3.05 | 1.44 | 1.50 |
| 14 | a | 509 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | c | 512 | CLA | C4D-ND | -3.05 | 1.33 | 1.37 |
| 14 | e | 1115 | CLA | C1D-ND | 3.05 | 1.41 | 1.37 |
| 14 | B | 1217 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | v | 506 | CLA | CHC-C1C | 3.05 | 1.42 | 1.35 |
| 14 | q | 512 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 14 | d | 504 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | 5 | 509 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | v | 512 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 14 | 1 | 513 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 14 | 4 | 509 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | G | 1013 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | a | 517 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | c | 509 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | G | 1104 | CLA | C1D-ND | 3.04 | 1.41 | 1.37 |
| 14 | v | 504 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 14 | u | 517 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | 4 | 511 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | e | 1106 | CLA | C1D-ND | 3.04 | 1.41 | 1.37 |
| 14 | n | 1502 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | e | 1135 | CLA | CMD-C2D | -3.04 | 1.44 | 1.50 |
| 14 | 3 | 509 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | A | 1130 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | b | 511 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | b | 516 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | L | 1502 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | c | 505 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | e | 1801 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | H | 1210 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | c | 504 | CLA | CHC-C1C | 3.04 | 1.42 | 1.35 |
| 14 | t | 506 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |
| 14 | t | 512 | CLA | C4D-ND | -3.04 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 5 | 505 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | 4 | 511 | CLA | C4D-ND | -3.03 | 1.33 | 1.37 |
| 14 | A | 1115 | CLA | C1D-ND | 3.03 | 1.41 | 1.37 |
| 14 | e | 1140 | CLA | C1D-ND | 3.03 | 1.41 | 1.37 |
| 14 | e | 1104 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | u | 505 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | e | 1013 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | v | 501 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | d | 516 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | f | 1210 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | H | 1021 | CLA | CMD-C2D | -3.03 | 1.44 | 1.50 |
| 14 | b | 513 | CLA | C4D-ND | -3.03 | 1.33 | 1.37 |
| 14 | H | 1206 | CLA | C1D-ND | 3.03 | 1.41 | 1.37 |
| 14 | 6 | 516 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | f | 1220 | CLA | C1D-ND | 3.03 | 1.41 | 1.37 |
| 14 | b | 509 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | s | 517 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | 4 | 506 | CLA | C4D-ND | -3.03 | 1.33 | 1.37 |
| 14 | 1 | 510 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | f | 1208 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | Y | 512 | CLA | C4D-ND | -3.03 | 1.33 | 1.37 |
| 14 | s | 509 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | Y | 513 | CLA | C4D-ND | -3.03 | 1.33 | 1.37 |
| 14 | A | 1109 | CLA | C1D-ND | 3.03 | 1.41 | 1.37 |
| 14 | Z | 510 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | q | 510 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | 3 | 517 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | B | 1210 | CLA | CHC-C1C | 3.03 | 1.42 | 1.35 |
| 14 | B | 1227 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | H | 1208 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | 3 | 504 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | 3 | 510 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | G | 1115 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | A | 1139 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | G | 1104 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | u | 503 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | A | 1104 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | A | 1117 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | G | 1124 | CLA | CMB-C2B | -3.02 | 1.45 | 1.51 |
| 14 | 5 | 512 | CLA | C4D-ND | -3.02 | 1.33 | 1.37 |
| 14 | 2 | 510 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | s | 504 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1227 | CLA | C3B-C2B | -3.02 | 1.36 | 1.40 |
| 14 | V | 1502 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | H | 1227 | CLA | C3B-C2B | -3.02 | 1.36 | 1.40 |
| 14 | s | 502 | CLA | C4D-ND | -3.02 | 1.33 | 1.37 |
| 14 | 3 | 511 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | b | 506 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | J | 1303 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | H | 1227 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | H | 1205 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | 5 | 512 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | G | 1106 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | G | 1117 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | 4 | 506 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | 4 | 516 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | G | 1105 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | G | 1801 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | A | 1124 | CLA | CMB-C2B | -3.02 | 1.45 | 1.51 |
| 14 | B | 1220 | CLA | C1D-ND | 3.02 | 1.41 | 1.37 |
| 14 | 5 | 506 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | f | 1227 | CLA | CMB-C2B | -3.02 | 1.45 | 1.51 |
| 14 | f | 1227 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | l | 1303 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | b | 505 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | e | 1130 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | a | 511 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | v | 505 | CLA | CHC-C1C | 3.02 | 1.42 | 1.35 |
| 14 | u | 512 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | 6 | 519 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | e | 1124 | CLA | CMB-C2B | -3.01 | 1.45 | 1.51 |
| 14 | A | 1104 | CLA | C1D-ND | 3.01 | 1.41 | 1.37 |
| 14 | s | 511 | CLA | C4D-ND | -3.01 | 1.33 | 1.37 |
| 14 | 6 | 511 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | c | 512 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | b | 506 | CLA | C4D-ND | -3.01 | 1.33 | 1.37 |
| 14 | a | 510 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | 5 | 504 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | r | 510 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | v | 519 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | a | 511 | CLA | C4D-ND | -3.01 | 1.33 | 1.37 |
| 14 | e | 1105 | CLA | C1D-ND | 3.01 | 1.41 | 1.37 |
| 14 | t | 503 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | u | 509 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1217 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | t | 518 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | f | 1227 | CLA | C3B-C2B | -3.01 | 1.36 | 1.40 |
| 14 | s | 510 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | u | 512 | CLA | C4D-ND | -3.01 | 1.33 | 1.37 |
| 14 | A | 1801 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | e | 1120 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | b | 518 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | d | 519 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | u | 516 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | 4 | 510 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | f | 1205 | CLA | C1D-ND | 3.01 | 1.41 | 1.37 |
| 14 | A | 1115 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | B | 1208 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | u | 504 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | b | 503 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | 5 | 503 | CLA | CHC-C1C | 3.01 | 1.42 | 1.35 |
| 14 | A | 1106 | CLA | C1D-ND | 3.00 | 1.41 | 1.37 |
| 14 | t | 510 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | 4 | 502 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | 4 | 512 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | c | 507 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | t | 504 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | d | 501 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | 3 | 511 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | 4 | 518 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | u | 501 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | G | 1121 | CLA | C1D-ND | 3.00 | 1.41 | 1.37 |
| 14 | e | 1011 | CLA | CMB-C2B | -3.00 | 1.45 | 1.51 |
| 14 | A | 1121 | CLA | C1D-ND | 3.00 | 1.41 | 1.37 |
| 14 | a | 516 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | c | 516 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | 5 | 516 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | c | 503 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | u | 513 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | e | 1115 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | f | 1023 | CLA | CMC-C2C | -3.00 | 1.44 | 1.50 |
| 14 | 4 | 505 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | s | 516 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | s | 513 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | t | 502 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | t | 510 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 6 | 501 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | t | 506 | CLA | CHC-C1C | 3.00 | 1.42 | 1.35 |
| 14 | 3 | 504 | CLA | C4D-ND | -3.00 | 1.33 | 1.37 |
| 14 | Z | 501 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | b | 510 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | f | 1235 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | A | 1013 | CLA | CMB-C2B | -2.99 | 1.45 | 1.51 |
| 14 | 3 | 516 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | 6 | 505 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | T | 1303 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 15 | f | 2002 | PQN | C5-C4 | -2.99 | 1.42 | 1.48 |
| 14 | 4 | 503 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | G | 1013 | CLA | CMB-C2B | -2.99 | 1.45 | 1.51 |
| 14 | u | 506 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | q | 501 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | G | 1126 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | A | 1105 | CLA | C1D-ND | 2.99 | 1.41 | 1.37 |
| 14 | 5 | 501 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | d | 505 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | A | 1120 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | Y | 507 | CLA | C4D-ND | -2.99 | 1.33 | 1.37 |
| 14 | G | 1139 | CLA | C1D-ND | 2.99 | 1.41 | 1.37 |
| 14 | c | 519 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | t | 505 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | A | 1126 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | s | 518 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | 1 | 518 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | G | 1120 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | H | 1216 | CLA | CHC-C1C | 2.99 | 1.42 | 1.35 |
| 14 | B | 1206 | CLA | C1D-ND | 2.99 | 1.41 | 1.37 |
| 14 | A | 1108 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | A | 1011 | CLA | CMB-C2B | -2.98 | 1.45 | 1.51 |
| 14 | c | 501 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | a | 504 | CLA | C4D-ND | -2.98 | 1.33 | 1.37 |
| 14 | u | 519 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | 5 | 519 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | H | 1220 | CLA | C1D-ND | 2.98 | 1.41 | 1.37 |
| 14 | e | 1113 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | B | 1232 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | A | 1124 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | 5 | 510 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | v | 513 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | d | 513 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | G | 1129 | CLA | CMD-C2D | -2.98 | 1.44 | 1.50 |
| 14 | 6 | 512 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | e | 1126 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | G | 1011 | CLA | CMB-C2B | -2.98 | 1.45 | 1.51 |
| 14 | q | 518 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | c | 510 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | q | 517 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | e | 1124 | CLA | C1D-ND | 2.98 | 1.41 | 1.37 |
| 14 | 4 | 504 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | d | 512 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | B | 1023 | CLA | CMC-C2C | -2.98 | 1.44 | 1.50 |
| 14 | 3 | 506 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | G | 1124 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | e | 1124 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | H | 1232 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | r | 509 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | t | 516 | CLA | CHC-C1C | 2.98 | 1.42 | 1.35 |
| 14 | G | 1115 | CLA | C1D-ND | 2.98 | 1.41 | 1.37 |
| 14 | 1 | 512 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | 4 | 504 | CLA | C4D-ND | -2.97 | 1.33 | 1.37 |
| 14 | b | 512 | CLA | C4D-ND | -2.97 | 1.33 | 1.37 |
| 14 | G | 1108 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | e | 1013 | CLA | CMB-C2B | -2.97 | 1.45 | 1.51 |
| 14 | e | 1109 | CLA | C1D-ND | 2.97 | 1.41 | 1.37 |
| 14 | B | 1216 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | Y | 517 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | v | 511 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | 1 | 501 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | 2 | 509 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | e | 1108 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | 1 | 517 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | e | 1013 | CLA | CMD-C2D | -2.97 | 1.44 | 1.50 |
| 14 | f | 1211 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | Y | 503 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | A | 1126 | CLA | C1D-ND | 2.97 | 1.41 | 1.37 |
| 14 | G | 1131 | CLA | CMB-C2B | -2.97 | 1.45 | 1.51 |
| 14 | b | 511 | CLA | C4D-ND | -2.97 | 1.33 | 1.37 |
| 14 | H | 1023 | CLA | CMC-C2C | -2.97 | 1.44 | 1.50 |
| 14 | 2 | 501 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | 3 | 519 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | Y | 518 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 5 | 511 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | s | 506 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | B | 1211 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | s | 519 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 15 | B | 2002 | PQN | C5-C4 | -2.97 | 1.42 | 1.48 |
| 14 | q | 504 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | d | 513 | CLA | C4D-ND | -2.97 | 1.33 | 1.37 |
| 14 | v | 513 | CLA | C4D-ND | -2.97 | 1.33 | 1.37 |
| 14 | 6 | 513 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | f | 1232 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | f | 1206 | CLA | C1D-ND | 2.97 | 1.41 | 1.37 |
| 14 | H | 1235 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | f | 1216 | CLA | CHC-C1C | 2.97 | 1.42 | 1.35 |
| 14 | A | 1113 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | G | 1131 | CLA | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 14 | Y | 512 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | a | 513 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | r | 501 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | e | 1131 | CLA | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 14 | G | 1126 | CLA | C1D-ND | 2.96 | 1.41 | 1.37 |
| 14 | f | 1221 | CLA | C1D-ND | 2.96 | 1.41 | 1.37 |
| 14 | B | 1235 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | a | 505 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | t | 504 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | a | 519 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | c | 511 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | 3 | 513 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | H | 1214 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | j | 1301 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | H | 1211 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | B | 1221 | CLA | C1D-ND | 2.96 | 1.41 | 1.37 |
| 14 | e | 1129 | CLA | CMD-C2D | -2.96 | 1.44 | 1.50 |
| 14 | a | 506 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | b | 504 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | G | 1113 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | v | 517 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | F | 1301 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | q | 512 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | u | 511 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | l | 504 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | Z | 509 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | Z | 518 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 4 | 510 | CLA | C4D-ND | -2.96 | 1.33 | 1.37 |
| 14 | b | 504 | CLA | C4D-ND | -2.96 | 1.33 | 1.37 |
| 14 | 6 | 513 | CLA | C4D-ND | -2.96 | 1.33 | 1.37 |
| 14 | R | 1301 | CLA | CHC-C1C | 2.96 | 1.42 | 1.35 |
| 14 | e | 1126 | CLA | C1D-ND | 2.96 | 1.41 | 1.37 |
| 14 | 6 | 518 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | G | 1124 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 14 | H | 1224 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | f | 1214 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | 3 | 518 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | J | 1302 | CLA | C4D-ND | -2.95 | 1.33 | 1.37 |
| 14 | b | 517 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | A | 1131 | CLA | C3B-C2B | -2.95 | 1.36 | 1.40 |
| 14 | H | 1205 | CLA | CMB-C2B | -2.95 | 1.45 | 1.51 |
| 14 | H | 1221 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 14 | B | 1214 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | A | 1125 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | e | 1123 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | e | 1125 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | f | 1203 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | 3 | 513 | CLA | C4D-ND | -2.95 | 1.33 | 1.37 |
| 14 | 4 | 517 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | f | 1236 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | u | 510 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | A | 1129 | CLA | CMD-C2D | -2.95 | 1.44 | 1.50 |
| 14 | B | 1230 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 14 | G | 1123 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | v | 512 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | B | 1205 | CLA | CMB-C2B | -2.95 | 1.45 | 1.51 |
| 14 | B | 1236 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | 6 | 517 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | u | 507 | CLA | C4D-ND | -2.95 | 1.33 | 1.37 |
| 14 | A | 1013 | CLA | CMD-C2D | -2.95 | 1.44 | 1.50 |
| 14 | A | 1107 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | v | 518 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | 2 | 518 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | s | 513 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 15 | H | 2002 | PQN | C5-C4 | -2.95 | 1.42 | 1.48 |
| 14 | B | 1220 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | 1 | 503 | CLA | CHC-C1C | 2.95 | 1.42 | 1.35 |
| 14 | A | 1124 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 14 | A | 1131 | CLA | CMB-C2B | -2.95 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | l | 511 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | H | 1231 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | H | 1236 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | r | 516 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | G | 1107 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 18 | G | 5001 | LHG | O7-C5 | -2.94 | 1.39 | 1.46 |
| 14 | s | 504 | CLA | C4D-ND | -2.94 | 1.33 | 1.37 |
| 14 | d | 518 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | e | 1136 | CLA | CMB-C2B | -2.94 | 1.45 | 1.51 |
| 14 | d | 517 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | l | 1302 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | b | 510 | CLA | C4D-ND | -2.94 | 1.33 | 1.37 |
| 14 | Z | 516 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | f | 1230 | CLA | C1D-ND | 2.94 | 1.41 | 1.37 |
| 14 | A | 1111 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 18 | A | 5001 | LHG | O7-C5 | -2.94 | 1.39 | 1.46 |
| 14 | r | 519 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | B | 1203 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | a | 518 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | Y | 509 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | H | 1230 | CLA | C1D-ND | 2.94 | 1.41 | 1.37 |
| 14 | e | 1130 | CLA | C1D-ND | 2.94 | 1.41 | 1.37 |
| 17 | n | 4219 | BCR | C10-C9 | -2.94 | 1.31 | 1.35 |
| 14 | Y | 501 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | Z | 519 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | H | 1220 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | Y | 504 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | l | 507 | CLA | C4D-ND | -2.94 | 1.33 | 1.37 |
| 14 | e | 1022 | CLA | C1D-ND | 2.94 | 1.41 | 1.37 |
| 14 | 2 | 516 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | e | 1107 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | A | 1123 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | J | 1302 | CLA | CHC-C1C | 2.94 | 1.42 | 1.35 |
| 14 | B | 1224 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | a | 513 | CLA | C4D-ND | -2.93 | 1.33 | 1.37 |
| 14 | 2 | 504 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | H | 1214 | CLA | CMB-C2B | -2.93 | 1.45 | 1.51 |
| 14 | t | 517 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | A | 1136 | CLA | CMB-C2B | -2.93 | 1.45 | 1.51 |
| 14 | 3 | 505 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | e | 1111 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | B | 1214 | CLA | CMB-C2B | -2.93 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | r | 506 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | b | 507 | CLA | C4D-ND | -2.93 | 1.33 | 1.37 |
| 14 | 6 | 503 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | q | 509 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 17 | L | 4219 | BCR | C10-C9 | -2.93 | 1.31 | 1.35 |
| 14 | q | 503 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | B | 1231 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | H | 1217 | CLA | C4D-ND | -2.93 | 1.33 | 1.37 |
| 14 | v | 503 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | A | 1140 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | Y | 511 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | Z | 504 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | f | 1021 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | G | 1106 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | G | 1111 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | 2 | 519 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | A | 1022 | CLA | C1D-ND | 2.93 | 1.41 | 1.37 |
| 14 | r | 504 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | Z | 512 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | r | 518 | CLA | CHC-C1C | 2.93 | 1.42 | 1.35 |
| 14 | f | 1214 | CLA | CMB-C2B | -2.93 | 1.45 | 1.51 |
| 14 | 1 | 509 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | e | 1237 | CLA | C3B-C2B | -2.92 | 1.36 | 1.40 |
| 14 | 2 | 506 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | 5 | 507 | CLA | C4D-ND | -2.92 | 1.33 | 1.37 |
| 14 | e | 1140 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | f | 1224 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | e | 1131 | CLA | CMB-C2B | -2.92 | 1.45 | 1.51 |
| 14 | e | 1106 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | H | 1219 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | d | 503 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | q | 511 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | G | 1125 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | Z | 506 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | e | 1119 | CLA | CMC-C2C | -2.92 | 1.44 | 1.50 |
| 14 | B | 1217 | CLA | C4D-ND | -2.92 | 1.33 | 1.37 |
| 14 | G | 1140 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | f | 1205 | CLA | CMB-C2B | -2.92 | 1.45 | 1.51 |
| 14 | B | 1021 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | A | 1130 | CLA | C1D-ND | 2.92 | 1.41 | 1.37 |
| 21 | s | 822 | SQD | O47-C7 | 2.92 | 1.42 | 1.34 |
| 14 | f | 1231 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1106 | CLA | CHC-C1C | 2.92 | 1.42 | 1.35 |
| 14 | G | 1136 | CLA | CMB-C2B | -2.92 | 1.45 | 1.51 |
| 14 | 3 | 512 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | 2 | 512 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | H | 1203 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | s | 512 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | 2 | 511 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 15 | H | 2002 | PQN | C10-C5 | -2.91 | 1.35 | 1.40 |
| 14 | 4 | 507 | CLA | C4D-ND | -2.91 | 1.33 | 1.37 |
| 14 | v | 507 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | e | 1117 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | 2 | 505 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | Z | 511 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | 2 | 517 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | Z | 517 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | r | 505 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | f | 1220 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | f | 1219 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | G | 1127 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 18 | e | 5001 | LHG | O7-C5 | -2.91 | 1.39 | 1.46 |
| 15 | B | 2002 | PQN | C10-C5 | -2.91 | 1.35 | 1.40 |
| 14 | H | 1021 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | s | 505 | CLA | CHC-C1C | 2.91 | 1.42 | 1.35 |
| 14 | e | 1022 | CLA | C3B-CAB | -2.90 | 1.42 | 1.47 |
| 14 | T | 1302 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 15 | G | 2001 | PQN | C11-C12 | 2.90 | 1.54 | 1.50 |
| 14 | r | 512 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 14 | 6 | 508 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 14 | G | 1022 | CLA | C1D-ND | 2.90 | 1.41 | 1.37 |
| 14 | T | 1302 | CLA | C4D-ND | -2.90 | 1.33 | 1.37 |
| 14 | v | 507 | CLA | C4D-ND | -2.90 | 1.33 | 1.37 |
| 14 | G | 1013 | CLA | CMD-C2D | -2.90 | 1.44 | 1.50 |
| 14 | Z | 503 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 17 | V | 4219 | BCR | C10-C9 | -2.90 | 1.31 | 1.35 |
| 14 | l | 1302 | CLA | C4D-ND | -2.90 | 1.33 | 1.37 |
| 21 | a | 822 | SQD | O47-C7 | 2.90 | 1.42 | 1.34 |
| 14 | 6 | 507 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 14 | r | 511 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 14 | b | 516 | CLA | C4D-ND | -2.90 | 1.33 | 1.37 |
| 14 | A | 1117 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 14 | Z | 507 | CLA | CHC-C1C | 2.90 | 1.42 | 1.35 |
| 14 | e | 1013 | CLA | CMC-C2C | -2.90 | 1.44 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 4 | 516 | CLA | C4D-ND | -2.89 | 1.33 | 1.37 |
| 14 | G | 1130 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 15 | e | 2001 | PQN | C3-C2 | 2.89 | 1.40 | 1.35 |
| 14 | q | 505 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | t | 503 | CLA | C4D-ND | -2.89 | 1.33 | 1.37 |
| 14 | A | 1237 | CLA | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 14 | B | 1218 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | f | 1218 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | q | 507 | CLA | C4D-ND | -2.89 | 1.33 | 1.37 |
| 14 | B | 1219 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | d | 508 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 20 | f | 5002 | LMG | O8-C9 | -2.89 | 1.38 | 1.45 |
| 15 | G | 2001 | PQN | C3-C2 | 2.89 | 1.40 | 1.35 |
| 14 | H | 1225 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 14 | G | 1237 | CLA | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 14 | t | 516 | CLA | C4D-ND | -2.89 | 1.33 | 1.37 |
| 14 | e | 1127 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 14 | r | 502 | CLA | CMB-C2B | -2.89 | 1.45 | 1.51 |
| 14 | G | 1117 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | A | 1013 | CLA | CMC-C2C | -2.89 | 1.44 | 1.50 |
| 14 | f | 1235 | CLA | CMB-C2B | -2.89 | 1.45 | 1.51 |
| 14 | e | 1127 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | B | 1225 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 14 | 6 | 507 | CLA | C4D-ND | -2.89 | 1.33 | 1.37 |
| 14 | A | 1127 | CLA | C1D-ND | 2.89 | 1.41 | 1.37 |
| 14 | a | 512 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 15 | f | 2002 | PQN | C10-C5 | -2.89 | 1.35 | 1.40 |
| 14 | Z | 505 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | v | 508 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | 4 | 503 | CLA | C4D-ND | -2.89 | 1.33 | 1.37 |
| 14 | G | 1110 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | r | 503 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | G | 1107 | CLA | C3B-C2B | -2.89 | 1.36 | 1.40 |
| 14 | A | 1127 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | A | 1119 | CLA | CMC-C2C | -2.89 | 1.44 | 1.50 |
| 14 | H | 1218 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | a | 502 | CLA | CHC-C1C | 2.89 | 1.42 | 1.35 |
| 14 | r | 517 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | t | 507 | CLA | C4D-ND | -2.88 | 1.33 | 1.37 |
| 14 | G | 1131 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | 1 | 505 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | A | 1022 | CLA | C3B-CAB | -2.88 | 1.42 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | t | 512 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 21 | 3 | 822 | SQD | O47-C7 | 2.88 | 1.42 | 1.34 |
| 14 | 2 | 507 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 21 | n | 5216 | SQD | O48-C23 | 2.88 | 1.41 | 1.33 |
| 14 | 2 | 502 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 14 | A | 1131 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | B | 1230 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 20 | B | 5002 | LMG | O8-C9 | -2.88 | 1.38 | 1.45 |
| 14 | e | 1131 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | f | 1021 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 14 | e | 1110 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | G | 1119 | CLA | CMC-C2C | -2.88 | 1.44 | 1.50 |
| 14 | G | 1013 | CLA | CMC-C2C | -2.88 | 1.44 | 1.50 |
| 15 | A | 2001 | PQN | C3-C2 | 2.88 | 1.40 | 1.35 |
| 14 | B | 1021 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 14 | B | 1235 | CLA | CMB-C2B | -2.88 | 1.45 | 1.51 |
| 14 | f | 1225 | CLA | C1D-ND | 2.88 | 1.41 | 1.37 |
| 14 | A | 1105 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | d | 507 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | q | 507 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | G | 1022 | CLA | C3B-CAB | -2.88 | 1.42 | 1.47 |
| 14 | e | 1105 | CLA | CHC-C1C | 2.88 | 1.42 | 1.35 |
| 14 | f | 1230 | CLA | CMB-C2B | -2.87 | 1.45 | 1.51 |
| 14 | 2 | 503 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 14 | 1 | 507 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 14 | H | 1021 | CLA | CMB-C2B | -2.87 | 1.45 | 1.51 |
| 14 | A | 1110 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 14 | A | 1022 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 14 | G | 1011 | CLA | CMD-C2D | -2.87 | 1.44 | 1.50 |
| 14 | d | 507 | CLA | C4D-ND | -2.87 | 1.33 | 1.37 |
| 21 | r | 822 | SQD | O47-C7 | 2.87 | 1.42 | 1.34 |
| 20 | H | 5002 | LMG | O8-C9 | -2.87 | 1.38 | 1.45 |
| 14 | G | 1022 | CLA | CHC-C1C | 2.87 | 1.42 | 1.35 |
| 14 | A | 1121 | CLA | CMD-C2D | -2.87 | 1.44 | 1.50 |
| 14 | G | 1121 | CLA | CMD-C2D | -2.87 | 1.44 | 1.50 |
| 14 | e | 1011 | CLA | CMD-C2D | -2.87 | 1.44 | 1.50 |
| 14 | b | 512 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | 4 | 512 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | Z | 502 | CLA | CMB-C2B | -2.86 | 1.45 | 1.51 |
| 14 | 1 | 516 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | G | 1102 | CLA | C1D-ND | 2.86 | 1.41 | 1.37 |
| 14 | d | 502 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1137 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | e | 1121 | CLA | CMD-C2D | -2.86 | 1.44 | 1.50 |
| 14 | f | 1217 | CLA | C4D-ND | -2.86 | 1.33 | 1.37 |
| 14 | j | 1302 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 21 | L | 5216 | SQD | O48-C23 | 2.86 | 1.41 | 1.33 |
| 14 | H | 1226 | CLA | MG-ND | -2.86 | 2.00 | 2.05 |
| 14 | e | 1129 | CLA | C3B-CAB | -2.86 | 1.42 | 1.47 |
| 14 | e | 1022 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | s | 502 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | f | 1223 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | e | 1130 | CLA | CMB-C2B | -2.86 | 1.45 | 1.51 |
| 14 | 3 | 507 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | 3 | 502 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 14 | B | 1223 | CLA | CHC-C1C | 2.86 | 1.42 | 1.35 |
| 21 | V | 5216 | SQD | O48-C23 | 2.85 | 1.41 | 1.33 |
| 15 | A | 2001 | PQN | C11-C12 | 2.85 | 1.54 | 1.50 |
| 15 | B | 2002 | PQN | C3-C2 | 2.85 | 1.40 | 1.35 |
| 14 | H | 1223 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | A | 1102 | CLA | C1D-ND | 2.85 | 1.41 | 1.37 |
| 14 | H | 1212 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 21 | 2 | 822 | SQD | O47-C7 | 2.85 | 1.42 | 1.34 |
| 14 | n | 1501 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | H | 1230 | CLA | CMB-C2B | -2.85 | 1.45 | 1.51 |
| 14 | A | 1137 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | r | 507 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | A | 1011 | CLA | CMD-C2D | -2.85 | 1.44 | 1.50 |
| 14 | Y | 516 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | B | 1212 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | G | 1137 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 15 | H | 2002 | PQN | C3-C2 | 2.85 | 1.40 | 1.35 |
| 14 | a | 507 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | 6 | 502 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | f | 1225 | CLA | CMB-C2B | -2.85 | 1.45 | 1.51 |
| 14 | F | 1302 | CLA | CHC-C1C | 2.85 | 1.42 | 1.35 |
| 14 | B | 1205 | CLA | CMD-C2D | -2.84 | 1.44 | 1.50 |
| 14 | K | 1105 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | e | 1102 | CLA | C1D-ND | 2.84 | 1.41 | 1.37 |
| 14 | R | 1302 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | G | 1138 | CLA | CMB-C2B | -2.84 | 1.45 | 1.51 |
| 14 | Y | 507 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 21 | Z | 822 | SQD | O47-C7 | 2.84 | 1.42 | 1.34 |
| 21 | q | 822 | SQD | O47-C7 | 2.84 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | f | 1226 | CLA | MG-ND | -2.84 | 2.00 | 2.05 |
| 14 | Y | 505 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | B | 1226 | CLA | MG-ND | -2.84 | 2.00 | 2.05 |
| 14 | B | 1221 | CLA | CMB-C2B | -2.84 | 1.45 | 1.51 |
| 14 | A | 1101 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | G | 1105 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | V | 1501 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | m | 1105 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | U | 1105 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | q | 516 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | e | 1114 | CLA | CHC-C1C | 2.84 | 1.42 | 1.35 |
| 14 | A | 1130 | CLA | CMB-C2B | -2.84 | 1.45 | 1.51 |
| 14 | H | 1235 | CLA | CMB-C2B | -2.84 | 1.45 | 1.51 |
| 14 | e | 1107 | CLA | C3B-C2B | -2.84 | 1.36 | 1.40 |
| 15 | e | 2001 | PQN | C11-C12 | 2.84 | 1.54 | 1.50 |
| 14 | b | 503 | CLA | C4D-ND | -2.84 | 1.33 | 1.37 |
| 14 | A | 1133 | CLA | C1D-ND | 2.84 | 1.41 | 1.37 |
| 14 | e | 1138 | CLA | CMB-C2B | -2.84 | 1.45 | 1.51 |
| 14 | G | 1101 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | G | 1129 | CLA | C3B-CAB | -2.83 | 1.42 | 1.47 |
| 14 | A | 1129 | CLA | C3B-CAB | -2.83 | 1.42 | 1.47 |
| 14 | G | 1122 | CLA | CMB-C2B | -2.83 | 1.45 | 1.51 |
| 14 | e | 1134 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | 5 | 502 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | G | 1127 | CLA | C1D-ND | 2.83 | 1.41 | 1.37 |
| 14 | f | 1212 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | A | 1107 | CLA | C3B-C2B | -2.83 | 1.36 | 1.40 |
| 14 | f | 1205 | CLA | CMD-C2D | -2.83 | 1.44 | 1.50 |
| 14 | s | 508 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 21 | B | 1852 | SQD | O2-C2 | -2.83 | 1.36 | 1.43 |
| 14 | L | 1501 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 21 | 1 | 822 | SQD | O47-C7 | 2.83 | 1.42 | 1.34 |
| 14 | H | 1205 | CLA | CMD-C2D | -2.83 | 1.44 | 1.50 |
| 14 | 5 | 508 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | G | 1114 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | s | 507 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | 4 | 502 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | A | 1114 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | b | 502 | CLA | CHC-C1C | 2.83 | 1.42 | 1.35 |
| 14 | G | 1130 | CLA | CMB-C2B | -2.83 | 1.45 | 1.51 |
| 14 | G | 1128 | CLA | C3B-C2B | -2.83 | 1.36 | 1.40 |
| 14 | G | 1129 | CLA | C1D-ND | 2.82 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21 | H | 1852 | SQD | O2-C2 | -2.82 | 1.36 | 1.43 |
| 14 | c | 508 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 14 | A | 1128 | CLA | C3B-C2B | -2.82 | 1.36 | 1.40 |
| 14 | e | 1101 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 14 | H | 1225 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 14 | A | 1138 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 14 | A | 1134 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 14 | B | 1225 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 14 | e | 1110 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 14 | f | 1221 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 14 | G | 1133 | CLA | C1D-ND | 2.82 | 1.41 | 1.37 |
| 14 | H | 1221 | CLA | CMB-C2B | -2.82 | 1.45 | 1.51 |
| 21 | Y | 822 | SQD | O47-C7 | 2.82 | 1.42 | 1.34 |
| 14 | u | 508 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 14 | t | 502 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 14 | f | 1204 | CLA | CHC-C1C | 2.82 | 1.42 | 1.35 |
| 14 | e | 1118 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | G | 1134 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 14 | v | 502 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | u | 502 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | u | 502 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 14 | A | 1134 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 21 | f | 1852 | SQD | O2-C2 | -2.81 | 1.36 | 1.43 |
| 14 | A | 1106 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 14 | G | 1134 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 15 | f | 2002 | PQN | C3-C2 | 2.81 | 1.40 | 1.35 |
| 14 | f | 1225 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | e | 1134 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 14 | 3 | 508 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | G | 1110 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 14 | e | 1140 | CLA | CMB-C2B | -2.81 | 1.45 | 1.51 |
| 14 | c | 502 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | B | 1238 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | B | 1204 | CLA | CHC-C1C | 2.81 | 1.42 | 1.35 |
| 14 | G | 1140 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | f | 1238 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | q | 502 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | G | 1111 | CLA | CMC-C2C | -2.80 | 1.44 | 1.50 |
| 14 | G | 1120 | CLA | C1D-ND | 2.80 | 1.41 | 1.37 |
| 14 | A | 1110 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | A | 1122 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | e | 1139 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1111 | CLA | CMC-C2C | -2.80 | 1.44 | 1.50 |
| 14 | f | 1239 | CLA | C3B-C2B | -2.80 | 1.36 | 1.40 |
| 14 | H | 1236 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | r | 508 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | 5 | 502 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | A | 1139 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | f | 1205 | CLA | C3B-C2B | -2.80 | 1.36 | 1.40 |
| 14 | f | 1238 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | r | 502 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | G | 1108 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | G | 1139 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | 2 | 502 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | e | 1108 | CLA | CMB-C2B | -2.80 | 1.45 | 1.51 |
| 14 | 2 | 508 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | G | 1101 | CLA | C1D-ND | 2.80 | 1.41 | 1.37 |
| 14 | H | 1204 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | A | 1118 | CLA | CHC-C1C | 2.80 | 1.42 | 1.35 |
| 14 | e | 1111 | CLA | CMC-C2C | -2.79 | 1.44 | 1.50 |
| 14 | B | 1239 | CLA | C3B-C2B | -2.79 | 1.36 | 1.40 |
| 14 | A | 1140 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 14 | e | 1133 | CLA | C1D-ND | 2.79 | 1.41 | 1.37 |
| 14 | G | 1106 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 14 | B | 1225 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 14 | 4 | 502 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 14 | e | 1103 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 14 | a | 508 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 14 | c | 507 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 14 | e | 1132 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 14 | B | 1219 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 14 | e | 1133 | CLA | CHC-C1C | 2.79 | 1.42 | 1.35 |
| 14 | A | 1101 | CLA | C1D-ND | 2.79 | 1.41 | 1.37 |
| 14 | V | 1502 | CLA | C1D-ND | 2.79 | 1.41 | 1.37 |
| 14 | m | 1105 | CLA | C4D-ND | -2.79 | 1.33 | 1.37 |
| 14 | v | 502 | CLA | CMB-C2B | -2.79 | 1.45 | 1.51 |
| 14 | A | 1108 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | 6 | 502 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | H | 1238 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | q | 509 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | t | 508 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | G | 1133 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | 5 | 507 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | Z | 502 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1238 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | e | 1122 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | H | 1225 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | d | 502 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | A | 1132 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | u | 507 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | e | 1128 | CLA | C3B-C2B | -2.78 | 1.36 | 1.40 |
| 14 | c | 502 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | A | 1120 | CLA | C1D-ND | 2.78 | 1.41 | 1.37 |
| 14 | l | 502 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | e | 1101 | CLA | C1D-ND | 2.78 | 1.41 | 1.37 |
| 14 | A | 1103 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | B | 1238 | CLA | CMB-C2B | -2.78 | 1.45 | 1.51 |
| 14 | G | 1118 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | A | 1136 | CLA | CHC-C1C | 2.78 | 1.42 | 1.35 |
| 14 | A | 1129 | CLA | C1D-ND | 2.78 | 1.41 | 1.37 |
| 14 | K | 1105 | CLA | C4D-ND | -2.77 | 1.33 | 1.37 |
| 14 | b | 502 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 14 | B | 1204 | CLA | C1D-ND | 2.77 | 1.41 | 1.37 |
| 14 | U | 1103 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | A | 1103 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | Y | 502 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | G | 1103 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 14 | Z | 508 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | e | 1136 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | f | 1230 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | U | 1105 | CLA | C4D-ND | -2.77 | 1.33 | 1.37 |
| 14 | H | 1230 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | K | 1103 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | q | 511 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 14 | 4 | 508 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | G | 1132 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | G | 1109 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 14 | H | 1239 | CLA | C3B-C2B | -2.77 | 1.36 | 1.40 |
| 14 | e | 1106 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 14 | A | 1133 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | G | 1136 | CLA | CHC-C1C | 2.77 | 1.42 | 1.35 |
| 14 | e | 1109 | CLA | CMB-C2B | -2.77 | 1.45 | 1.51 |
| 14 | e | 1103 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 14 | H | 1209 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | B | 1236 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 21 | n | 5216 | SQD | O47-C7 | 2.76 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1127 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | B | 1209 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | t | 502 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | j | 1302 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | 4 | 507 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 14 | F | 1302 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | G | 1127 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | b | 508 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 14 | A | 1129 | CLA | CHC-C1C | 2.76 | 1.42 | 1.35 |
| 14 | Y | 511 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | A | 1109 | CLA | CMB-C2B | -2.76 | 1.45 | 1.51 |
| 14 | f | 1204 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 14 | m | 1103 | CLA | CHC-C1C | 2.75 | 1.42 | 1.35 |
| 14 | V | 1503 | CLA | CHC-C1C | 2.75 | 1.42 | 1.35 |
| 14 | H | 1232 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | B | 1230 | CLA | CHC-C1C | 2.75 | 1.42 | 1.35 |
| 14 | G | 1103 | CLA | CHC-C1C | 2.75 | 1.42 | 1.35 |
| 14 | f | 1219 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | e | 1137 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | R | 1302 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | H | 1204 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 14 | A | 1103 | CLA | CMC-C2C | -2.75 | 1.45 | 1.50 |
| 14 | l | 511 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | H | 1219 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | A | 1128 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 14 | e | 1237 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 14 | f | 1236 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | H | 1208 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | Z | 511 | CLA | CMB-C2B | -2.75 | 1.45 | 1.51 |
| 14 | B | 1205 | CLA | C3B-C2B | -2.75 | 1.36 | 1.40 |
| 14 | L | 1503 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 14 | B | 1232 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 15 | A | 2001 | PQN | C10-C5 | -2.74 | 1.36 | 1.40 |
| 15 | e | 2001 | PQN | C10-C5 | -2.74 | 1.36 | 1.40 |
| 14 | n | 1502 | CLA | C1D-ND | 2.74 | 1.41 | 1.37 |
| 21 | L | 5216 | SQD | O47-C7 | 2.74 | 1.42 | 1.34 |
| 14 | e | 1129 | CLA | C1D-ND | 2.74 | 1.41 | 1.37 |
| 15 | G | 2001 | PQN | C10-C5 | -2.74 | 1.36 | 1.40 |
| 14 | G | 1122 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 14 | l | 502 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | e | 1128 | CLA | C1D-ND | 2.74 | 1.41 | 1.37 |
| 14 | e | 1129 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 2 | 511 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | G | 1136 | CLA | C3B-C2B | -2.74 | 1.36 | 1.40 |
| 14 | b | 507 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 14 | f | 1209 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | l | 509 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | Y | 509 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | e | 1127 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | r | 511 | CLA | CMB-C2B | -2.74 | 1.45 | 1.51 |
| 14 | l | 508 | CLA | CHC-C1C | 2.74 | 1.42 | 1.35 |
| 14 | j | 1301 | CLA | CMB-C2B | -2.73 | 1.46 | 1.51 |
| 14 | t | 507 | CLA | CHC-C1C | 2.73 | 1.42 | 1.35 |
| 14 | G | 1129 | CLA | CHC-C1C | 2.73 | 1.42 | 1.35 |
| 14 | H | 1205 | CLA | C3B-C2B | -2.73 | 1.36 | 1.40 |
| 14 | q | 502 | CLA | CMB-C2B | -2.73 | 1.46 | 1.51 |
| 14 | Y | 516 | CLA | C1D-ND | 2.73 | 1.41 | 1.37 |
| 14 | e | 1120 | CLA | C1D-ND | 2.73 | 1.41 | 1.37 |
| 14 | G | 1101 | CLA | CMB-C2B | -2.73 | 1.46 | 1.51 |
| 14 | s | 502 | CLA | CMB-C2B | -2.73 | 1.46 | 1.51 |
| 14 | G | 1103 | CLA | CMC-C2C | -2.73 | 1.45 | 1.50 |
| 14 | e | 1129 | CLA | C3B-C2B | -2.73 | 1.36 | 1.40 |
| 14 | Y | 502 | CLA | CMB-C2B | -2.73 | 1.46 | 1.51 |
| 14 | G | 1129 | CLA | C3B-C2B | -2.73 | 1.36 | 1.40 |
| 21 | V | 5216 | SQD | O47-C7 | 2.73 | 1.42 | 1.34 |
| 14 | Y | 508 | CLA | CHC-C1C | 2.72 | 1.42 | 1.35 |
| 14 | f | 1208 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |
| 14 | e | 1103 | CLA | CMC-C2C | -2.72 | 1.45 | 1.50 |
| 14 | A | 1237 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |
| 14 | G | 1103 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |
| 14 | q | 516 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |
| 14 | G | 1115 | CLA | CMC-C2C | -2.72 | 1.45 | 1.50 |
| 14 | H | 1012 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |
| 14 | q | 508 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 14 | f | 1012 | CLA | C1D-ND | 2.72 | 1.41 | 1.37 |
| 14 | A | 1115 | CLA | CMC-C2C | -2.72 | 1.45 | 1.50 |
| 14 | n | 1503 | CLA | CHC-C1C | 2.72 | 1.41 | 1.35 |
| 14 | B | 1208 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |
| 14 | G | 1125 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |
| 14 | f | 1232 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |
| 14 | A | 1129 | CLA | C3B-C2B | -2.72 | 1.36 | 1.40 |
| 14 | A | 1136 | CLA | C3B-C2B | -2.72 | 1.36 | 1.40 |
| 14 | A | 1135 | CLA | MG-ND | -2.72 | 2.00 | 2.05 |
| 14 | e | 1125 | CLA | CMB-C2B | -2.72 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1136 | CLA | C3B-C2B | -2.71 | 1.36 | 1.40 |
| 14 | f | 1210 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 14 | A | 1137 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 14 | H | 1210 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 14 | e | 1122 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 14 | B | 1210 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 14 | G | 1237 | CLA | C1D-ND | 2.71 | 1.41 | 1.37 |
| 14 | F | 1301 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 14 | l | 516 | CLA | C1D-ND | 2.71 | 1.41 | 1.37 |
| 14 | H | 1205 | CLA | CHC-C1C | 2.71 | 1.41 | 1.35 |
| 14 | G | 1137 | CLA | CMB-C2B | -2.71 | 1.46 | 1.51 |
| 14 | L | 1502 | CLA | C1D-ND | 2.70 | 1.41 | 1.37 |
| 14 | e | 1101 | CLA | CMB-C2B | -2.70 | 1.46 | 1.51 |
| 14 | B | 1205 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 14 | e | 1135 | CLA | CMB-C2B | -2.70 | 1.46 | 1.51 |
| 14 | e | 1107 | CLA | C1D-ND | 2.70 | 1.41 | 1.37 |
| 14 | A | 1103 | CLA | C1D-ND | 2.70 | 1.41 | 1.37 |
| 14 | r | 506 | CLA | CMB-C2B | -2.70 | 1.46 | 1.51 |
| 14 | A | 1122 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 14 | f | 1205 | CLA | CHC-C1C | 2.70 | 1.41 | 1.35 |
| 14 | R | 1301 | CLA | CMB-C2B | -2.70 | 1.46 | 1.51 |
| 14 | Z | 506 | CLA | CMB-C2B | -2.70 | 1.46 | 1.51 |
| 14 | f | 1221 | CLA | CMD-C2D | -2.70 | 1.45 | 1.50 |
| 14 | f | 1215 | CLA | CHC-C1C | 2.69 | 1.41 | 1.35 |
| 14 | A | 1101 | CLA | CMB-C2B | -2.69 | 1.46 | 1.51 |
| 14 | B | 1012 | CLA | C1D-ND | 2.69 | 1.41 | 1.37 |
| 14 | 3 | 502 | CLA | CMB-C2B | -2.69 | 1.46 | 1.51 |
| 14 | G | 1128 | CLA | C1D-ND | 2.69 | 1.41 | 1.37 |
| 14 | f | 1205 | CLA | CMC-C2C | -2.69 | 1.45 | 1.50 |
| 14 | G | 1135 | CLA | MG-ND | -2.69 | 2.00 | 2.05 |
| 14 | A | 1125 | CLA | CMB-C2B | -2.69 | 1.46 | 1.51 |
| 14 | H | 1230 | CLA | C3B-C2B | -2.69 | 1.36 | 1.40 |
| 14 | a | 502 | CLA | CMB-C2B | -2.68 | 1.46 | 1.51 |
| 14 | G | 1135 | CLA | CMB-C2B | -2.68 | 1.46 | 1.51 |
| 14 | A | 1135 | CLA | CMB-C2B | -2.68 | 1.46 | 1.51 |
| 14 | A | 1107 | CLA | C1D-ND | 2.68 | 1.41 | 1.37 |
| 14 | G | 1129 | CLA | MG-ND | -2.68 | 2.00 | 2.05 |
| 14 | e | 1135 | CLA | MG-ND | -2.68 | 2.00 | 2.05 |
| 14 | e | 1103 | CLA | C1D-ND | 2.68 | 1.41 | 1.37 |
| 14 | a | 512 | CLA | CMB-C2B | -2.68 | 1.46 | 1.51 |
| 14 | G | 1124 | CLA | CMD-C2D | -2.68 | 1.45 | 1.50 |
| 14 | e | 1103 | CLA | CMD-C2D | -2.68 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1115 | CLA | CMC-C2C | -2.68 | 1.45 | 1.50 |
| 14 | e | 1124 | CLA | CMD-C2D | -2.68 | 1.45 | 1.50 |
| 14 | f | 1220 | CLA | CMC-C2C | -2.68 | 1.45 | 1.50 |
| 14 | e | 1101 | CLA | CMD-C2D | -2.68 | 1.45 | 1.50 |
| 14 | B | 1234 | CLA | CMB-C2B | -2.67 | 1.46 | 1.51 |
| 14 | G | 1103 | CLA | CMD-C2D | -2.67 | 1.45 | 1.50 |
| 14 | G | 1111 | CLA | C1D-ND | 2.67 | 1.41 | 1.37 |
| 14 | L | 1502 | CLA | CMB-C2B | -2.67 | 1.46 | 1.51 |
| 14 | H | 1234 | CLA | CMB-C2B | -2.67 | 1.46 | 1.51 |
| 14 | A | 1124 | CLA | CMD-C2D | -2.67 | 1.45 | 1.50 |
| 14 | B | 1215 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 14 | H | 1229 | CLA | C1D-ND | 2.67 | 1.41 | 1.37 |
| 14 | H | 1220 | CLA | CMC-C2C | -2.67 | 1.45 | 1.50 |
| 14 | v | 512 | CLA | CMB-C2B | -2.67 | 1.46 | 1.51 |
| 14 | G | 1011 | CLA | CHC-C1C | 2.67 | 1.41 | 1.35 |
| 14 | B | 1205 | CLA | CMC-C2C | -2.66 | 1.45 | 1.50 |
| 14 | n | 1503 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 14 | A | 1111 | CLA | C1D-ND | 2.66 | 1.41 | 1.37 |
| 14 | 2 | 506 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 14 | G | 1118 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 14 | B | 1221 | CLA | CMD-C2D | -2.66 | 1.45 | 1.50 |
| 14 | H | 1205 | CLA | CMC-C2C | -2.66 | 1.45 | 1.50 |
| 14 | A | 1103 | CLA | CMD-C2D | -2.66 | 1.45 | 1.50 |
| 14 | f | 1230 | CLA | C3B-C2B | -2.66 | 1.36 | 1.40 |
| 14 | 3 | 512 | CLA | CMB-C2B | -2.66 | 1.46 | 1.51 |
| 14 | 6 | 512 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | e | 1109 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 14 | H | 1215 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 14 | A | 1011 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 14 | e | 1117 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 14 | A | 1101 | CLA | CMD-C2D | -2.65 | 1.45 | 1.50 |
| 14 | f | 1211 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | A | 1109 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 14 | f | 1236 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 14 | e | 1011 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 14 | A | 1119 | CLA | CHC-C1C | 2.65 | 1.41 | 1.35 |
| 14 | B | 1220 | CLA | CMC-C2C | -2.65 | 1.45 | 1.50 |
| 14 | n | 1502 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | T | 1302 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | V | 1502 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | B | 1230 | CLA | C3B-C2B | -2.65 | 1.36 | 1.40 |
| 14 | G | 1107 | CLA | C1D-ND | 2.65 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1101 | CLA | CMD-C2D | -2.65 | 1.45 | 1.50 |
| 14 | f | 1234 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | A | 1118 | CLA | CMB-C2B | -2.65 | 1.46 | 1.51 |
| 14 | A | 1129 | CLA | MG-ND | -2.65 | 2.00 | 2.05 |
| 14 | e | 1129 | CLA | MG-ND | -2.65 | 2.00 | 2.05 |
| 14 | H | 1211 | CLA | CMD-C2D | -2.64 | 1.45 | 1.50 |
| 14 | e | 1131 | CLA | C3B-CAB | -2.64 | 1.42 | 1.47 |
| 14 | G | 1109 | CLA | CHC-C1C | 2.64 | 1.41 | 1.35 |
| 14 | A | 1117 | CLA | C3B-C2B | -2.64 | 1.36 | 1.40 |
| 14 | A | 1131 | CLA | C1D-ND | 2.64 | 1.41 | 1.37 |
| 14 | L | 1503 | CLA | CMB-C2B | -2.64 | 1.46 | 1.51 |
| 14 | f | 1229 | CLA | C1D-ND | 2.64 | 1.41 | 1.37 |
| 14 | f | 1214 | CLA | C3B-C2B | -2.63 | 1.36 | 1.40 |
| 14 | J | 1302 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | Z | 519 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 18 | V | 5218 | LHG | O7-C5 | -2.63 | 1.40 | 1.46 |
| 14 | B | 1229 | CLA | C1D-ND | 2.63 | 1.41 | 1.37 |
| 14 | G | 1117 | CLA | C3B-C2B | -2.63 | 1.36 | 1.40 |
| 14 | e | 1118 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | s | 506 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 18 | e | 5003 | LHG | O7-C5 | -2.63 | 1.40 | 1.46 |
| 14 | s | 512 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | V | 1503 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | H | 1221 | CLA | CMD-C2D | -2.63 | 1.45 | 1.50 |
| 14 | A | 1121 | CLA | CHC-C1C | 2.63 | 1.41 | 1.35 |
| 14 | d | 512 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | Z | 509 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | v | 519 | CLA | CMB-C2B | -2.63 | 1.46 | 1.51 |
| 14 | e | 1022 | CLA | CMD-C2D | -2.63 | 1.45 | 1.50 |
| 14 | G | 1131 | CLA | C1D-ND | 2.62 | 1.41 | 1.37 |
| 14 | e | 1121 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 14 | B | 1211 | CLA | CMD-C2D | -2.62 | 1.45 | 1.50 |
| 14 | e | 1119 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 14 | f | 1218 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | B | 1231 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | B | 1236 | CLA | C3B-C2B | -2.62 | 1.36 | 1.40 |
| 14 | 4 | 506 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | G | 1111 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | A | 1111 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | 2 | 519 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 21 | f | 1852 | SQD | O47-C7 | 2.62 | 1.41 | 1.34 |
| 14 | G | 1132 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 2 | 509 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | G | 1121 | CLA | CHC-C1C | 2.62 | 1.41 | 1.35 |
| 14 | 6 | 519 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | G | 1131 | CLA | C3B-CAB | -2.62 | 1.42 | 1.47 |
| 14 | H | 1203 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | H | 1224 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | l | 1302 | CLA | CMB-C2B | -2.62 | 1.46 | 1.51 |
| 14 | s | 518 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 21 | H | 1852 | SQD | O47-C7 | 2.61 | 1.41 | 1.34 |
| 14 | A | 1022 | CLA | CMD-C2D | -2.61 | 1.45 | 1.50 |
| 14 | e | 1115 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | B | 1211 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | f | 1231 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 18 | L | 5218 | LHG | O7-C5 | -2.61 | 1.40 | 1.46 |
| 14 | B | 1218 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | H | 1231 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | Y | 504 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | f | 1211 | CLA | CMD-C2D | -2.61 | 1.45 | 1.50 |
| 14 | G | 1119 | CLA | CHC-C1C | 2.61 | 1.41 | 1.35 |
| 14 | H | 1021 | CLA | C1D-ND | 2.61 | 1.41 | 1.37 |
| 14 | A | 1131 | CLA | C3B-CAB | -2.61 | 1.42 | 1.47 |
| 18 | A | 5003 | LHG | O7-C5 | -2.61 | 1.40 | 1.46 |
| 14 | e | 1111 | CLA | C1D-ND | 2.61 | 1.41 | 1.37 |
| 14 | 3 | 506 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | Y | 516 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | Z | 512 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 14 | r | 512 | CLA | CMB-C2B | -2.61 | 1.46 | 1.51 |
| 18 | G | 5003 | LHG | O7-C5 | -2.61 | 1.40 | 1.46 |
| 21 | B | 1852 | SQD | O47-C7 | 2.60 | 1.41 | 1.34 |
| 18 | n | 5218 | LHG | O7-C5 | -2.60 | 1.40 | 1.46 |
| 14 | r | 519 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | b | 506 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | q | 510 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | G | 1115 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | e | 1111 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | B | 1224 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | 4 | 512 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | b | 511 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | A | 1132 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | q | 504 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | a | 506 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | e | 1132 | CLA | C3B-C2B | -2.60 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | m | 1103 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | r | 509 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | v | 511 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | A | 1115 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | K | 1103 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | r | 501 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | B | 1214 | CLA | C3B-C2B | -2.60 | 1.36 | 1.40 |
| 14 | u | 511 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | B | 1021 | CLA | C1D-ND | 2.60 | 1.41 | 1.37 |
| 14 | U | 1103 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | s | 519 | CLA | CMB-C2B | -2.60 | 1.46 | 1.51 |
| 14 | G | 1022 | CLA | CMD-C2D | -2.59 | 1.45 | 1.50 |
| 14 | d | 519 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | G | 1022 | CLA | C3B-C2B | -2.59 | 1.36 | 1.40 |
| 14 | B | 1203 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | A | 1022 | CLA | C3B-C2B | -2.59 | 1.36 | 1.40 |
| 14 | 2 | 512 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | t | 506 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | B | 1220 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | H | 1211 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | e | 1112 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | f | 1023 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | f | 1220 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | f | 1210 | CLA | CMC-C2C | -2.59 | 1.45 | 1.50 |
| 14 | f | 1224 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | H | 1023 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | 2 | 501 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | H | 1227 | CLA | C3B-CAB | -2.59 | 1.42 | 1.47 |
| 14 | a | 518 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | a | 519 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | b | 509 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | b | 512 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | e | 1116 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | f | 1203 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | 3 | 519 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | 1 | 504 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | G | 1801 | CLA | CMB-C2B | -2.59 | 1.46 | 1.51 |
| 14 | u | 513 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | A | 1116 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | e | 1131 | CLA | C1D-ND | 2.58 | 1.41 | 1.37 |
| 14 | A | 1112 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | B | 1023 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 3 | 518 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | H | 1218 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | 4 | 509 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | H | 1210 | CLA | CMC-C2C | -2.58 | 1.45 | 1.50 |
| 14 | e | 1140 | CLA | CMC-C2C | -2.58 | 1.45 | 1.50 |
| 14 | G | 1112 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | G | 1132 | CLA | C3B-C2B | -2.58 | 1.36 | 1.40 |
| 14 | A | 1801 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | n | 1501 | CLA | C3B-C2B | -2.58 | 1.36 | 1.40 |
| 14 | B | 1212 | CLA | CMC-C2C | -2.58 | 1.45 | 1.50 |
| 14 | f | 1238 | CLA | CMD-C2D | -2.58 | 1.45 | 1.50 |
| 14 | c | 513 | CLA | CMB-C2B | -2.58 | 1.46 | 1.51 |
| 14 | d | 518 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | F | 1302 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 14 | 1 | 510 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | t | 511 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | A | 1132 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 14 | Z | 513 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | A | 1140 | CLA | CMC-C2C | -2.57 | 1.45 | 1.50 |
| 14 | G | 1140 | CLA | CMC-C2C | -2.57 | 1.45 | 1.50 |
| 14 | 3 | 511 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | 4 | 511 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | Y | 517 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | 2 | 504 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | Y | 510 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | H | 1236 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 14 | c | 518 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | f | 1227 | CLA | C3B-CAB | -2.57 | 1.42 | 1.47 |
| 14 | H | 1212 | CLA | CMC-C2C | -2.57 | 1.45 | 1.50 |
| 14 | e | 1132 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | B | 1227 | CLA | C3B-CAB | -2.57 | 1.42 | 1.47 |
| 14 | f | 1204 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | 1 | 516 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | 6 | 511 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | a | 509 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | H | 1220 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | t | 509 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | 5 | 511 | CLA | CMB-C2B | -2.57 | 1.46 | 1.51 |
| 14 | j | 1302 | CLA | C3B-C2B | -2.57 | 1.36 | 1.40 |
| 14 | 2 | 513 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | e | 1801 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | q | 516 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | t | 512 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | G | 1104 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | c | 509 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | s | 511 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | A | 1104 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | e | 1104 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | B | 1210 | CLA | CMC-C2C | -2.56 | 1.45 | 1.50 |
| 14 | Y | 519 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | 5 | 513 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | G | 1118 | CLA | CMD-C2D | -2.56 | 1.45 | 1.50 |
| 14 | 1 | 519 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | 3 | 509 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | G | 1116 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | f | 1223 | CLA | CMC-C2C | -2.56 | 1.45 | 1.50 |
| 14 | d | 511 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | s | 509 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | 4 | 501 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | 6 | 518 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | Z | 501 | CLA | CMB-C2B | -2.56 | 1.46 | 1.51 |
| 14 | v | 501 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | Z | 504 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | f | 1212 | CLA | CMC-C2C | -2.55 | 1.45 | 1.50 |
| 14 | B | 1223 | CLA | CMC-C2C | -2.55 | 1.45 | 1.50 |
| 14 | H | 1238 | CLA | CMD-C2D | -2.55 | 1.45 | 1.50 |
| 14 | u | 512 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | e | 1139 | CLA | CMD-C2D | -2.55 | 1.45 | 1.50 |
| 14 | H | 1204 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | b | 501 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | 5 | 518 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | L | 1501 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 14 | H | 1214 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 14 | B | 1238 | CLA | CMD-C2D | -2.55 | 1.45 | 1.50 |
| 14 | a | 504 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | B | 1204 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | c | 511 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | V | 1501 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 14 | 3 | 504 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | 5 | 509 | CLA | CMB-C2B | -2.55 | 1.46 | 1.51 |
| 14 | G | 1114 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 14 | e | 1022 | CLA | C3B-C2B | -2.55 | 1.36 | 1.40 |
| 14 | f | 1021 | CLA | C1D-ND | 2.55 | 1.40 | 1.37 |
| 14 | A | 1105 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1105 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | 6 | 501 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | A | 1114 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 14 | B | 1219 | CLA | CMD-C2D | -2.54 | 1.45 | 1.50 |
| 14 | l | 517 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | a | 511 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | G | 1105 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | t | 501 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | 6 | 510 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | H | 1223 | CLA | CMC-C2C | -2.54 | 1.45 | 1.50 |
| 14 | d | 510 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | f | 1240 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | Y | 513 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | r | 504 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | r | 513 | CLA | CMB-C2B | -2.54 | 1.46 | 1.51 |
| 14 | e | 1101 | CLA | C3B-C2B | -2.54 | 1.36 | 1.40 |
| 14 | A | 1135 | CLA | CHC-C1C | 2.53 | 1.41 | 1.35 |
| 14 | G | 1135 | CLA | CHC-C1C | 2.53 | 1.41 | 1.35 |
| 14 | 5 | 512 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | q | 519 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | v | 518 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | 4 | 504 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | A | 1139 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |
| 14 | G | 1139 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |
| 14 | R | 1302 | CLA | C3B-C2B | -2.53 | 1.36 | 1.40 |
| 14 | A | 1113 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | s | 504 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | G | 1237 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |
| 14 | 3 | 513 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | A | 1237 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |
| 14 | e | 1113 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | q | 501 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | G | 1101 | CLA | CMC-C2C | -2.53 | 1.45 | 1.50 |
| 14 | Y | 503 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | A | 1118 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |
| 14 | d | 509 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | e | 1135 | CLA | CHC-C1C | 2.53 | 1.41 | 1.35 |
| 14 | Y | 501 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | a | 513 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | c | 507 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | u | 518 | CLA | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 14 | a | 505 | CLA | CMD-C2D | -2.53 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1219 | CLA | CMD-C2D | -2.52 | 1.45 | 1.50 |
| 14 | A | 1102 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | l | 501 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | c | 512 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | A | 1101 | CLA | CMC-C2C | -2.52 | 1.45 | 1.50 |
| 14 | f | 1219 | CLA | CMD-C2D | -2.52 | 1.45 | 1.50 |
| 14 | q | 513 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | B | 1240 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | H | 1206 | CLA | CHC-C1C | 2.52 | 1.41 | 1.35 |
| 14 | A | 1101 | CLA | C3B-C2B | -2.52 | 1.36 | 1.40 |
| 14 | G | 1138 | CLA | C3B-C2B | -2.52 | 1.36 | 1.40 |
| 14 | l | 513 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | u | 509 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | e | 1237 | CLA | CMD-C2D | -2.52 | 1.45 | 1.50 |
| 14 | 5 | 510 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | v | 510 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | A | 1126 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | q | 517 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | d | 501 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | H | 1240 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | b | 518 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | e | 1102 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | G | 1126 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | e | 1126 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | t | 504 | CLA | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 14 | 3 | 505 | CLA | CMD-C2D | -2.52 | 1.45 | 1.50 |
| 14 | 5 | 503 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | H | 1240 | CLA | CMD-C2D | -2.51 | 1.45 | 1.50 |
| 14 | l | 503 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | t | 518 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | B | 1206 | CLA | CHC-C1C | 2.51 | 1.41 | 1.35 |
| 14 | e | 1114 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |
| 14 | 6 | 503 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | c | 519 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 21 | f | 1852 | SQD | O47-C45 | -2.51 | 1.40 | 1.46 |
| 14 | 4 | 518 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | r | 517 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | H | 1217 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | f | 1234 | CLA | MG-ND | -2.51 | 2.00 | 2.05 |
| 14 | e | 1118 | CLA | CMD-C2D | -2.51 | 1.45 | 1.50 |
| 14 | B | 1217 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | u | 510 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 5 | 501 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | G | 1101 | CLA | C3B-C2B | -2.51 | 1.36 | 1.40 |
| 14 | B | 1212 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | u | 504 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | 5 | 507 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | c | 510 | CLA | CMB-C2B | -2.51 | 1.46 | 1.51 |
| 14 | r | 510 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | B | 1240 | CLA | CMD-C2D | -2.50 | 1.45 | 1.50 |
| 14 | b | 504 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | f | 1206 | CLA | CHC-C1C | 2.50 | 1.41 | 1.35 |
| 14 | d | 503 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | c | 501 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | e | 1136 | CLA | CMD-C2D | -2.50 | 1.45 | 1.50 |
| 14 | 6 | 509 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | G | 1113 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | H | 1212 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | A | 1138 | CLA | C3B-C2B | -2.50 | 1.36 | 1.40 |
| 14 | c | 503 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | s | 513 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | A | 1123 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | f | 1012 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | G | 1102 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | G | 1123 | CLA | CMD-C2D | -2.50 | 1.45 | 1.50 |
| 14 | a | 517 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | f | 1212 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | G | 1120 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | G | 1137 | CLA | C3B-C2B | -2.50 | 1.36 | 1.40 |
| 14 | s | 505 | CLA | CMD-C2D | -2.50 | 1.45 | 1.50 |
| 14 | H | 1228 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | c | 517 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | e | 1101 | CLA | CMC-C2C | -2.50 | 1.45 | 1.50 |
| 14 | K | 1401 | CLA | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 14 | U | 1401 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | 5 | 519 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | B | 1234 | CLA | MG-ND | -2.49 | 2.00 | 2.05 |
| 14 | B | 1228 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | b | 510 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | v | 516 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | G | 1123 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | e | 1123 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | f | 1228 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | b | 516 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1120 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | b | 507 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | q | 503 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | t | 510 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | G | 1109 | CLA | CMD-C2D | -2.49 | 1.45 | 1.50 |
| 14 | B | 1012 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 15 | A | 2001 | PQN | C10-C1 | -2.49 | 1.43 | 1.48 |
| 14 | l | 1303 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | H | 1012 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | e | 1128 | CLA | MG-ND | -2.49 | 2.00 | 2.05 |
| 14 | G | 1131 | CLA | CMD-C2D | -2.49 | 1.45 | 1.50 |
| 14 | G | 1128 | CLA | MG-ND | -2.49 | 2.00 | 2.05 |
| 14 | 2 | 517 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | H | 1226 | CLA | C1D-ND | 2.49 | 1.40 | 1.37 |
| 14 | H | 1230 | CLA | CMC-C2C | -2.49 | 1.45 | 1.50 |
| 21 | B | 1852 | SQD | O47-C45 | -2.49 | 1.40 | 1.46 |
| 14 | 5 | 506 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | A | 1119 | CLA | C3B-C2B | -2.49 | 1.36 | 1.40 |
| 14 | m | 1401 | CLA | CMB-C2B | -2.49 | 1.46 | 1.51 |
| 14 | B | 1214 | CLA | CMC-C2C | -2.49 | 1.45 | 1.50 |
| 14 | a | 501 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | e | 1127 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 14 | T | 1303 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | A | 1128 | CLA | MG-ND | -2.48 | 2.00 | 2.05 |
| 14 | H | 1214 | CLA | CMC-C2C | -2.48 | 1.45 | 1.50 |
| 14 | b | 505 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 14 | H | 1234 | CLA | MG-ND | -2.48 | 2.00 | 2.05 |
| 14 | H | 1202 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | u | 516 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | A | 1120 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | t | 519 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | f | 1240 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 14 | Z | 503 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | 4 | 507 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | b | 519 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | v | 506 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | e | 1123 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 14 | b | 503 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 17 | n | 4219 | BCR | C21-C22 | -2.48 | 1.32 | 1.35 |
| 21 | H | 1852 | SQD | O47-C45 | -2.48 | 1.40 | 1.46 |
| 14 | 4 | 519 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | u | 517 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 5 | 504 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | u | 501 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | 4 | 505 | CLA | CMD-C2D | -2.48 | 1.45 | 1.50 |
| 14 | G | 1122 | CLA | CMC-C2C | -2.48 | 1.45 | 1.50 |
| 14 | v | 503 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | 4 | 516 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | e | 1107 | CLA | MG-ND | -2.48 | 2.00 | 2.05 |
| 14 | 2 | 510 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | q | 512 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | f | 1217 | CLA | CMB-C2B | -2.48 | 1.46 | 1.51 |
| 14 | d | 516 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | v | 509 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | A | 1123 | CLA | CMD-C2D | -2.47 | 1.45 | 1.50 |
| 14 | f | 1214 | CLA | CMC-C2C | -2.47 | 1.45 | 1.50 |
| 14 | B | 1213 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | 5 | 517 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | 6 | 516 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | f | 1202 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | A | 1131 | CLA | CMD-C2D | -2.47 | 1.45 | 1.50 |
| 14 | f | 1213 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | Z | 507 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | A | 1122 | CLA | CMC-C2C | -2.47 | 1.45 | 1.50 |
| 14 | u | 503 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | t | 505 | CLA | CMD-C2D | -2.47 | 1.45 | 1.50 |
| 14 | 4 | 503 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | 4 | 510 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | u | 506 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | v | 517 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | e | 1122 | CLA | CMC-C2C | -2.47 | 1.45 | 1.50 |
| 14 | t | 516 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 15 | G | 2001 | PQN | C10-C1 | -2.47 | 1.43 | 1.48 |
| 14 | 2 | 507 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | B | 1230 | CLA | CMC-C2C | -2.47 | 1.45 | 1.50 |
| 14 | 3 | 510 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | t | 507 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | Z | 517 | CLA | CMB-C2B | -2.47 | 1.46 | 1.51 |
| 14 | A | 1136 | CLA | CMD-C2D | -2.47 | 1.45 | 1.50 |
| 14 | c | 504 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | v | 513 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | d | 513 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | u | 519 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | 5 | 501 | CLA | CMC-C2C | -2.46 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1225 | CLA | MG-ND | -2.46 | 2.00 | 2.05 |
| 14 | r | 518 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | Z | 510 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | B | 1226 | CLA | C1D-ND | 2.46 | 1.40 | 1.37 |
| 14 | s | 510 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | s | 517 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | 6 | 506 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | a | 507 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | G | 1136 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | 2 | 516 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | 3 | 517 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | G | 1107 | CLA | MG-ND | -2.46 | 2.00 | 2.05 |
| 14 | A | 1109 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | B | 1202 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | s | 501 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | A | 1109 | CLA | CMC-C2C | -2.46 | 1.45 | 1.50 |
| 14 | H | 1207 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | 5 | 516 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | e | 1109 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | e | 1131 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | 3 | 501 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | B | 1207 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | Y | 512 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | Z | 518 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | e | 1119 | CLA | CMD-C2D | -2.46 | 1.45 | 1.50 |
| 14 | c | 506 | CLA | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 14 | e | 1138 | CLA | C3B-C2B | -2.46 | 1.37 | 1.40 |
| 14 | d | 507 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | u | 507 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | e | 1119 | CLA | C3B-C2B | -2.45 | 1.37 | 1.40 |
| 14 | e | 1135 | CLA | C3B-CAB | -2.45 | 1.42 | 1.47 |
| 14 | 2 | 503 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | c | 501 | CLA | CMC-C2C | -2.45 | 1.45 | 1.50 |
| 14 | A | 1107 | CLA | MG-ND | -2.45 | 2.00 | 2.05 |
| 14 | n | 1503 | CLA | CMC-C2C | -2.45 | 1.45 | 1.50 |
| 14 | Z | 516 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | A | 1127 | CLA | CMD-C2D | -2.45 | 1.45 | 1.50 |
| 14 | G | 1127 | CLA | CMD-C2D | -2.45 | 1.45 | 1.50 |
| 14 | c | 516 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | 2 | 518 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | v | 507 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | V | 1503 | CLA | CMC-C2C | -2.45 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 1 | 512 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | B | 1021 | CLA | CMC-C2C | -2.45 | 1.45 | 1.50 |
| 14 | J | 1303 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | A | 1119 | CLA | CMD-C2D | -2.45 | 1.45 | 1.50 |
| 17 | V | 4219 | BCR | C21-C22 | -2.45 | 1.32 | 1.35 |
| 14 | 6 | 507 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | d | 506 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | t | 503 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | G | 1119 | CLA | C3B-C2B | -2.45 | 1.37 | 1.40 |
| 14 | H | 1225 | CLA | MG-ND | -2.45 | 2.00 | 2.05 |
| 14 | 3 | 503 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | 2 | 505 | CLA | CMD-C2D | -2.45 | 1.45 | 1.50 |
| 14 | 6 | 513 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | G | 1112 | CLA | C3B-C2B | -2.45 | 1.37 | 1.40 |
| 14 | b | 513 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | B | 1223 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | r | 516 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | f | 1021 | CLA | CMC-C2C | -2.45 | 1.45 | 1.50 |
| 14 | 2 | 505 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | H | 1213 | CLA | CMB-C2B | -2.45 | 1.46 | 1.51 |
| 14 | u | 501 | CLA | CMC-C2C | -2.44 | 1.45 | 1.50 |
| 14 | G | 1119 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 14 | f | 1207 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 14 | 3 | 507 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | r | 507 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | r | 505 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 14 | f | 1230 | CLA | CMC-C2C | -2.44 | 1.45 | 1.50 |
| 14 | f | 1207 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | A | 1135 | CLA | C3B-CAB | -2.44 | 1.43 | 1.47 |
| 14 | H | 1230 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 14 | a | 503 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 15 | e | 2001 | PQN | C10-C1 | -2.44 | 1.43 | 1.48 |
| 14 | Z | 505 | CLA | CMD-C2D | -2.44 | 1.45 | 1.50 |
| 14 | t | 505 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | 6 | 517 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | e | 1128 | CLA | CHC-C1C | 2.44 | 1.41 | 1.35 |
| 14 | a | 510 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | L | 1503 | CLA | CMC-C2C | -2.44 | 1.45 | 1.50 |
| 14 | H | 1207 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | r | 503 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | H | 1223 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | d | 517 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1107 | CLA | CMC-C2C | -2.44 | 1.45 | 1.50 |
| 14 | l | 518 | CLA | CMB-C2B | -2.44 | 1.46 | 1.51 |
| 14 | A | 1137 | CLA | C3B-C2B | -2.44 | 1.37 | 1.40 |
| 14 | A | 1107 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | B | 1225 | CLA | C3B-CAB | -2.43 | 1.43 | 1.47 |
| 14 | m | 1103 | CLA | CMD-C2D | -2.43 | 1.45 | 1.50 |
| 14 | G | 1109 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | e | 1113 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | G | 1113 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 17 | L | 4219 | BCR | C21-C22 | -2.43 | 1.32 | 1.35 |
| 14 | s | 505 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | 4 | 513 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | f | 1225 | CLA | MG-ND | -2.43 | 2.01 | 2.05 |
| 14 | A | 1022 | CLA | MG-ND | -2.43 | 2.01 | 2.05 |
| 14 | A | 1113 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | G | 1128 | CLA | CMD-C2D | -2.43 | 1.45 | 1.50 |
| 14 | d | 505 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | A | 1112 | CLA | C3B-C2B | -2.43 | 1.37 | 1.40 |
| 14 | H | 1207 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | 3 | 516 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | r | 505 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | f | 1226 | CLA | C1D-ND | 2.43 | 1.40 | 1.37 |
| 14 | H | 1225 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | e | 1109 | CLA | CMC-C2C | -2.43 | 1.45 | 1.50 |
| 14 | t | 513 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | u | 505 | CLA | CMD-C2D | -2.43 | 1.45 | 1.50 |
| 14 | Y | 518 | CLA | CMB-C2B | -2.43 | 1.46 | 1.51 |
| 14 | G | 1107 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | c | 505 | CLA | CMD-C2D | -2.42 | 1.45 | 1.50 |
| 14 | G | 1135 | CLA | C3B-CAB | -2.42 | 1.43 | 1.47 |
| 14 | f | 1239 | CLA | CHC-C1C | 2.42 | 1.41 | 1.35 |
| 14 | m | 1105 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |
| 14 | A | 1237 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | e | 1237 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | f | 1225 | CLA | C3B-CAB | -2.42 | 1.43 | 1.47 |
| 14 | e | 1022 | CLA | MG-ND | -2.42 | 2.01 | 2.05 |
| 14 | A | 1130 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | B | 1239 | CLA | CHC-C1C | 2.42 | 1.41 | 1.35 |
| 14 | H | 1239 | CLA | CHC-C1C | 2.42 | 1.41 | 1.35 |
| 18 | B | 1842 | LHG | O8-C6 | -2.42 | 1.39 | 1.45 |
| 14 | 5 | 505 | CLA | CMD-C2D | -2.42 | 1.45 | 1.50 |
| 14 | 6 | 505 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | s | 503 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |
| 14 | s | 507 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |
| 14 | G | 1130 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | G | 1022 | CLA | MG-ND | -2.42 | 2.01 | 2.05 |
| 14 | H | 1021 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | B | 1209 | CLA | CMC-C2C | -2.42 | 1.45 | 1.50 |
| 14 | K | 1103 | CLA | CMD-C2D | -2.42 | 1.45 | 1.50 |
| 14 | Z | 505 | CLA | CMB-C2B | -2.42 | 1.46 | 1.51 |
| 14 | H | 1225 | CLA | C3B-CAB | -2.42 | 1.43 | 1.47 |
| 14 | A | 1128 | CLA | CMD-C2D | -2.41 | 1.45 | 1.50 |
| 14 | f | 1230 | CLA | CMD-C2D | -2.41 | 1.45 | 1.50 |
| 14 | 1 | 505 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 14 | Z | 502 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 14 | B | 1230 | CLA | CMD-C2D | -2.41 | 1.45 | 1.50 |
| 14 | G | 1128 | CLA | CHC-C1C | 2.41 | 1.41 | 1.35 |
| 14 | B | 1207 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 18 | H | 1842 | LHG | O8-C6 | -2.41 | 1.39 | 1.45 |
| 14 | 5 | 505 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 14 | q | 505 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 14 | 2 | 502 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 14 | e | 1126 | CLA | CMD-C2D | -2.41 | 1.45 | 1.50 |
| 14 | e | 1130 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 14 | e | 1137 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 14 | B | 1207 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 14 | f | 1203 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 14 | f | 1209 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 14 | v | 502 | CLA | C3B-C2B | -2.41 | 1.37 | 1.40 |
| 14 | q | 518 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 14 | u | 505 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 14 | H | 1209 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 14 | B | 1201 | CLA | CMB-C2B | -2.41 | 1.46 | 1.51 |
| 14 | A | 1126 | CLA | CMD-C2D | -2.41 | 1.45 | 1.50 |
| 14 | H | 1203 | CLA | CMC-C2C | -2.41 | 1.45 | 1.50 |
| 14 | A | 1128 | CLA | CHC-C1C | 2.41 | 1.41 | 1.35 |
| 14 | v | 505 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | 3 | 505 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | U | 1105 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | a | 516 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | G | 1237 | CLA | CMC-C2C | -2.40 | 1.45 | 1.50 |
| 14 | B | 1203 | CLA | CMC-C2C | -2.40 | 1.45 | 1.50 |
| 14 | b | 505 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 15 | e | 2001 | PQN | C5-C4 | -2.40 | 1.43 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 4 | 505 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | 4 | 517 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | G | 1132 | CLA | CMD-C2D | -2.40 | 1.45 | 1.50 |
| 14 | U | 1103 | CLA | CMD-C2D | -2.40 | 1.45 | 1.50 |
| 14 | f | 1223 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | G | 1110 | CLA | C3B-C2B | -2.40 | 1.37 | 1.40 |
| 14 | e | 1121 | CLA | MG-ND | -2.40 | 2.01 | 2.05 |
| 15 | H | 2002 | PQN | C11-C12 | 2.40 | 1.54 | 1.50 |
| 14 | A | 1121 | CLA | MG-ND | -2.40 | 2.01 | 2.05 |
| 14 | f | 1226 | CLA | CHC-C1C | 2.40 | 1.41 | 1.35 |
| 14 | e | 1112 | CLA | C3B-C2B | -2.40 | 1.37 | 1.40 |
| 14 | G | 1119 | CLA | MG-ND | -2.40 | 2.01 | 2.05 |
| 14 | t | 517 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | s | 516 | CLA | CMB-C2B | -2.40 | 1.46 | 1.51 |
| 14 | f | 1225 | CLA | CMC-C2C | -2.40 | 1.45 | 1.50 |
| 14 | A | 1132 | CLA | CMD-C2D | -2.39 | 1.45 | 1.50 |
| 21 | f | 1852 | SQD | O4-C4 | -2.39 | 1.37 | 1.43 |
| 15 | A | 2001 | PQN | C5-C4 | -2.39 | 1.43 | 1.48 |
| 14 | B | 1235 | CLA | CMD-C2D | -2.39 | 1.45 | 1.50 |
| 14 | Y | 505 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 14 | f | 1221 | CLA | MG-ND | -2.39 | 2.01 | 2.05 |
| 14 | H | 1222 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 14 | B | 1225 | CLA | CMC-C2C | -2.39 | 1.45 | 1.50 |
| 14 | e | 1128 | CLA | CMD-C2D | -2.39 | 1.45 | 1.50 |
| 14 | L | 1502 | CLA | C3B-CAB | -2.39 | 1.43 | 1.47 |
| 14 | f | 1201 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 14 | G | 1121 | CLA | MG-ND | -2.39 | 2.01 | 2.05 |
| 18 | f | 1842 | LHG | O8-C6 | -2.39 | 1.39 | 1.45 |
| 14 | e | 1119 | CLA | MG-ND | -2.39 | 2.01 | 2.05 |
| 14 | H | 1226 | CLA | CHC-C1C | 2.39 | 1.41 | 1.35 |
| 14 | e | 1132 | CLA | CMD-C2D | -2.39 | 1.45 | 1.50 |
| 14 | f | 1222 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 14 | f | 1207 | CLA | CMC-C2C | -2.39 | 1.45 | 1.50 |
| 14 | e | 1237 | CLA | MG-ND | -2.39 | 2.01 | 2.05 |
| 14 | H | 1201 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 14 | q | 507 | CLA | CMB-C2B | -2.39 | 1.46 | 1.51 |
| 14 | G | 1140 | CLA | CMD-C2D | -2.38 | 1.45 | 1.50 |
| 14 | K | 1105 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 14 | A | 1119 | CLA | MG-ND | -2.38 | 2.01 | 2.05 |
| 14 | B | 1222 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 14 | n | 1502 | CLA | C3B-CAB | -2.38 | 1.43 | 1.47 |
| 14 | c | 505 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1226 | CLA | CHC-C1C | 2.38 | 1.41 | 1.35 |
| 14 | G | 1126 | CLA | CMD-C2D | -2.38 | 1.45 | 1.50 |
| 14 | 6 | 502 | CLA | C3B-C2B | -2.38 | 1.37 | 1.40 |
| 14 | b | 517 | CLA | CMB-C2B | -2.38 | 1.46 | 1.51 |
| 14 | G | 1112 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | e | 1140 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 14 | H | 1235 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 14 | e | 1138 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 14 | V | 1502 | CLA | C3B-CAB | -2.37 | 1.43 | 1.47 |
| 14 | A | 1237 | CLA | MG-ND | -2.37 | 2.01 | 2.05 |
| 14 | e | 1112 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | e | 1126 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | a | 505 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 14 | B | 1206 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 14 | 2 | 501 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | G | 1132 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | f | 1235 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 15 | B | 2002 | PQN | C11-C12 | 2.37 | 1.54 | 1.50 |
| 21 | B | 1852 | SQD | O4-C4 | -2.37 | 1.37 | 1.43 |
| 14 | A | 1112 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | B | 1229 | CLA | CMB-C2B | -2.37 | 1.46 | 1.51 |
| 14 | H | 1206 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 14 | Z | 501 | CLA | CMC-C2C | -2.37 | 1.45 | 1.50 |
| 14 | q | 516 | CLA | CMD-C2D | -2.37 | 1.45 | 1.50 |
| 14 | B | 1221 | CLA | MG-ND | -2.37 | 2.01 | 2.05 |
| 14 | r | 502 | CLA | C3B-C2B | -2.36 | 1.37 | 1.40 |
| 14 | H | 1201 | CLA | CMD-C2D | -2.36 | 1.45 | 1.50 |
| 14 | r | 501 | CLA | CMC-C2C | -2.36 | 1.45 | 1.50 |
| 14 | d | 502 | CLA | C3B-C2B | -2.36 | 1.37 | 1.40 |
| 14 | l | 516 | CLA | CMD-C2D | -2.36 | 1.45 | 1.50 |
| 14 | Z | 513 | CLA | C3B-C2B | -2.36 | 1.37 | 1.40 |
| 14 | H | 1226 | CLA | CMC-C2C | -2.36 | 1.45 | 1.50 |
| 14 | G | 1111 | CLA | CMD-C2D | -2.36 | 1.45 | 1.50 |
| 14 | A | 1126 | CLA | CMC-C2C | -2.36 | 1.45 | 1.50 |
| 14 | H | 1221 | CLA | MG-ND | -2.36 | 2.01 | 2.05 |
| 14 | G | 1126 | CLA | CMC-C2C | -2.36 | 1.45 | 1.50 |
| 14 | Y | 516 | CLA | CMD-C2D | -2.36 | 1.45 | 1.50 |
| 14 | H | 1229 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 14 | A | 1140 | CLA | CMD-C2D | -2.36 | 1.45 | 1.50 |
| 14 | l | 507 | CLA | CMB-C2B | -2.36 | 1.46 | 1.51 |
| 14 | Y | 507 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 15 | G | 2001 | PQN | C5-C4 | -2.35 | 1.43 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1202 | CLA | CMD-C2D | -2.35 | 1.45 | 1.50 |
| 14 | f | 1201 | CLA | CMD-C2D | -2.35 | 1.45 | 1.50 |
| 14 | 6 | 504 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 14 | f | 1202 | CLA | CMD-C2D | -2.35 | 1.45 | 1.50 |
| 14 | Y | 506 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 14 | v | 505 | CLA | CMD-C2D | -2.35 | 1.45 | 1.50 |
| 14 | G | 1237 | CLA | MG-ND | -2.35 | 2.01 | 2.05 |
| 14 | v | 504 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 15 | f | 2002 | PQN | C11-C3 | 2.35 | 1.55 | 1.51 |
| 14 | A | 1111 | CLA | CMD-C2D | -2.35 | 1.45 | 1.50 |
| 14 | l | 506 | CLA | CMB-C2B | -2.35 | 1.46 | 1.51 |
| 14 | t | 508 | CLA | C3B-C2B | -2.34 | 1.37 | 1.40 |
| 14 | q | 506 | CLA | CMB-C2B | -2.34 | 1.46 | 1.51 |
| 17 | G | 4003 | BCR | C30-C25 | -2.34 | 1.50 | 1.53 |
| 14 | A | 1132 | CLA | CMC-C2C | -2.34 | 1.45 | 1.50 |
| 14 | d | 505 | CLA | CMD-C2D | -2.34 | 1.45 | 1.50 |
| 14 | e | 1111 | CLA | CMD-C2D | -2.34 | 1.45 | 1.50 |
| 14 | 6 | 505 | CLA | CMD-C2D | -2.34 | 1.45 | 1.50 |
| 21 | H | 1852 | SQD | O4-C4 | -2.34 | 1.37 | 1.43 |
| 15 | e | 2001 | PQN | C11-C3 | 2.34 | 1.55 | 1.51 |
| 15 | f | 2002 | PQN | C11-C12 | 2.34 | 1.54 | 1.50 |
| 14 | f | 1201 | CLA | CMC-C2C | -2.34 | 1.45 | 1.50 |
| 14 | u | 518 | CLA | CMD-C2D | -2.34 | 1.45 | 1.50 |
| 14 | B | 1201 | CLA | CMC-C2C | -2.34 | 1.45 | 1.50 |
| 14 | B | 1226 | CLA | CMC-C2C | -2.34 | 1.45 | 1.50 |
| 14 | 2 | 502 | CLA | CMD-C2D | -2.34 | 1.45 | 1.50 |
| 14 | B | 1202 | CLA | CMD-C2D | -2.34 | 1.45 | 1.50 |
| 14 | e | 1130 | CLA | MG-ND | -2.34 | 2.01 | 2.05 |
| 14 | A | 1117 | CLA | CMC-C2C | -2.34 | 1.45 | 1.50 |
| 14 | c | 518 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | e | 1132 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | Z | 502 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | e | 1113 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | d | 504 | CLA | CMB-C2B | -2.33 | 1.46 | 1.51 |
| 14 | H | 1201 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | A | 1132 | CLA | C3B-CAB | -2.33 | 1.43 | 1.47 |
| 14 | A | 1138 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | G | 1113 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | e | 1128 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | f | 1206 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | A | 1113 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | G | 1132 | CLA | C3B-CAB | -2.33 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | f | 1226 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | A | 1110 | CLA | C3B-C2B | -2.33 | 1.37 | 1.40 |
| 14 | r | 513 | CLA | C3B-C2B | -2.33 | 1.37 | 1.40 |
| 14 | f | 1229 | CLA | CMB-C2B | -2.33 | 1.46 | 1.51 |
| 14 | f | 1206 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | G | 1138 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | f | 1216 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | s | 502 | CLA | CMD-C2D | -2.33 | 1.45 | 1.50 |
| 14 | B | 1234 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | H | 1234 | CLA | CMC-C2C | -2.33 | 1.45 | 1.50 |
| 14 | G | 1112 | CLA | C3B-CAB | -2.32 | 1.43 | 1.47 |
| 14 | b | 502 | CLA | C3B-C2B | -2.32 | 1.37 | 1.40 |
| 17 | B | 4017 | BCR | C10-C9 | -2.32 | 1.32 | 1.35 |
| 14 | 4 | 511 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 14 | A | 1112 | CLA | C3B-CAB | -2.32 | 1.43 | 1.47 |
| 14 | G | 1128 | CLA | C4B-CHC | -2.32 | 1.34 | 1.41 |
| 15 | H | 2002 | PQN | C11-C3 | 2.32 | 1.55 | 1.51 |
| 20 | l | 5104 | LMG | O7-C8 | -2.32 | 1.40 | 1.46 |
| 17 | f | 4017 | BCR | C10-C9 | -2.32 | 1.32 | 1.35 |
| 14 | G | 1117 | CLA | CMC-C2C | -2.32 | 1.45 | 1.50 |
| 14 | 5 | 518 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 20 | T | 5104 | LMG | O7-C8 | -2.32 | 1.40 | 1.46 |
| 14 | B | 1201 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 14 | Y | 503 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 20 | J | 5104 | LMG | O7-C8 | -2.32 | 1.40 | 1.46 |
| 14 | A | 1130 | CLA | MG-ND | -2.32 | 2.01 | 2.05 |
| 15 | A | 2001 | PQN | C11-C3 | 2.32 | 1.55 | 1.51 |
| 14 | G | 1110 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 15 | B | 2002 | PQN | C11-C3 | 2.32 | 1.55 | 1.51 |
| 14 | f | 1216 | CLA | CMD-C2D | -2.32 | 1.45 | 1.50 |
| 14 | 3 | 502 | CLA | CMD-C2D | -2.31 | 1.45 | 1.50 |
| 14 | B | 1226 | CLA | C4B-CHC | -2.31 | 1.34 | 1.41 |
| 14 | H | 1215 | CLA | CMD-C2D | -2.31 | 1.45 | 1.50 |
| 14 | b | 511 | CLA | CMD-C2D | -2.31 | 1.45 | 1.50 |
| 14 | f | 1213 | CLA | CMD-C2D | -2.31 | 1.45 | 1.50 |
| 14 | f | 1215 | CLA | CMD-C2D | -2.31 | 1.45 | 1.50 |
| 14 | s | 506 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |
| 14 | 4 | 502 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | H | 1226 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | j | 1301 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | B | 1021 | CLA | MG-ND | -2.31 | 2.01 | 2.05 |
| 14 | H | 1216 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | u | 502 | CLA | CMD-C2D | -2.31 | 1.45 | 1.50 |
| 14 | e | 1128 | CLA | C4B-CHC | -2.31 | 1.34 | 1.41 |
| 14 | 2 | 513 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | e | 1107 | CLA | C3B-CAB | -2.31 | 1.43 | 1.47 |
| 15 | G | 2001 | PQN | C11-C3 | 2.31 | 1.55 | 1.51 |
| 14 | f | 1226 | CLA | C4B-CHC | -2.31 | 1.34 | 1.41 |
| 14 | B | 1216 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |
| 17 | H | 4017 | BCR | C10-C9 | -2.31 | 1.32 | 1.35 |
| 14 | G | 1133 | CLA | MG-ND | -2.31 | 2.01 | 2.05 |
| 14 | f | 1021 | CLA | MG-ND | -2.31 | 2.01 | 2.05 |
| 14 | A | 1135 | CLA | C1D-ND | 2.31 | 1.40 | 1.37 |
| 14 | A | 1128 | CLA | CMC-C2C | -2.31 | 1.45 | 1.50 |
| 14 | Z | 512 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 17 | A | 4003 | BCR | C30-C25 | -2.31 | 1.50 | 1.53 |
| 14 | 4 | 508 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | G | 1121 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | e | 1121 | CLA | C3B-C2B | -2.31 | 1.37 | 1.40 |
| 14 | H | 1023 | CLA | MG-ND | -2.31 | 2.01 | 2.05 |
| 14 | H | 1216 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | G | 1120 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | F | 1301 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 14 | t | 502 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 14 | B | 1206 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | f | 1234 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | A | 1120 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | R | 1301 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 14 | G | 1123 | CLA | MG-ND | -2.30 | 2.01 | 2.05 |
| 14 | f | 1226 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 14 | e | 1108 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | Z | 517 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | G | 1105 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | e | 1117 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | B | 1216 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | A | 1107 | CLA | C3B-CAB | -2.30 | 1.43 | 1.47 |
| 14 | A | 1128 | CLA | C4B-CHC | -2.30 | 1.34 | 1.41 |
| 14 | t | 503 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | e | 1112 | CLA | C3B-CAB | -2.30 | 1.43 | 1.47 |
| 14 | j | 1302 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | A | 1237 | CLA | CHC-C1C | 2.30 | 1.40 | 1.35 |
| 14 | e | 1137 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | G | 1130 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | a | 502 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1133 | CLA | MG-ND | -2.30 | 2.01 | 2.05 |
| 14 | t | 511 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | A | 1122 | CLA | C3B-C2B | -2.30 | 1.37 | 1.40 |
| 14 | G | 1022 | CLA | CMC-C2C | -2.30 | 1.45 | 1.50 |
| 14 | r | 502 | CLA | CMD-C2D | -2.30 | 1.45 | 1.50 |
| 14 | G | 1135 | CLA | C1D-ND | 2.29 | 1.40 | 1.37 |
| 14 | B | 1220 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | B | 1023 | CLA | MG-ND | -2.29 | 2.01 | 2.05 |
| 14 | f | 1023 | CLA | MG-ND | -2.29 | 2.01 | 2.05 |
| 14 | B | 1213 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | A | 1108 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | Z | 512 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | e | 1110 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 14 | e | 1112 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | d | 502 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | e | 1117 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | A | 1125 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | A | 1136 | CLA | CMC-C2C | -2.29 | 1.45 | 1.50 |
| 14 | e | 1135 | CLA | C1D-ND | 2.29 | 1.40 | 1.37 |
| 14 | H | 1213 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | f | 1012 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | 3 | 506 | CLA | CMC-C2C | -2.29 | 1.45 | 1.50 |
| 14 | f | 1219 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 14 | e | 1132 | CLA | C3B-CAB | -2.29 | 1.43 | 1.47 |
| 14 | A | 1130 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | G | 1125 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | e | 1122 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 14 | 4 | 503 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | 6 | 502 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | H | 1220 | CLA | CMD-C2D | -2.29 | 1.45 | 1.50 |
| 14 | B | 1215 | CLA | CMD-C2D | -2.29 | 1.46 | 1.50 |
| 14 | B | 1226 | CLA | C3B-C2B | -2.29 | 1.37 | 1.40 |
| 17 | V | 4219 | BCR | C17-C18 | -2.29 | 1.32 | 1.35 |
| 14 | r | 508 | CLA | CMC-C2C | -2.29 | 1.46 | 1.50 |
| 14 | e | 1133 | CLA | MG-ND | -2.29 | 2.01 | 2.05 |
| 14 | 2 | 512 | CLA | CMD-C2D | -2.29 | 1.46 | 1.50 |
| 14 | q | 502 | CLA | CMD-C2D | -2.29 | 1.46 | 1.50 |
| 14 | Z | 506 | CLA | CMC-C2C | -2.29 | 1.46 | 1.50 |
| 14 | e | 1120 | CLA | CMC-C2C | -2.29 | 1.46 | 1.50 |
| 14 | e | 1022 | CLA | CMC-C2C | -2.29 | 1.46 | 1.50 |
| 14 | r | 517 | CLA | CMC-C2C | -2.29 | 1.46 | 1.50 |
| 14 | H | 1226 | CLA | C4B-CHC | -2.28 | 1.34 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1110 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | G | 1128 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 14 | f | 1220 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | G | 1108 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | e | 1105 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | l | 502 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | Y | 502 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | t | 518 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | H | 1021 | CLA | MG-ND | -2.28 | 2.01 | 2.05 |
| 14 | V | 1502 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 14 | A | 1105 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | H | 1206 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 14 | b | 503 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | G | 1237 | CLA | CHC-C1C | 2.28 | 1.40 | 1.35 |
| 21 | n | 5216 | SQD | O2-C2 | -2.28 | 1.37 | 1.43 |
| 22 | X | 170 | FMN | C10-N1 | 2.28 | 1.37 | 1.33 |
| 14 | 2 | 517 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 14 | A | 1133 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | U | 1105 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | r | 512 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | G | 1107 | CLA | C3B-CAB | -2.28 | 1.43 | 1.47 |
| 14 | A | 1022 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 14 | b | 508 | CLA | C3B-C2B | -2.28 | 1.37 | 1.40 |
| 14 | A | 1112 | CLA | CMD-C2D | -2.28 | 1.46 | 1.50 |
| 14 | G | 1110 | CLA | CMC-C2C | -2.28 | 1.46 | 1.50 |
| 14 | n | 1502 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | A | 1137 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | 5 | 502 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | G | 1136 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | q | 503 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | G | 1122 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 14 | f | 1012 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | A | 1115 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | e | 1115 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | Z | 519 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 14 | G | 1130 | CLA | MG-ND | -2.27 | 2.01 | 2.05 |
| 14 | e | 1104 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | A | 1013 | CLA | MG-ND | -2.27 | 2.01 | 2.05 |
| 14 | e | 1125 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | n | 1503 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | G | 1112 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | G | 1137 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 3 | 509 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | e | 1237 | CLA | CHC-C1C | 2.27 | 1.40 | 1.35 |
| 14 | A | 1104 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | 1 | 503 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 22 | P | 170 | FMN | C10-N1 | 2.27 | 1.37 | 1.33 |
| 14 | B | 1222 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | G | 1129 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 22 | p | 170 | FMN | C10-N1 | 2.27 | 1.37 | 1.33 |
| 14 | A | 1110 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | A | 1123 | CLA | MG-ND | -2.27 | 2.01 | 2.05 |
| 17 | e | 4003 | BCR | C30-C25 | -2.27 | 1.50 | 1.53 |
| 14 | f | 1209 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 14 | r | 519 | CLA | C3B-C2B | -2.27 | 1.37 | 1.40 |
| 14 | B | 1012 | CLA | CMD-C2D | -2.27 | 1.46 | 1.50 |
| 17 | H | 4017 | BCR | C21-C22 | -2.27 | 1.32 | 1.35 |
| 14 | e | 1136 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | A | 1801 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | e | 1110 | CLA | CMC-C2C | -2.27 | 1.46 | 1.50 |
| 14 | H | 1222 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | a | 506 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | G | 1104 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | K | 1105 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | d | 518 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | q | 512 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | A | 1104 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | Z | 508 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | q | 505 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | e | 1801 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 21 | V | 5216 | SQD | O2-C2 | -2.26 | 1.37 | 1.43 |
| 14 | F | 1302 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | L | 1502 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | 4 | 518 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | G | 1013 | CLA | MG-ND | -2.26 | 2.01 | 2.05 |
| 14 | A | 1116 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | q | 516 | CLA | MG-ND | -2.26 | 2.01 | 2.05 |
| 14 | B | 1206 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 14 | e | 1130 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | s | 509 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | A | 1129 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 21 | L | 5216 | SQD | O2-C2 | -2.26 | 1.37 | 1.43 |
| 14 | A | 1121 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |
| 14 | v | 519 | CLA | C3B-C2B | -2.26 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1133 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | e | 1123 | CLA | MG-ND | -2.26 | 2.01 | 2.05 |
| 14 | f | 1222 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 14 | m | 1105 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | G | 1103 | CLA | MG-ND | -2.26 | 2.01 | 2.05 |
| 14 | Y | 512 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | e | 1116 | CLA | CMC-C2C | -2.26 | 1.46 | 1.50 |
| 20 | H | 5002 | LMG | O7-C8 | -2.26 | 1.41 | 1.46 |
| 14 | A | 1118 | CLA | MG-ND | -2.26 | 2.01 | 2.05 |
| 14 | Y | 511 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | b | 518 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | f | 1227 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | G | 1115 | CLA | CMD-C2D | -2.26 | 1.46 | 1.50 |
| 14 | v | 502 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | e | 1133 | CLA | C3B-CAB | -2.25 | 1.43 | 1.47 |
| 17 | n | 4219 | BCR | C17-C18 | -2.25 | 1.32 | 1.35 |
| 14 | f | 1206 | CLA | C4B-CHC | -2.25 | 1.34 | 1.41 |
| 20 | B | 5002 | LMG | O7-C8 | -2.25 | 1.41 | 1.46 |
| 14 | e | 1118 | CLA | MG-ND | -2.25 | 2.01 | 2.05 |
| 14 | R | 1302 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | e | 1133 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 20 | f | 5002 | LMG | O7-C8 | -2.25 | 1.41 | 1.46 |
| 14 | 2 | 508 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 14 | 6 | 519 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 14 | a | 509 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 17 | L | 4219 | BCR | C17-C18 | -2.25 | 1.32 | 1.35 |
| 14 | G | 1801 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 14 | H | 1012 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | H | 1209 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | 5 | 508 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 14 | B | 1206 | CLA | C4B-CHC | -2.25 | 1.34 | 1.41 |
| 14 | L | 1503 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | 2 | 506 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 14 | c | 508 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |
| 14 | 1 | 512 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | q | 502 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 14 | B | 1227 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | f | 1217 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | 2 | 519 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 14 | d | 503 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | B | 1217 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | A | 1138 | CLA | CMC-C2C | -2.25 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | 2 | 503 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | e | 1103 | CLA | MG-ND | -2.25 | 2.01 | 2.05 |
| 14 | Z | 503 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | c | 502 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | l | 511 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | H | 1206 | CLA | C3B-C2B | -2.25 | 1.37 | 1.40 |
| 14 | A | 1117 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | r | 503 | CLA | CMD-C2D | -2.25 | 1.46 | 1.50 |
| 14 | A | 1124 | CLA | MG-ND | -2.25 | 2.01 | 2.05 |
| 14 | G | 1133 | CLA | C3B-CAB | -2.24 | 1.43 | 1.47 |
| 14 | n | 1501 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | s | 502 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 14 | V | 1503 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | H | 1206 | CLA | C4B-CHC | -2.24 | 1.34 | 1.41 |
| 14 | G | 1124 | CLA | MG-ND | -2.24 | 2.01 | 2.05 |
| 14 | 2 | 512 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 17 | B | 4017 | BCR | C21-C22 | -2.24 | 1.32 | 1.35 |
| 17 | f | 4017 | BCR | C21-C22 | -2.24 | 1.32 | 1.35 |
| 14 | Y | 516 | CLA | MG-ND | -2.24 | 2.01 | 2.05 |
| 14 | B | 1023 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | e | 1104 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | G | 1116 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 14 | e | 1138 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 14 | r | 512 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 14 | B | 1012 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 14 | f | 1023 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | G | 1114 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | B | 1203 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | V | 1502 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | 6 | 518 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | G | 1104 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 14 | v | 517 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | c | 502 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 14 | B | 1209 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | l | 1302 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 14 | G | 1138 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 14 | H | 1217 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | 6 | 517 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | G | 1117 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | a | 509 | CLA | CMD-C2D | -2.24 | 1.46 | 1.50 |
| 14 | u | 508 | CLA | CMC-C2C | -2.24 | 1.46 | 1.50 |
| 14 | A | 1103 | CLA | MG-ND | -2.24 | 2.01 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1219 | CLA | C3B-C2B | -2.24 | 1.37 | 1.40 |
| 14 | 1 | 516 | CLA | MG-ND | -2.23 | 2.01 | 2.05 |
| 21 | H | 1852 | SQD | O3-C3 | -2.23 | 1.37 | 1.43 |
| 14 | 1 | 519 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 21 | 2 | 822 | SQD | O2-C2 | -2.23 | 1.37 | 1.43 |
| 14 | H | 1210 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 17 | n | 4219 | BCR | C1-C6 | -2.23 | 1.50 | 1.53 |
| 14 | r | 506 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 18 | A | 5005 | LHG | O7-C5 | -2.23 | 1.41 | 1.46 |
| 18 | G | 5005 | LHG | O7-C5 | -2.23 | 1.41 | 1.46 |
| 14 | f | 1234 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | m | 1401 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 14 | f | 1021 | CLA | C3B-CAB | -2.23 | 1.43 | 1.47 |
| 14 | G | 1106 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 18 | e | 5005 | LHG | O7-C5 | -2.23 | 1.41 | 1.46 |
| 14 | e | 1122 | CLA | C3B-CAB | -2.23 | 1.43 | 1.47 |
| 14 | J | 1302 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 14 | A | 1114 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | 1 | 505 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | e | 1110 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 21 | B | 1852 | SQD | O3-C3 | -2.23 | 1.37 | 1.43 |
| 14 | R | 1301 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | f | 1212 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | f | 1235 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 14 | 1 | 502 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 14 | 3 | 502 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 14 | B | 1204 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | d | 519 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 14 | H | 1203 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | n | 1502 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | G | 1125 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 14 | f | 1231 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | 6 | 503 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | a | 519 | CLA | C3B-C2B | -2.23 | 1.37 | 1.40 |
| 14 | B | 1234 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | F | 1301 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | 1 | 506 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 14 | H | 1221 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 14 | v | 518 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | A | 1106 | CLA | CMC-C2C | -2.23 | 1.46 | 1.50 |
| 14 | f | 1203 | CLA | CMD-C2D | -2.23 | 1.46 | 1.50 |
| 14 | A | 1133 | CLA | C3B-CAB | -2.22 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1021 | CLA | C3B-CAB | -2.22 | 1.43 | 1.47 |
| 14 | e | 1124 | CLA | MG-ND | -2.22 | 2.01 | 2.05 |
| 14 | A | 1122 | CLA | C3B-CAB | -2.22 | 1.43 | 1.47 |
| 14 | Y | 505 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | d | 517 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | e | 1129 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | f | 1213 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | v | 506 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | A | 1125 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 14 | Y | 506 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | e | 1013 | CLA | MG-ND | -2.22 | 2.01 | 2.05 |
| 14 | Y | 502 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 14 | l | 507 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | q | 506 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | H | 1012 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | e | 1114 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 21 | r | 822 | SQD | O2-C2 | -2.22 | 1.37 | 1.43 |
| 21 | u | 822 | SQD | O2-C2 | -2.22 | 1.37 | 1.43 |
| 14 | H | 1021 | CLA | C3B-CAB | -2.22 | 1.43 | 1.47 |
| 21 | Z | 822 | SQD | O2-C2 | -2.22 | 1.37 | 1.43 |
| 14 | a | 502 | CLA | C3B-C2B | -2.22 | 1.37 | 1.40 |
| 14 | H | 1234 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | Y | 507 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | u | 517 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | j | 1301 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | H | 1206 | CLA | MG-ND | -2.22 | 2.01 | 2.05 |
| 21 | 5 | 822 | SQD | O2-C2 | -2.22 | 1.37 | 1.43 |
| 14 | d | 519 | CLA | C3B-CAB | -2.22 | 1.43 | 1.47 |
| 14 | t | 508 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | A | 1125 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | B | 1235 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | K | 1401 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | f | 1211 | CLA | CMC-C2C | -2.22 | 1.46 | 1.50 |
| 14 | G | 1237 | CLA | C4B-CHC | -2.22 | 1.34 | 1.41 |
| 14 | L | 1502 | CLA | CMD-C2D | -2.22 | 1.46 | 1.50 |
| 14 | m | 1103 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | e | 1132 | CLA | MG-ND | -2.21 | 2.01 | 2.05 |
| 14 | B | 1219 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | T | 1302 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | H | 1023 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | H | 1223 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | H | 1224 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1120 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | e | 1125 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | B | 1207 | CLA | C3B-CAB | -2.21 | 1.43 | 1.47 |
| 14 | L | 1501 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | G | 1102 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | G | 1120 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | B | 1225 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 17 | V | 4219 | BCR | C1-C6 | -2.21 | 1.50 | 1.53 |
| 14 | 2 | 509 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | H | 1227 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | A | 1132 | CLA | MG-ND | -2.21 | 2.01 | 2.05 |
| 14 | f | 1216 | CLA | MG-ND | -2.21 | 2.01 | 2.05 |
| 14 | H | 1231 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | U | 1103 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | f | 1206 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | u | 502 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | e | 1102 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | G | 1118 | CLA | MG-ND | -2.21 | 2.01 | 2.05 |
| 14 | G | 1132 | CLA | MG-ND | -2.21 | 2.01 | 2.05 |
| 17 | n | 4219 | BCR | C14-C13 | -2.21 | 1.32 | 1.35 |
| 14 | B | 1231 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | B | 1202 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | 3 | 509 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 14 | Y | 508 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | v | 501 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | 5 | 517 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | H | 1202 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | G | 1122 | CLA | C3B-CAB | -2.21 | 1.43 | 1.47 |
| 14 | H | 1212 | CLA | CMD-C2D | -2.21 | 1.46 | 1.50 |
| 21 | f | 1852 | SQD | O3-C3 | -2.21 | 1.37 | 1.43 |
| 14 | H | 1214 | CLA | C3B-CAB | -2.21 | 1.43 | 1.47 |
| 21 | d | 822 | SQD | O2-C2 | -2.21 | 1.37 | 1.43 |
| 14 | 5 | 502 | CLA | C3B-C2B | -2.21 | 1.37 | 1.40 |
| 14 | 1 | 508 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | f | 1202 | CLA | CMC-C2C | -2.21 | 1.46 | 1.50 |
| 14 | 6 | 519 | CLA | C3B-CAB | -2.20 | 1.43 | 1.47 |
| 14 | a | 503 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | q | 507 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | e | 1140 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 14 | A | 1237 | CLA | C4B-CHC | -2.20 | 1.34 | 1.41 |
| 14 | f | 1207 | CLA | C3B-CAB | -2.20 | 1.43 | 1.47 |
| 14 | v | 503 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1102 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | H | 1220 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 14 | H | 1235 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | v | 519 | CLA | C3B-CAB | -2.20 | 1.43 | 1.47 |
| 14 | Z | 509 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | f | 1204 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | H | 1216 | CLA | MG-ND | -2.20 | 2.01 | 2.05 |
| 17 | A | 4008 | BCR | C10-C9 | -2.20 | 1.32 | 1.35 |
| 14 | 3 | 508 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 14 | a | 512 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | d | 501 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 21 | c | 822 | SQD | O2-C2 | -2.20 | 1.37 | 1.43 |
| 18 | A | 5002 | LHG | O7-C5 | -2.20 | 1.41 | 1.46 |
| 14 | B | 1216 | CLA | MG-ND | -2.20 | 2.01 | 2.05 |
| 14 | G | 1111 | CLA | C3B-CAB | -2.20 | 1.43 | 1.47 |
| 14 | f | 1214 | CLA | C3B-CAB | -2.20 | 1.43 | 1.47 |
| 14 | 4 | 508 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | H | 1213 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | U | 1401 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | U | 1103 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | A | 1120 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | B | 1212 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | q | 508 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | B | 1221 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | f | 1225 | CLA | C3B-C2B | -2.20 | 1.37 | 1.40 |
| 14 | H | 1218 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | B | 1215 | CLA | CAC-C3C | -2.20 | 1.45 | 1.51 |
| 14 | G | 1135 | CLA | CMC-C2C | -2.20 | 1.46 | 1.50 |
| 14 | e | 1117 | CLA | C3B-CAB | -2.20 | 1.43 | 1.47 |
| 14 | 4 | 512 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | V | 1501 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 21 | 6 | 822 | SQD | O2-C2 | -2.20 | 1.37 | 1.43 |
| 14 | 3 | 518 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | 5 | 509 | CLA | CMD-C2D | -2.20 | 1.46 | 1.50 |
| 14 | B | 1210 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | B | 1223 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | 3 | 503 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | G | 1102 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | b | 512 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | e | 1237 | CLA | C4B-CHC | -2.19 | 1.34 | 1.41 |
| 14 | f | 1215 | CLA | CAC-C3C | -2.19 | 1.45 | 1.51 |
| 14 | A | 1135 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1135 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | f | 1210 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | B | 1206 | CLA | MG-ND | -2.19 | 2.01 | 2.05 |
| 14 | G | 1125 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | H | 1239 | CLA | C4B-CHC | -2.19 | 1.34 | 1.41 |
| 14 | Y | 519 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | A | 1127 | CLA | MG-ND | -2.19 | 2.01 | 2.05 |
| 17 | f | 4010 | BCR | C17-C18 | -2.19 | 1.32 | 1.35 |
| 14 | s | 504 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 18 | e | 5002 | LHG | O7-C5 | -2.19 | 1.41 | 1.46 |
| 21 | v | 822 | SQD | O2-C2 | -2.19 | 1.37 | 1.43 |
| 14 | B | 1224 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | a | 504 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | q | 511 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | f | 1206 | CLA | MG-ND | -2.19 | 2.01 | 2.05 |
| 17 | S | 4018 | BCR | C1-C6 | -2.19 | 1.50 | 1.53 |
| 14 | f | 1220 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 14 | B | 1213 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | 3 | 512 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | s | 512 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | b | 508 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | H | 1225 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | q | 519 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | K | 1103 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | 1 | 501 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | B | 1235 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | e | 1125 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | H | 1220 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 14 | H | 1215 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | G | 1117 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 14 | H | 1204 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | d | 506 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | e | 1106 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | H | 1228 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | c | 509 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | B | 1214 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 14 | u | 512 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 21 | a | 822 | SQD | O2-C2 | -2.19 | 1.37 | 1.43 |
| 17 | L | 4219 | BCR | C1-C6 | -2.19 | 1.50 | 1.53 |
| 14 | H | 1207 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 14 | B | 1228 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | 6 | 506 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1220 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | K | 1103 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | c | 512 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | B | 1239 | CLA | C4B-CHC | -2.19 | 1.34 | 1.41 |
| 14 | 6 | 501 | CLA | CMC-C2C | -2.19 | 1.46 | 1.50 |
| 14 | f | 1223 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | A | 1117 | CLA | C3B-CAB | -2.19 | 1.43 | 1.47 |
| 14 | H | 1215 | CLA | C3B-C2B | -2.19 | 1.37 | 1.40 |
| 14 | s | 509 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | e | 1116 | CLA | CMD-C2D | -2.19 | 1.46 | 1.50 |
| 14 | A | 1111 | CLA | C3B-CAB | -2.18 | 1.43 | 1.47 |
| 14 | Z | 512 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 17 | B | 4010 | BCR | C17-C18 | -2.18 | 1.32 | 1.35 |
| 14 | r | 512 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | 5 | 512 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | f | 1221 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | R | 1301 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | A | 1102 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | c | 517 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | H | 1218 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 14 | v | 512 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | f | 1218 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | G | 1140 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 14 | s | 519 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 14 | A | 1102 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | a | 508 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | B | 1216 | CLA | C3B-CAB | -2.18 | 1.43 | 1.47 |
| 14 | f | 1238 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | r | 509 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | u | 506 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | 2 | 512 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 17 | H | 4010 | BCR | C17-C18 | -2.18 | 1.32 | 1.35 |
| 14 | 2 | 507 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | e | 1134 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 21 | t | 822 | SQD | O3-C3 | -2.18 | 1.37 | 1.43 |
| 14 | B | 1214 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | H | 1208 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | 3 | 512 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | e | 1127 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | A | 1140 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 14 | Y | 501 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 21 | q | 822 | SQD | O2-C2 | -2.18 | 1.37 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | j | 1301 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | e | 1138 | CLA | C3B-CAB | -2.18 | 1.43 | 1.47 |
| 14 | f | 1208 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | f | 1236 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | s | 503 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | m | 1103 | CLA | CMC-C2C | -2.18 | 1.46 | 1.50 |
| 14 | B | 1218 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | G | 1131 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 17 | G | 4008 | BCR | C10-C9 | -2.18 | 1.32 | 1.35 |
| 14 | s | 518 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | e | 1124 | CLA | C3B-C2B | -2.18 | 1.37 | 1.40 |
| 14 | a | 512 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | s | 512 | CLA | MG-ND | -2.18 | 2.01 | 2.05 |
| 14 | A | 1116 | CLA | CMD-C2D | -2.18 | 1.46 | 1.50 |
| 14 | e | 1105 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | A | 1118 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | G | 1116 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | B | 1211 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | A | 1106 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | B | 1220 | CLA | C3B-CAB | -2.17 | 1.43 | 1.47 |
| 14 | c | 508 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 14 | A | 1138 | CLA | C3B-CAB | -2.17 | 1.43 | 1.47 |
| 14 | 3 | 508 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | H | 1224 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | f | 1224 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | B | 1208 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | H | 1236 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | c | 503 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | q | 501 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | f | 1239 | CLA | C4B-CHC | -2.17 | 1.35 | 1.41 |
| 14 | A | 1133 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 14 | B | 1236 | CLA | CMC-C2C | -2.17 | 1.46 | 1.50 |
| 17 | k | 4018 | BCR | C30-C25 | -2.17 | 1.50 | 1.53 |
| 14 | f | 1220 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 14 | B | 1230 | CLA | MG-ND | -2.17 | 2.01 | 2.05 |
| 14 | H | 1215 | CLA | CAC-C3C | -2.17 | 1.45 | 1.51 |
| 14 | H | 1222 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | s | 508 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 14 | H | 1236 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 14 | 5 | 513 | CLA | C3B-C2B | -2.17 | 1.37 | 1.40 |
| 14 | A | 1134 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 17 | L | 4219 | BCR | C14-C13 | -2.17 | 1.32 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1236 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 17 | e | 4008 | BCR | C10-C9 | -2.17 | 1.32 | 1.35 |
| 14 | B | 1222 | CLA | CMD-C2D | -2.17 | 1.46 | 1.50 |
| 17 | I | 4018 | BCR | C1-C6 | -2.17 | 1.50 | 1.53 |
| 17 | I | 4018 | BCR | C30-C25 | -2.16 | 1.50 | 1.53 |
| 14 | A | 1122 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 18 | G | 5002 | LHG | O7-C5 | -2.16 | 1.41 | 1.46 |
| 14 | e | 1122 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | G | 1118 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | Z | 513 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | 3 | 822 | SQD | O2-C2 | -2.16 | 1.37 | 1.43 |
| 21 | 4 | 822 | SQD | O3-C3 | -2.16 | 1.37 | 1.43 |
| 14 | G | 1122 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | e | 1106 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 21 | b | 822 | SQD | O3-C3 | -2.16 | 1.37 | 1.43 |
| 14 | 3 | 504 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | r | 507 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | f | 1235 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 14 | f | 1222 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | l | 1303 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | G | 1138 | CLA | C3B-CAB | -2.16 | 1.43 | 1.47 |
| 14 | f | 1216 | CLA | C3B-CAB | -2.16 | 1.43 | 1.47 |
| 21 | d | 822 | SQD | O4-C4 | -2.16 | 1.37 | 1.43 |
| 14 | G | 1127 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | B | 1224 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | B | 1215 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 14 | B | 1215 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | 6 | 512 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | e | 1118 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | H | 1203 | CLA | MG-ND | -2.16 | 2.01 | 2.05 |
| 14 | f | 1230 | CLA | MG-ND | -2.16 | 2.01 | 2.05 |
| 14 | c | 506 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | e | 1124 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | G | 1124 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 21 | 1 | 822 | SQD | O2-C2 | -2.16 | 1.37 | 1.43 |
| 14 | B | 1238 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | G | 1106 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | B | 1203 | CLA | MG-ND | -2.16 | 2.01 | 2.05 |
| 14 | e | 1127 | CLA | C3B-CAB | -2.16 | 1.43 | 1.47 |
| 14 | 3 | 519 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 14 | d | 507 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | a | 508 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | f | 1232 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | 5 | 506 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | f | 1214 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | a | 501 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | H | 1235 | CLA | C3B-C2B | -2.16 | 1.37 | 1.40 |
| 14 | u | 513 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | A | 1011 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | A | 1131 | CLA | MG-ND | -2.16 | 2.01 | 2.05 |
| 14 | f | 1203 | CLA | MG-ND | -2.16 | 2.01 | 2.05 |
| 14 | b | 519 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | e | 1011 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | e | 1127 | CLA | CMC-C2C | -2.16 | 1.46 | 1.50 |
| 14 | f | 1236 | CLA | CMD-C2D | -2.16 | 1.46 | 1.50 |
| 14 | F | 1301 | CLA | MG-ND | -2.15 | 2.01 | 2.05 |
| 14 | u | 509 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 21 | r | 822 | SQD | O4-C4 | -2.15 | 1.37 | 1.43 |
| 14 | A | 1124 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | j | 1302 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | 5 | 503 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | 6 | 507 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | e | 1137 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | B | 1218 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | V | 1501 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | G | 1133 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | r | 518 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | s | 517 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | e | 1111 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | 2 | 519 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | f | 1228 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | r | 519 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | s | 511 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | e | 1125 | CLA | MG-ND | -2.15 | 2.01 | 2.05 |
| 21 | Y | 822 | SQD | O2-C2 | -2.15 | 1.37 | 1.43 |
| 14 | 5 | 513 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | q | 504 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | r | 508 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | G | 1126 | CLA | MG-ND | -2.15 | 2.01 | 2.05 |
| 17 | A | 4002 | BCR | C30-C25 | -2.15 | 1.50 | 1.53 |
| 14 | A | 1105 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | t | 512 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | 5 | 508 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | 6 | 508 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | H | 1239 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | G | 1127 | CLA | MG-ND | -2.15 | 2.01 | 2.05 |
| 14 | G | 1134 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | r | 513 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | u | 508 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | H | 1232 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | v | 507 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | t | 505 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | A | 1125 | CLA | MG-ND | -2.15 | 2.01 | 2.05 |
| 14 | f | 1215 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | B | 1232 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | G | 1127 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | A | 1127 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 21 | s | 822 | SQD | O2-C2 | -2.15 | 1.37 | 1.43 |
| 14 | 3 | 511 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | a | 518 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | e | 1133 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | q | 510 | CLA | CMD-C2D | -2.15 | 1.46 | 1.50 |
| 14 | l | 512 | CLA | C3B-C2B | -2.15 | 1.37 | 1.40 |
| 14 | G | 1124 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | H | 1216 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | 3 | 517 | CLA | CMC-C2C | -2.15 | 1.46 | 1.50 |
| 14 | e | 1105 | CLA | C3B-CAB | -2.15 | 1.43 | 1.47 |
| 14 | Y | 510 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 14 | a | 511 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 14 | u | 519 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | f | 1222 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 14 | H | 1214 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 14 | Z | 519 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | s | 501 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | s | 508 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | A | 1139 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | H | 1230 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 14 | Z | 508 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | B | 1230 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 14 | R | 1302 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 14 | G | 1133 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | q | 504 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | e | 1131 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | r | 509 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 21 | 6 | 822 | SQD | O4-C4 | -2.14 | 1.37 | 1.43 |
| 21 | V | 5216 | SQD | O4-C4 | -2.14 | 1.37 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1134 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | e | 1131 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | G | 1139 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | A | 1127 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 18 | B | 1855 | LHG | P-O6 | 2.14 | 1.68 | 1.59 |
| 14 | c | 513 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | Z | 507 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 14 | d | 508 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | f | 1224 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | A | 1102 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | 2 | 513 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 14 | K | 1105 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | f | 1228 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | e | 1133 | CLA | C3B-C2B | -2.14 | 1.37 | 1.40 |
| 14 | f | 1012 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 17 | e | 4002 | BCR | C30-C25 | -2.14 | 1.50 | 1.53 |
| 14 | 5 | 507 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 14 | R | 1301 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | A | 1111 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | e | 1102 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | G | 1112 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 14 | e | 1125 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 14 | A | 1137 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | 3 | 518 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | e | 1134 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | j | 1302 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | G | 1118 | CLA | C3B-CAB | -2.14 | 1.43 | 1.47 |
| 14 | G | 1011 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | a | 517 | CLA | CMC-C2C | -2.14 | 1.46 | 1.50 |
| 14 | b | 509 | CLA | CMD-C2D | -2.14 | 1.46 | 1.50 |
| 21 | 2 | 822 | SQD | O4-C4 | -2.14 | 1.37 | 1.43 |
| 18 | H | 1855 | LHG | P-O6 | 2.14 | 1.67 | 1.59 |
| 21 | Z | 822 | SQD | O4-C4 | -2.14 | 1.37 | 1.43 |
| 14 | A | 1109 | CLA | MG-ND | -2.14 | 2.01 | 2.05 |
| 21 | v | 822 | SQD | O4-C4 | -2.13 | 1.37 | 1.43 |
| 14 | H | 1238 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 14 | d | 509 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | H | 1232 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 14 | Y | 512 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 14 | u | 513 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 21 | L | 5216 | SQD | O4-C4 | -2.13 | 1.37 | 1.43 |
| 14 | B | 1228 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | v | 508 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 14 | A | 1115 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | G | 1125 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 14 | e | 1135 | CLA | C4B-CHC | -2.13 | 1.35 | 1.41 |
| 18 | f | 1855 | LHG | P-O6 | 2.13 | 1.67 | 1.59 |
| 14 | n | 1501 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | q | 512 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 21 | t | 822 | SQD | O2-C2 | -2.13 | 1.38 | 1.43 |
| 14 | A | 1126 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 17 | k | 4018 | BCR | C1-C6 | -2.13 | 1.50 | 1.53 |
| 14 | 2 | 518 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | Y | 504 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | c | 507 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | 4 | 822 | SQD | O2-C2 | -2.13 | 1.38 | 1.43 |
| 14 | B | 1023 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | B | 1222 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | v | 507 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 14 | u | 517 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | 1 | 504 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 14 | F | 1302 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | 4 | 519 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 14 | c | 513 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | e | 1118 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 21 | Z | 822 | SQD | O3-C3 | -2.13 | 1.38 | 1.43 |
| 14 | s | 518 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 14 | A | 1124 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |
| 14 | H | 1222 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | 1 | 510 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | G | 1109 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 14 | f | 1215 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 14 | r | 508 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | b | 505 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | H | 1230 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 14 | A | 1125 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | G | 1115 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | 1 | 504 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | q | 504 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | f | 1211 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 17 | V | 4020 | BCR | C21-C22 | -2.13 | 1.33 | 1.35 |
| 14 | A | 1105 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | L | 1501 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | A | 1139 | CLA | C3B-C2B | -2.13 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | d | 512 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 14 | A | 1118 | CLA | C3B-CAB | -2.13 | 1.43 | 1.47 |
| 14 | a | 518 | CLA | CMC-C2C | -2.13 | 1.46 | 1.50 |
| 14 | a | 510 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 21 | b | 822 | SQD | O2-C2 | -2.13 | 1.38 | 1.43 |
| 14 | e | 1139 | CLA | MG-ND | -2.13 | 2.01 | 2.05 |
| 14 | J | 1303 | CLA | CMD-C2D | -2.13 | 1.46 | 1.50 |
| 18 | V | 5220 | LHG | O7-C5 | -2.12 | 1.41 | 1.46 |
| 14 | A | 1131 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | 3 | 501 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | Z | 518 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | 4 | 505 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 14 | Z | 508 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 17 | A | 4008 | BCR | C21-C22 | -2.12 | 1.33 | 1.35 |
| 14 | v | 509 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | G | 1137 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 14 | B | 1012 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 14 | 2 | 510 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 18 | n | 5220 | LHG | O7-C5 | -2.12 | 1.41 | 1.46 |
| 14 | c | 519 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | A | 1801 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | 2 | 508 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | G | 1105 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | G | 1122 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 14 | B | 1218 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | G | 1105 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 14 | U | 1105 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | H | 1211 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | u | 508 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | A | 1137 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 14 | f | 1023 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 14 | t | 519 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | G | 1123 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | Z | 508 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | u | 507 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | A | 1237 | CLA | CAC-C3C | -2.12 | 1.45 | 1.51 |
| 14 | H | 1023 | CLA | C3B-CAB | -2.12 | 1.43 | 1.47 |
| 14 | A | 1134 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | A | 1135 | CLA | C4B-CHC | -2.12 | 1.35 | 1.41 |
| 14 | e | 1111 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 14 | F | 1302 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | 5 | 517 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | q | 513 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | A | 1112 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 14 | F | 1301 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | u | 513 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 18 | L | 5220 | LHG | O7-C5 | -2.12 | 1.41 | 1.46 |
| 14 | H | 1206 | CLA | CAC-C3C | -2.12 | 1.45 | 1.51 |
| 14 | f | 1206 | CLA | CAC-C3C | -2.12 | 1.45 | 1.51 |
| 14 | R | 1302 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | 2 | 508 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | 6 | 509 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | f | 1239 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 17 | L | 4020 | BCR | C21-C22 | -2.12 | 1.33 | 1.35 |
| 14 | G | 1121 | CLA | C4B-CHC | -2.12 | 1.35 | 1.41 |
| 14 | j | 1301 | CLA | CMC-C2C | -2.12 | 1.46 | 1.50 |
| 14 | A | 1133 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | 3 | 517 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | 6 | 507 | CLA | C3B-C2B | -2.12 | 1.37 | 1.40 |
| 14 | B | 1239 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | c | 517 | CLA | CMD-C2D | -2.12 | 1.46 | 1.50 |
| 14 | d | 507 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | 4 | 509 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | 2 | 508 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | f | 1230 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |
| 14 | 5 | 508 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | U | 1401 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | u | 503 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | B | 1211 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | 5 | 519 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | G | 1139 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | B | 1206 | CLA | CAC-C3C | -2.11 | 1.45 | 1.51 |
| 14 | e | 1116 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | A | 1134 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 14 | T | 1303 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | r | 504 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | e | 1106 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | e | 1237 | CLA | CAC-C3C | -2.11 | 1.45 | 1.51 |
| 14 | f | 1218 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | u | 517 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | f | 1210 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | e | 1115 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |
| 14 | G | 1111 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 17 | V | 4219 | BCR | C14-C13 | -2.11 | 1.33 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | T | 1303 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 14 | c | 508 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | G | 1116 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | H | 1205 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | H | 1211 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 17 | n | 4020 | BCR | C21-C22 | -2.11 | 1.33 | 1.35 |
| 14 | l | 513 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 14 | Z | 509 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 14 | G | 1237 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |
| 21 | n | 5216 | SQD | O4-C4 | -2.11 | 1.38 | 1.43 |
| 14 | G | 1134 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | e | 1139 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | G | 1125 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |
| 14 | b | 510 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | e | 1126 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | K | 1401 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | b | 508 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | H | 1012 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | A | 1011 | CLA | C3B-CAB | -2.11 | 1.43 | 1.47 |
| 14 | G | 1114 | CLA | CMC-C2C | -2.11 | 1.46 | 1.50 |
| 14 | b | 516 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | m | 1105 | CLA | C3C-C2C | 2.11 | 1.41 | 1.36 |
| 14 | B | 1205 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 14 | 4 | 516 | CLA | CMD-C2D | -2.11 | 1.46 | 1.50 |
| 14 | e | 1011 | CLA | C3B-C2B | -2.11 | 1.37 | 1.40 |
| 14 | 2 | 511 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | 6 | 509 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | Z | 510 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | e | 1011 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 14 | 3 | 510 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | 5 | 513 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | r | 510 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | f | 1205 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | B | 1229 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | G | 1137 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | r | 508 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | H | 1229 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | e | 1801 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | e | 1137 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 14 | m | 1105 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 14 | H | 1204 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | u | 516 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1237 | CLA | CAC-C3C | -2.10 | 1.45 | 1.51 |
| 17 | G | 4002 | BCR | C30-C25 | -2.10 | 1.50 | 1.53 |
| 14 | H | 1235 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 14 | J | 1303 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | s | 510 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | A | 1116 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | G | 1106 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | H | 1218 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | b | 502 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | t | 516 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | G | 1121 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | m | 1401 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | e | 1117 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 17 | e | 4008 | BCR | C21-C22 | -2.10 | 1.33 | 1.35 |
| 14 | Z | 504 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | v | 519 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | e | 1115 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | e | 1134 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 14 | n | 1501 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | K | 1105 | CLA | C3C-C2C | 2.10 | 1.41 | 1.36 |
| 14 | A | 1237 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 21 | n | 5216 | SQD | O3-C3 | -2.10 | 1.38 | 1.43 |
| 14 | l | 517 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | G | 1135 | CLA | C4B-CHC | -2.10 | 1.35 | 1.41 |
| 14 | f | 1235 | CLA | C3B-CAB | -2.10 | 1.43 | 1.47 |
| 17 | S | 4018 | BCR | C30-C25 | -2.10 | 1.50 | 1.53 |
| 14 | B | 1204 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | l | 504 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | a | 519 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | s | 513 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 14 | A | 1115 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | A | 1106 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | 2 | 504 | CLA | CMD-C2D | -2.10 | 1.46 | 1.50 |
| 14 | H | 1231 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | e | 1121 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 14 | e | 1109 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | f | 1223 | CLA | MG-ND | -2.10 | 2.01 | 2.05 |
| 14 | A | 1011 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 14 | 2 | 516 | CLA | C3B-C2B | -2.10 | 1.37 | 1.40 |
| 21 | s | 822 | SQD | O3-C3 | -2.10 | 1.38 | 1.43 |
| 14 | 2 | 509 | CLA | CMC-C2C | -2.10 | 1.46 | 1.50 |
| 21 | L | 5216 | SQD | O3-C3 | -2.10 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 1121 | CLA | C4B-CHC | -2.09 | 1.35 | 1.41 |
| 14 | 2 | 519 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | G | 1102 | CLA | MG-ND | -2.09 | 2.01 | 2.05 |
| 14 | f | 1218 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | d | 501 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 20 | J | 5104 | LMG | O8-C9 | -2.09 | 1.40 | 1.45 |
| 14 | e | 1237 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | f | 1204 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | H | 1228 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | Z | 511 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | A | 1117 | CLA | MG-ND | -2.09 | 2.01 | 2.05 |
| 14 | Z | 519 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | G | 1131 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | u | 510 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | v | 516 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | B | 1227 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | 3 | 513 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 21 | 2 | 822 | SQD | O3-C3 | -2.09 | 1.38 | 1.43 |
| 20 | T | 5104 | LMG | O8-C9 | -2.09 | 1.40 | 1.45 |
| 17 | n | 4020 | BCR | C10-C9 | -2.09 | 1.33 | 1.35 |
| 20 | l | 5104 | LMG | O8-C9 | -2.09 | 1.40 | 1.45 |
| 14 | e | 1112 | CLA | MG-ND | -2.09 | 2.01 | 2.05 |
| 14 | B | 1235 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | G | 1011 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | s | 519 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 17 | G | 4008 | BCR | C21-C22 | -2.09 | 1.33 | 1.35 |
| 14 | 6 | 501 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | a | 517 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | 3 | 508 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | r | 516 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | e | 1109 | CLA | C4B-CHC | -2.09 | 1.35 | 1.41 |
| 14 | q | 513 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | H | 1205 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | e | 1114 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 21 | r | 822 | SQD | O3-C3 | -2.09 | 1.38 | 1.43 |
| 14 | 3 | 519 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | a | 508 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | Z | 516 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 14 | A | 1123 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | r | 511 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | v | 509 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | L | 1501 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | a | 507 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | 5 | 517 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 14 | a | 513 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 14 | T | 1302 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | t | 509 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | Y | 513 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | f | 1231 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | v | 508 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | A | 1114 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | e | 1119 | CLA | C3B-CAB | -2.09 | 1.43 | 1.47 |
| 14 | r | 516 | CLA | C3B-C2B | -2.09 | 1.37 | 1.40 |
| 14 | Y | 504 | CLA | CMC-C2C | -2.09 | 1.46 | 1.50 |
| 14 | Y | 517 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | u | 501 | CLA | CMD-C2D | -2.09 | 1.46 | 1.50 |
| 14 | s | 508 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | B | 1232 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | c | 506 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | d | 519 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | J | 1302 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | A | 1022 | CLA | O2D-CED | -2.08 | 1.40 | 1.45 |
| 14 | 6 | 519 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | G | 1801 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | s | 517 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | e | 1022 | CLA | O2D-CED | -2.08 | 1.40 | 1.45 |
| 14 | f | 1229 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | H | 1223 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | e | 1123 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | s | 508 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 21 | 4 | 822 | SQD | O4-C4 | -2.08 | 1.38 | 1.43 |
| 14 | B | 1223 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | n | 1503 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | f | 1209 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 14 | Z | 506 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | q | 508 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 21 | a | 822 | SQD | O3-C3 | -2.08 | 1.38 | 1.43 |
| 14 | e | 1121 | CLA | C4B-CHC | -2.08 | 1.35 | 1.41 |
| 14 | B | 1210 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | G | 1115 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 21 | t | 822 | SQD | O4-C4 | -2.08 | 1.38 | 1.43 |
| 14 | B | 1231 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | G | 1139 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | v | 504 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | Y | 508 | CLA | C3B-C2B | -2.08 | 1.37 | 1.40 |
| 14 | d | 504 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | f | 1208 | CLA | C3B-CAB | -2.08 | 1.43 | 1.47 |
| 14 | H | 1210 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | J | 1302 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | q | 518 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | 3 | 519 | CLA | C3B-CAB | -2.08 | 1.43 | 1.47 |
| 14 | f | 1203 | CLA | C3B-CAB | -2.08 | 1.43 | 1.47 |
| 14 | a | 510 | CLA | O2A-CGA | 2.08 | 1.37 | 1.30 |
| 14 | 2 | 517 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | c | 513 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | v | 501 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | 1 | 509 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | 3 | 507 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | Y | 510 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | t | 507 | CLA | CMD-C2D | -2.08 | 1.46 | 1.50 |
| 14 | H | 1203 | CLA | C3B-CAB | -2.08 | 1.43 | 1.47 |
| 21 | V | 5216 | SQD | O3-C3 | -2.08 | 1.38 | 1.43 |
| 14 | d | 509 | CLA | CMC-C2C | -2.08 | 1.46 | 1.50 |
| 14 | H | 1204 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 14 | d | 519 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | 3 | 510 | CLA | O2A-CGA | 2.07 | 1.37 | 1.30 |
| 14 | a | 506 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | s | 510 | CLA | O2A-CGA | 2.07 | 1.37 | 1.30 |
| 14 | U | 1105 | CLA | C3C-C2C | 2.07 | 1.41 | 1.36 |
| 14 | 4 | 513 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | u | 822 | SQD | O4-C4 | -2.07 | 1.38 | 1.43 |
| 14 | 6 | 519 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 14 | t | 502 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 17 | V | 4020 | BCR | C10-C9 | -2.07 | 1.33 | 1.35 |
| 14 | 4 | 508 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | d | 510 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 14 | A | 1121 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 14 | 4 | 510 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | d | 508 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 21 | c | 822 | SQD | O4-C4 | -2.07 | 1.38 | 1.43 |
| 14 | a | 513 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | r | 513 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |
| 21 | 5 | 822 | SQD | O4-C4 | -2.07 | 1.38 | 1.43 |
| 14 | A | 1122 | CLA | MG-ND | -2.07 | 2.01 | 2.05 |
| 14 | q | 517 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | r | 519 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21 | Y | 822 | SQD | O3-C3 | -2.07 | 1.38 | 1.43 |
| 14 | l | 1303 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 14 | b | 505 | CLA | MG-ND | -2.07 | 2.01 | 2.05 |
| 14 | t | 508 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | G | 1117 | CLA | MG-ND | -2.07 | 2.01 | 2.05 |
| 14 | Y | 503 | CLA | C3B-C2B | -2.07 | 1.37 | 1.40 |
| 14 | G | 1022 | CLA | O2D-CED | -2.07 | 1.40 | 1.45 |
| 14 | H | 1208 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |
| 14 | q | 503 | CLA | C3B-C2B | -2.07 | 1.37 | 1.40 |
| 14 | A | 1104 | CLA | MG-ND | -2.07 | 2.01 | 2.05 |
| 14 | 2 | 506 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | 6 | 504 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | B | 1203 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |
| 18 | n | 5218 | LHG | P-O6 | 2.07 | 1.67 | 1.59 |
| 14 | d | 513 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | b | 508 | CLA | MG-ND | -2.07 | 2.01 | 2.05 |
| 14 | a | 510 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |
| 14 | T | 1302 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | r | 504 | CLA | C3B-C2B | -2.07 | 1.37 | 1.40 |
| 14 | f | 1227 | CLA | CMC-C2C | -2.07 | 1.46 | 1.50 |
| 14 | 2 | 513 | CLA | C3B-CAB | -2.07 | 1.43 | 1.47 |
| 14 | 6 | 513 | CLA | C3B-C2B | -2.07 | 1.37 | 1.40 |
| 18 | L | 5218 | LHG | P-O6 | 2.07 | 1.67 | 1.59 |
| 21 | d | 822 | SQD | O3-C3 | -2.07 | 1.38 | 1.43 |
| 14 | 4 | 502 | CLA | CMD-C2D | -2.07 | 1.46 | 1.50 |
| 14 | d | 510 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | v | 519 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | f | 1220 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | Y | 513 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | b | 519 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | 1 | 503 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | 3 | 512 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | 1 | 513 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | 4 | 519 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | t | 519 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 18 | V | 5218 | LHG | P-O6 | 2.06 | 1.67 | 1.59 |
| 18 | e | 5008 | LHG | P-O6 | 2.06 | 1.67 | 1.59 |
| 14 | 3 | 513 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | 6 | 508 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | e | 1104 | CLA | CAC-C3C | -2.06 | 1.45 | 1.51 |
| 21 | b | 822 | SQD | O4-C4 | -2.06 | 1.38 | 1.43 |
| 14 | Z | 519 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | t | 513 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | a | 519 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | n | 1501 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | A | 1139 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | 5 | 516 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | Z | 517 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | s | 519 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | G | 1011 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | a | 512 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | d | 516 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | v | 513 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | G | 1109 | CLA | C4B-CHC | -2.06 | 1.35 | 1.41 |
| 14 | s | 512 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | 5 | 510 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | B | 1208 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | s | 513 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | Y | 512 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | a | 508 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | A | 1011 | CLA | C4B-CHC | -2.06 | 1.35 | 1.41 |
| 14 | Z | 513 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | G | 1108 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | q | 508 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 21 | Y | 822 | SQD | O4-C4 | -2.06 | 1.38 | 1.43 |
| 14 | a | 505 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | B | 1204 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 21 | q | 822 | SQD | O4-C4 | -2.06 | 1.38 | 1.43 |
| 14 | 3 | 505 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | c | 510 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | s | 510 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 18 | A | 5008 | LHG | P-O6 | 2.06 | 1.67 | 1.59 |
| 21 | 1 | 822 | SQD | O4-C4 | -2.06 | 1.38 | 1.43 |
| 14 | L | 1503 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | H | 1220 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | e | 1139 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | r | 513 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | 1 | 508 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | 3 | 506 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | 4 | 502 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | G | 1139 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | r | 506 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 21 | 6 | 822 | SQD | O3-C3 | -2.06 | 1.38 | 1.43 |
| 14 | V | 1501 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | u | 510 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 17 | f | 4017 | BCR | C30-C25 | -2.06 | 1.50 | 1.53 |
| 14 | A | 1109 | CLA | C4B-CHC | -2.06 | 1.35 | 1.41 |
| 14 | B | 1205 | CLA | C3B-CAB | -2.06 | 1.43 | 1.47 |
| 14 | 4 | 508 | CLA | MG-ND | -2.06 | 2.01 | 2.05 |
| 14 | r | 517 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | L | 1502 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | 5 | 503 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 21 | 3 | 822 | SQD | O3-C3 | -2.06 | 1.38 | 1.43 |
| 14 | Y | 509 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | H | 1209 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | c | 503 | CLA | C3B-C2B | -2.06 | 1.37 | 1.40 |
| 14 | 2 | 513 | CLA | CMC-C2C | -2.06 | 1.46 | 1.50 |
| 14 | q | 519 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | s | 507 | CLA | CMD-C2D | -2.06 | 1.46 | 1.50 |
| 14 | e | 1011 | CLA | C4B-CHC | -2.05 | 1.35 | 1.41 |
| 14 | 5 | 501 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | V | 1501 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | s | 513 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | B | 1220 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | 4 | 505 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | G | 1011 | CLA | C4B-CHC | -2.05 | 1.35 | 1.41 |
| 14 | 1 | 518 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | 1 | 508 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 14 | Y | 504 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 14 | 6 | 516 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | q | 510 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | 1 | 508 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | t | 508 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | A | 1136 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 14 | f | 1236 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 14 | B | 1232 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | 3 | 508 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | A | 1104 | CLA | CAC-C3C | -2.05 | 1.45 | 1.51 |
| 14 | u | 503 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 14 | 1 | 510 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | f | 1204 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | f | 1235 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 18 | G | 5008 | LHG | P-O6 | 2.05 | 1.67 | 1.59 |
| 14 | q | 503 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 14 | Z | 516 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | l | 1302 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | q | 505 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | e | 1104 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | e | 1122 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | f | 1232 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | 2 | 516 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | L | 1501 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | c | 516 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | G | 1104 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | H | 1236 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 21 | q | 822 | SQD | O3-C3 | -2.05 | 1.38 | 1.43 |
| 14 | l | 519 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | b | 513 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | q | 519 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | f | 1012 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 17 | H | 4017 | BCR | C30-C25 | -2.05 | 1.50 | 1.53 |
| 14 | Y | 519 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | r | 511 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | A | 1128 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 17 | L | 4020 | BCR | C10-C9 | -2.05 | 1.33 | 1.35 |
| 14 | A | 1140 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | H | 1227 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | B | 1209 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |
| 14 | Z | 513 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | G | 1140 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | 3 | 513 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | G | 1104 | CLA | CAC-C3C | -2.05 | 1.45 | 1.51 |
| 14 | Y | 508 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | B | 1236 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 21 | s | 822 | SQD | O4-C4 | -2.05 | 1.38 | 1.43 |
| 14 | l | 505 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | b | 506 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | f | 1232 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | G | 1101 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 14 | f | 1205 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 14 | s | 506 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | 6 | 513 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | b | 502 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | q | 509 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | t | 510 | CLA | CMD-C2D | -2.05 | 1.46 | 1.50 |
| 14 | e | 1136 | CLA | C3B-CAB | -2.05 | 1.43 | 1.47 |
| 14 | t | 517 | CLA | CMC-C2C | -2.05 | 1.46 | 1.50 |
| 14 | u | 512 | CLA | C3B-C2B | -2.05 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | B | 1227 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | r | 507 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 14 | A | 1119 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | H | 1222 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | V | 1503 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | 2 | 519 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | a | 822 | SQD | O4-C4 | -2.04 | 1.38 | 1.43 |
| 14 | B | 1215 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | 2 | 506 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | e | 1140 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 21 | 3 | 822 | SQD | O4-C4 | -2.04 | 1.38 | 1.43 |
| 14 | e | 1102 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | 2 | 504 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | u | 509 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 14 | a | 513 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | q | 512 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 18 | G | 5006 | LHG | O7-C5 | -2.04 | 1.41 | 1.46 |
| 14 | B | 1229 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | Y | 518 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | A | 1139 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | f | 1229 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | r | 519 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | q | 508 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | A | 1119 | CLA | C4B-CHC | -2.04 | 1.35 | 1.41 |
| 14 | e | 1128 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | 5 | 506 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | V | 1502 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | d | 513 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | r | 501 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 21 | v | 822 | SQD | O3-C3 | -2.04 | 1.38 | 1.43 |
| 14 | 1 | 512 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | f | 1227 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | 1 | 516 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | l | 1302 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | H | 1229 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | 4 | 507 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | B | 1235 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | H | 1215 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | b | 508 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | B | 1222 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 21 | u | 822 | SQD | O3-C3 | -2.04 | 1.38 | 1.43 |
| 14 | 3 | 510 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1119 | CLA | C4B-CHC | -2.04 | 1.35 | 1.41 |
| 14 | Z | 504 | CLA | C3B-C2B | -2.04 | 1.37 | 1.40 |
| 14 | f | 1219 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | e | 1119 | CLA | C4B-CHC | -2.04 | 1.35 | 1.41 |
| 14 | l | 519 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | 6 | 510 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | b | 517 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 14 | l | 1302 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 14 | G | 1102 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | Y | 516 | CLA | O2A-CGA | 2.04 | 1.37 | 1.30 |
| 14 | 5 | 510 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 14 | A | 1102 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | G | 1119 | CLA | C3B-CAB | -2.04 | 1.43 | 1.47 |
| 14 | c | 501 | CLA | CMD-C2D | -2.04 | 1.46 | 1.50 |
| 21 | c | 822 | SQD | O3-C3 | -2.04 | 1.38 | 1.43 |
| 14 | H | 1219 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 14 | 4 | 517 | CLA | CMC-C2C | -2.04 | 1.46 | 1.50 |
| 14 | u | 506 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | c | 517 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 14 | u | 504 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | v | 504 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 21 | 5 | 822 | SQD | O3-C3 | -2.03 | 1.38 | 1.43 |
| 17 | B | 4017 | BCR | C30-C25 | -2.03 | 1.51 | 1.53 |
| 17 | c | 523 | BCR | C1-C6 | -2.03 | 1.51 | 1.53 |
| 14 | A | 1120 | CLA | CAC-C3C | -2.03 | 1.45 | 1.51 |
| 14 | f | 1215 | CLA | C3B-CAB | -2.03 | 1.43 | 1.47 |
| 14 | Y | 511 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 14 | 2 | 501 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | q | 516 | CLA | O2A-CGA | 2.03 | 1.37 | 1.30 |
| 14 | Y | 505 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 14 | A | 1101 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 14 | r | 507 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 14 | e | 1139 | CLA | C3B-CAB | -2.03 | 1.43 | 1.47 |
| 14 | e | 1103 | CLA | CAC-C3C | -2.03 | 1.45 | 1.51 |
| 14 | Z | 511 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 14 | c | 504 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | s | 501 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | a | 505 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 14 | l | 503 | CLA | C3B-CAB | -2.03 | 1.43 | 1.47 |
| 14 | H | 1012 | CLA | C3B-CAB | -2.03 | 1.43 | 1.47 |
| 14 | H | 1235 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 21 | 1 | 822 | SQD | O3-C3 | -2.03 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | t | 505 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 14 | 2 | 511 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 14 | Y | 508 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | b | 507 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | v | 505 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 14 | T | 1302 | CLA | C3B-CAB | -2.03 | 1.43 | 1.47 |
| 14 | Y | 519 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | t | 502 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | H | 1232 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 14 | v | 510 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | Y | 517 | CLA | CMC-C2C | -2.03 | 1.46 | 1.50 |
| 14 | u | 505 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 14 | q | 501 | CLA | CMD-C2D | -2.03 | 1.46 | 1.50 |
| 14 | B | 1219 | CLA | MG-ND | -2.03 | 2.01 | 2.05 |
| 14 | G | 1111 | CLA | C3B-C2B | -2.03 | 1.37 | 1.40 |
| 18 | e | 5006 | LHG | O7-C5 | -2.02 | 1.41 | 1.46 |
| 14 | Y | 507 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | G | 1128 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 14 | B | 1012 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 14 | b | 503 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | c | 505 | CLA | MG-ND | -2.02 | 2.01 | 2.05 |
| 20 | H | 5002 | LMG | O1-C7 | -2.02 | 1.40 | 1.43 |
| 14 | 4 | 503 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | 5 | 512 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | c | 512 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | 5 | 509 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | Z | 501 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | c | 510 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | t | 504 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | 2 | 507 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | 3 | 501 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | 6 | 510 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | e | 1101 | CLA | MG-ND | -2.02 | 2.01 | 2.05 |
| 14 | 1 | 517 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | Y | 509 | CLA | MG-ND | -2.02 | 2.01 | 2.05 |
| 14 | 1 | 516 | CLA | O2A-CGA | 2.02 | 1.37 | 1.30 |
| 14 | 1 | 510 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | 5 | 504 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | Y | 506 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | t | 505 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | Z | 506 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | t | 503 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | G | 1136 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 14 | 3 | 517 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | b | 517 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | c | 508 | CLA | C4B-CHC | -2.02 | 1.35 | 1.41 |
| 14 | e | 1122 | CLA | C4B-CHC | -2.02 | 1.35 | 1.41 |
| 17 | 5 | 523 | BCR | C1-C6 | -2.02 | 1.51 | 1.53 |
| 14 | t | 508 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 14 | Z | 502 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | Z | 501 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | n | 1502 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | H | 1207 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 18 | A | 5006 | LHG | O7-C5 | -2.02 | 1.41 | 1.46 |
| 14 | a | 501 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | B | 1210 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 14 | a | 504 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | G | 1120 | CLA | CAC-C3C | -2.02 | 1.45 | 1.51 |
| 14 | 1 | 509 | CLA | MG-ND | -2.02 | 2.01 | 2.05 |
| 14 | 4 | 506 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | v | 517 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | H | 1227 | CLA | MG-ND | -2.02 | 2.01 | 2.05 |
| 14 | u | 504 | CLA | C3B-C2B | -2.02 | 1.37 | 1.40 |
| 14 | 4 | 504 | CLA | CMD-C2D | -2.02 | 1.46 | 1.50 |
| 14 | H | 1208 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | 6 | 504 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | s | 505 | CLA | CMC-C2C | -2.02 | 1.46 | 1.50 |
| 14 | q | 509 | CLA | MG-ND | -2.02 | 2.01 | 2.05 |
| 14 | Y | 504 | CLA | C3B-CAB | -2.02 | 1.43 | 1.47 |
| 14 | b | 501 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | v | 510 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | 3 | 518 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | 2 | 507 | CLA | MG-ND | -2.01 | 2.01 | 2.05 |
| 14 | f | 1222 | CLA | MG-ND | -2.01 | 2.01 | 2.05 |
| 14 | A | 1103 | CLA | CAC-C3C | -2.01 | 1.45 | 1.51 |
| 14 | d | 504 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | r | 501 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | v | 506 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | c | 504 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | H | 1234 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | Z | 510 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | 4 | 517 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | Y | 501 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | c | 509 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | r | 505 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | t | 501 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | t | 506 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 17 | H | 4017 | BCR | C17-C18 | -2.01 | 1.33 | 1.35 |
| 14 | b | 509 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | A | 1013 | CLA | CAC-C3C | -2.01 | 1.45 | 1.51 |
| 14 | A | 1105 | CLA | MG-ND | -2.01 | 2.01 | 2.05 |
| 14 | q | 507 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | r | 518 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | l | 508 | CLA | C4B-CHC | -2.01 | 1.35 | 1.41 |
| 14 | d | 506 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | Y | 510 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | v | 513 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | l | 506 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | 2 | 505 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | 4 | 513 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | 6 | 505 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | Z | 518 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | Y | 503 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | 3 | 504 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | 6 | 517 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | b | 511 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | A | 1108 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | 5 | 504 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | b | 506 | CLA | CMD-C2D | -2.01 | 1.46 | 1.50 |
| 14 | Z | 502 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 20 | B | 5002 | LMG | O1-C7 | -2.01 | 1.40 | 1.43 |
| 14 | A | 1108 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | a | 517 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | u | 504 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | G | 1013 | CLA | CAC-C3C | -2.01 | 1.46 | 1.51 |
| 14 | J | 1302 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | H | 1210 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | A | 1118 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | a | 502 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | v | 517 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | 5 | 505 | CLA | MG-ND | -2.01 | 2.01 | 2.05 |
| 14 | 2 | 502 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | l | 1303 | CLA | C3B-CAB | -2.01 | 1.43 | 1.47 |
| 14 | 4 | 511 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | v | 512 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | B | 1207 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | e | 1013 | CLA | CAC-C3C | -2.01 | 1.46 | 1.51 |
| 17 | f | 4014 | BCR | C10-C9 | -2.01 | 1.33 | 1.35 |
| 14 | e | 1120 | CLA | CAC-C3C | -2.01 | 1.46 | 1.51 |
| 14 | 4 | 509 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | q | 502 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | e | 1118 | CLA | C3B-C2B | -2.01 | 1.37 | 1.40 |
| 14 | A | 1136 | CLA | MG-ND | -2.01 | 2.01 | 2.05 |
| 14 | 5 | 508 | CLA | C4B-CHC | -2.01 | 1.35 | 1.41 |
| 14 | G | 1103 | CLA | CAC-C3C | -2.01 | 1.46 | 1.51 |
| 14 | 1 | 502 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | Z | 507 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | t | 509 | CLA | CMC-C2C | -2.01 | 1.46 | 1.50 |
| 14 | a | 518 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 14 | u | 508 | CLA | C4B-CHC | -2.00 | 1.35 | 1.41 |
| 14 | 2 | 510 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | t | 506 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | 6 | 506 | CLA | CMD-C2D | -2.00 | 1.46 | 1.50 |
| 14 | d | 512 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | q | 519 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 14 | f | 1219 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | e | 1105 | CLA | MG-ND | -2.00 | 2.01 | 2.05 |
| 14 | Y | 516 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 14 | f | 1229 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 14 | 1 | 507 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | f | 1234 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 14 | 4 | 505 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | d | 503 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 14 | q | 516 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 14 | H | 1219 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | 1 | 511 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 14 | e | 1108 | CLA | C3B-CAB | -2.00 | 1.43 | 1.47 |
| 14 | G | 1108 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | s | 517 | CLA | C3B-C2B | -2.00 | 1.37 | 1.40 |
| 14 | 3 | 505 | CLA | MG-ND | -2.00 | 2.01 | 2.05 |
| 14 | A | 1108 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | Y | 502 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | d | 505 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | q | 511 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | r | 510 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 17 | B | 4014 | BCR | C10-C9 | -2.00 | 1.33 | 1.35 |
| 14 | s | 502 | CLA | CMC-C2C | -2.00 | 1.46 | 1.50 |
| 14 | G | 1122 | CLA | C4B-CHC | -2.00 | 1.35 | 1.41 |

All (7680) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1023 | CLA | C4A-NA-C1A | 9.67 | 111.06 | 106.71 |
| 14 | B | 1023 | CLA | C4A-NA-C1A | 9.59 | 111.02 | 106.71 |
| 14 | f | 1023 | CLA | C4A-NA-C1A | 9.53 | 110.99 | 106.71 |
| 15 | G | 2001 | PQN | C11-C12-C13 | -9.51 | 110.96 | 126.79 |
| 15 | A | 2001 | PQN | C11-C12-C13 | -9.50 | 110.98 | 126.79 |
| 15 | e | 2001 | PQN | C11-C12-C13 | -9.49 | 110.99 | 126.79 |
| 15 | f | 2002 | PQN | C11-C12-C13 | -9.11 | 111.63 | 126.79 |
| 15 | B | 2002 | PQN | C11-C12-C13 | -9.10 | 111.64 | 126.79 |
| 15 | H | 2002 | PQN | C11-C12-C13 | -9.09 | 111.67 | 126.79 |
| 14 | e | 1103 | CLA | C4A-NA-C1A | 8.34 | 110.46 | 106.71 |
| 17 | G | 4008 | BCR | C24-C23-C22 | -8.34 | 113.63 | 126.23 |
| 17 | e | 4008 | BCR | C24-C23-C22 | -8.32 | 113.66 | 126.23 |
| 17 | A | 4008 | BCR | C24-C23-C22 | -8.32 | 113.66 | 126.23 |
| 14 | A | 1103 | CLA | C4A-NA-C1A | 8.32 | 110.45 | 106.71 |
| 14 | G | 1103 | CLA | C4A-NA-C1A | 8.31 | 110.44 | 106.71 |
| 14 | f | 1239 | CLA | C4A-NA-C1A | 8.20 | 110.39 | 106.71 |
| 14 | H | 1239 | CLA | C4A-NA-C1A | 8.14 | 110.37 | 106.71 |
| 14 | B | 1239 | CLA | C4A-NA-C1A | 8.12 | 110.36 | 106.71 |
| 14 | G | 1109 | CLA | C4A-NA-C1A | 7.99 | 110.30 | 106.71 |
| 14 | A | 1109 | CLA | C4A-NA-C1A | 7.99 | 110.30 | 106.71 |
| 14 | G | 1101 | CLA | C4A-NA-C1A | 7.97 | 110.29 | 106.71 |
| 14 | H | 1214 | CLA | C4A-NA-C1A | 7.94 | 110.28 | 106.71 |
| 14 | n | 1503 | CLA | C4A-NA-C1A | 7.93 | 110.27 | 106.71 |
| 14 | Z | 502 | CLA | C4A-NA-C1A | 7.91 | 110.26 | 106.71 |
| 14 | e | 1109 | CLA | C4A-NA-C1A | 7.91 | 110.26 | 106.71 |
| 14 | H | 1226 | CLA | CMB-C2B-C1B | -7.91 | 116.31 | 128.46 |
| 14 | f | 1226 | CLA | CMB-C2B-C1B | -7.89 | 116.34 | 128.46 |
| 14 | B | 1226 | CLA | CMB-C2B-C1B | -7.88 | 116.35 | 128.46 |
| 14 | L | 1503 | CLA | C4A-NA-C1A | 7.88 | 110.25 | 106.71 |
| 14 | B | 1214 | CLA | C4A-NA-C1A | 7.87 | 110.25 | 106.71 |
| 14 | e | 1101 | CLA | C4A-NA-C1A | 7.87 | 110.25 | 106.71 |
| 14 | A | 1115 | CLA | C4A-NA-C1A | 7.86 | 110.24 | 106.71 |
| 14 | f | 1214 | CLA | C4A-NA-C1A | 7.85 | 110.24 | 106.71 |
| 14 | B | 1205 | CLA | C4A-NA-C1A | 7.85 | 110.24 | 106.71 |
| 14 | s | 502 | CLA | C4A-NA-C1A | 7.85 | 110.23 | 106.71 |
| 14 | V | 1503 | CLA | C4A-NA-C1A | 7.85 | 110.23 | 106.71 |
| 14 | 2 | 502 | CLA | C4A-NA-C1A | 7.83 | 110.22 | 106.71 |
| 14 | f | 1205 | CLA | C4A-NA-C1A | 7.82 | 110.22 | 106.71 |
| 14 | G | 1115 | CLA | C4A-NA-C1A | 7.81 | 110.22 | 106.71 |
| 14 | r | 502 | CLA | C4A-NA-C1A | 7.81 | 110.22 | 106.71 |
| 14 | A | 1101 | CLA | C4A-NA-C1A | 7.81 | 110.22 | 106.71 |
| 14 | 3 | 502 | CLA | C4A-NA-C1A | 7.79 | 110.21 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1201 | CLA | C4A-NA-C1A | 7.78 | 110.20 | 106.71 |
| 14 | a | 502 | CLA | C4A-NA-C1A | 7.78 | 110.20 | 106.71 |
| 14 | t | 502 | CLA | C4A-NA-C1A | 7.78 | 110.20 | 106.71 |
| 14 | f | 1201 | CLA | C4A-NA-C1A | 7.77 | 110.20 | 106.71 |
| 14 | e | 1115 | CLA | C4A-NA-C1A | 7.77 | 110.20 | 106.71 |
| 14 | H | 1205 | CLA | C4A-NA-C1A | 7.76 | 110.19 | 106.71 |
| 14 | q | 508 | CLA | C4A-NA-C1A | 7.76 | 110.19 | 106.71 |
| 14 | G | 1137 | CLA | C4A-NA-C1A | 7.74 | 110.19 | 106.71 |
| 14 | f | 1215 | CLA | C4A-NA-C1A | 7.74 | 110.18 | 106.71 |
| 14 | A | 1137 | CLA | C4A-NA-C1A | 7.72 | 110.18 | 106.71 |
| 14 | H | 1201 | CLA | C4A-NA-C1A | 7.72 | 110.18 | 106.71 |
| 14 | b | 502 | CLA | C4A-NA-C1A | 7.72 | 110.17 | 106.71 |
| 14 | 4 | 502 | CLA | C4A-NA-C1A | 7.70 | 110.17 | 106.71 |
| 14 | e | 1237 | CLA | C4A-NA-C1A | 7.70 | 110.17 | 106.71 |
| 14 | Z | 501 | CLA | C4A-NA-C1A | 7.68 | 110.16 | 106.71 |
| 14 | e | 1137 | CLA | C4A-NA-C1A | 7.68 | 110.16 | 106.71 |
| 14 | G | 1013 | CLA | CMB-C2B-C1B | -7.68 | 116.66 | 128.46 |
| 14 | A | 1013 | CLA | CMB-C2B-C1B | -7.67 | 116.67 | 128.46 |
| 14 | 5 | 502 | CLA | C4A-NA-C1A | 7.67 | 110.15 | 106.71 |
| 14 | e | 1013 | CLA | CMB-C2B-C1B | -7.67 | 116.68 | 128.46 |
| 14 | B | 1215 | CLA | C4A-NA-C1A | 7.66 | 110.15 | 106.71 |
| 14 | f | 1213 | CLA | C4A-NA-C1A | 7.66 | 110.15 | 106.71 |
| 14 | H | 1215 | CLA | C4A-NA-C1A | 7.63 | 110.14 | 106.71 |
| 14 | l | 508 | CLA | C4A-NA-C1A | 7.63 | 110.14 | 106.71 |
| 14 | G | 1104 | CLA | C4A-NA-C1A | 7.63 | 110.14 | 106.71 |
| 14 | A | 1120 | CLA | C4A-NA-C1A | 7.62 | 110.13 | 106.71 |
| 14 | A | 1237 | CLA | C4A-NA-C1A | 7.62 | 110.13 | 106.71 |
| 14 | G | 1237 | CLA | C4A-NA-C1A | 7.61 | 110.13 | 106.71 |
| 14 | B | 1213 | CLA | C4A-NA-C1A | 7.60 | 110.12 | 106.71 |
| 14 | H | 1212 | CLA | C4A-NA-C1A | 7.60 | 110.12 | 106.71 |
| 14 | A | 1122 | CLA | C4A-NA-C1A | 7.60 | 110.12 | 106.71 |
| 14 | Y | 508 | CLA | C4A-NA-C1A | 7.60 | 110.12 | 106.71 |
| 14 | 2 | 501 | CLA | C4A-NA-C1A | 7.60 | 110.12 | 106.71 |
| 14 | H | 1213 | CLA | C4A-NA-C1A | 7.60 | 110.12 | 106.71 |
| 14 | e | 1104 | CLA | C4A-NA-C1A | 7.59 | 110.12 | 106.71 |
| 14 | r | 501 | CLA | C4A-NA-C1A | 7.58 | 110.11 | 106.71 |
| 14 | c | 502 | CLA | C4A-NA-C1A | 7.58 | 110.11 | 106.71 |
| 14 | l | 1303 | CLA | C4A-NA-C1A | 7.58 | 110.11 | 106.71 |
| 14 | A | 1104 | CLA | C4A-NA-C1A | 7.57 | 110.11 | 106.71 |
| 14 | l | 502 | CLA | C4A-NA-C1A | 7.56 | 110.10 | 106.71 |
| 14 | u | 502 | CLA | C4A-NA-C1A | 7.55 | 110.10 | 106.71 |
| 14 | G | 1120 | CLA | C4A-NA-C1A | 7.54 | 110.10 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14 | e | 1120 | CLA | C4A-NA-C1A | 7.54 | 110.10 | 106.71 |
| 14 | q | 502 | CLA | C4A-NA-C1A | 7.54 | 110.10 | 106.71 |
| 14 | H | 1218 | CLA | C4A-NA-C1A | 7.54 | 110.10 | 106.71 |
| 14 | e | 1122 | CLA | C4A-NA-C1A | 7.54 | 110.09 | 106.71 |
| 14 | d | 502 | CLA | C4A-NA-C1A | 7.53 | 110.09 | 106.71 |
| 14 | v | 501 | CLA | C4A-NA-C1A | 7.52 | 110.09 | 106.71 |
| 14 | G | 1133 | CLA | C4A-NA-C1A | 7.52 | 110.08 | 106.71 |
| 14 | f | 1212 | CLA | C4A-NA-C1A | 7.52 | 110.08 | 106.71 |
| 14 | e | 1133 | CLA | C4A-NA-C1A | 7.50 | 110.08 | 106.71 |
| 14 | G | 1122 | CLA | C4A-NA-C1A | 7.50 | 110.08 | 106.71 |
| 14 | G | 1118 | CLA | C4A-NA-C1A | 7.50 | 110.08 | 106.71 |
| 14 | f | 1223 | CLA | C4A-NA-C1A | 7.50 | 110.08 | 106.71 |
| 14 | J | 1303 | CLA | C4A-NA-C1A | 7.49 | 110.07 | 106.71 |
| 14 | Y | 502 | CLA | C4A-NA-C1A | 7.49 | 110.07 | 106.71 |
| 14 | e | 1118 | CLA | C4A-NA-C1A | 7.49 | 110.07 | 106.71 |
| 14 | 6 | 502 | CLA | C4A-NA-C1A | 7.48 | 110.07 | 106.71 |
| 14 | u | 508 | CLA | C4A-NA-C1A | 7.48 | 110.07 | 106.71 |
| 14 | B | 1212 | CLA | C4A-NA-C1A | 7.48 | 110.07 | 106.71 |
| 14 | T | 1303 | CLA | C4A-NA-C1A | 7.47 | 110.06 | 106.71 |
| 14 | 6 | 501 | CLA | C4A-NA-C1A | 7.47 | 110.06 | 106.71 |
| 14 | d | 501 | CLA | C4A-NA-C1A | 7.46 | 110.06 | 106.71 |
| 14 | A | 1118 | CLA | C4A-NA-C1A | 7.46 | 110.06 | 106.71 |
| 14 | Y | 518 | CLA | C4A-NA-C1A | 7.46 | 110.06 | 106.71 |
| 14 | B | 1223 | CLA | C4A-NA-C1A | 7.45 | 110.06 | 106.71 |
| 14 | A | 1133 | CLA | C4A-NA-C1A | 7.45 | 110.06 | 106.71 |
| 14 | u | 501 | CLA | C4A-NA-C1A | 7.45 | 110.06 | 106.71 |
| 14 | b | 517 | CLA | C4A-NA-C1A | 7.44 | 110.05 | 106.71 |
| 14 | f | 1218 | CLA | C4A-NA-C1A | 7.44 | 110.05 | 106.71 |
| 14 | A | 1112 | CLA | C4A-NA-C1A | 7.44 | 110.05 | 106.71 |
| 14 | 4 | 517 | CLA | C4A-NA-C1A | 7.44 | 110.05 | 106.71 |
| 14 | v | 502 | CLA | C4A-NA-C1A | 7.44 | 110.05 | 106.71 |
| 14 | 5 | 508 | CLA | C4A-NA-C1A | 7.43 | 110.05 | 106.71 |
| 14 | 5 | 501 | CLA | C4A-NA-C1A | 7.41 | 110.04 | 106.71 |
| 14 | e | 1112 | CLA | C4A-NA-C1A | 7.40 | 110.03 | 106.71 |
| 14 | H | 1220 | CLA | C4A-NA-C1A | 7.39 | 110.03 | 106.71 |
| 14 | B | 1218 | CLA | C4A-NA-C1A | 7.39 | 110.03 | 106.71 |
| 14 | c | 508 | CLA | C4A-NA-C1A | 7.39 | 110.03 | 106.71 |
| 14 | v | 503 | CLA | C4A-NA-C1A | 7.39 | 110.03 | 106.71 |
| 14 | H | 1223 | CLA | C4A-NA-C1A | 7.38 | 110.03 | 106.71 |
| 14 | G | 1134 | CLA | C4A-NA-C1A | 7.38 | 110.02 | 106.71 |
| 14 | Y | 501 | CLA | C4A-NA-C1A | 7.38 | 110.02 | 106.71 |
| 14 | 6 | 503 | CLA | C4A-NA-C1A | 7.37 | 110.02 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | t | 517 | CLA | C4A-NA-C1A | 7.37 | 110.02 | 106.71 |
| 14 | l | 501 | CLA | C4A-NA-C1A | 7.36 | 110.02 | 106.71 |
| 14 | l | 518 | CLA | C4A-NA-C1A | 7.36 | 110.01 | 106.71 |
| 14 | H | 1211 | CLA | C4A-NA-C1A | 7.36 | 110.01 | 106.71 |
| 14 | A | 1140 | CLA | C4A-NA-C1A | 7.35 | 110.01 | 106.71 |
| 15 | B | 2002 | PQN | C15-C13-C12 | -7.34 | 106.26 | 121.12 |
| 14 | B | 1220 | CLA | C4A-NA-C1A | 7.34 | 110.01 | 106.71 |
| 14 | G | 1112 | CLA | C4A-NA-C1A | 7.34 | 110.01 | 106.71 |
| 15 | H | 2002 | PQN | C15-C13-C12 | -7.34 | 106.26 | 121.12 |
| 14 | H | 1228 | CLA | C4A-NA-C1A | 7.34 | 110.00 | 106.71 |
| 14 | B | 1228 | CLA | C4A-NA-C1A | 7.34 | 110.00 | 106.71 |
| 14 | f | 1211 | CLA | C4A-NA-C1A | 7.33 | 110.00 | 106.71 |
| 14 | f | 1228 | CLA | C4A-NA-C1A | 7.33 | 110.00 | 106.71 |
| 14 | J | 1302 | CLA | C4A-NA-C1A | 7.32 | 110.00 | 106.71 |
| 14 | 4 | 501 | CLA | C4A-NA-C1A | 7.32 | 110.00 | 106.71 |
| 14 | e | 1134 | CLA | C4A-NA-C1A | 7.32 | 110.00 | 106.71 |
| 15 | f | 2002 | PQN | C15-C13-C12 | -7.32 | 106.30 | 121.12 |
| 14 | A | 1134 | CLA | C4A-NA-C1A | 7.32 | 110.00 | 106.71 |
| 14 | A | 1119 | CLA | C4A-NA-C1A | 7.32 | 110.00 | 106.71 |
| 14 | n | 1502 | CLA | C4A-NA-C1A | 7.31 | 109.99 | 106.71 |
| 14 | e | 1126 | CLA | C4A-NA-C1A | 7.31 | 109.99 | 106.71 |
| 14 | q | 501 | CLA | C4A-NA-C1A | 7.31 | 109.99 | 106.71 |
| 14 | 5 | 504 | CLA | C4A-NA-C1A | 7.31 | 109.99 | 106.71 |
| 14 | c | 501 | CLA | C4A-NA-C1A | 7.30 | 109.99 | 106.71 |
| 14 | f | 1220 | CLA | C4A-NA-C1A | 7.30 | 109.99 | 106.71 |
| 14 | l | 1302 | CLA | C4A-NA-C1A | 7.30 | 109.99 | 106.71 |
| 14 | t | 501 | CLA | C4A-NA-C1A | 7.30 | 109.99 | 106.71 |
| 14 | e | 1119 | CLA | C4A-NA-C1A | 7.29 | 109.98 | 106.71 |
| 14 | e | 1140 | CLA | C4A-NA-C1A | 7.29 | 109.98 | 106.71 |
| 14 | G | 1126 | CLA | C4A-NA-C1A | 7.29 | 109.98 | 106.71 |
| 14 | 4 | 509 | CLA | C4A-NA-C1A | 7.28 | 109.98 | 106.71 |
| 14 | G | 1119 | CLA | C4A-NA-C1A | 7.28 | 109.98 | 106.71 |
| 14 | d | 503 | CLA | C4A-NA-C1A | 7.28 | 109.98 | 106.71 |
| 14 | f | 1204 | CLA | C4A-NA-C1A | 7.28 | 109.98 | 106.71 |
| 14 | G | 1140 | CLA | C4A-NA-C1A | 7.28 | 109.98 | 106.71 |
| 14 | T | 1302 | CLA | C4A-NA-C1A | 7.27 | 109.98 | 106.71 |
| 14 | a | 509 | CLA | C4A-NA-C1A | 7.27 | 109.97 | 106.71 |
| 14 | B | 1211 | CLA | C4A-NA-C1A | 7.26 | 109.97 | 106.71 |
| 14 | r | 517 | CLA | C4A-NA-C1A | 7.26 | 109.97 | 106.71 |
| 14 | q | 518 | CLA | C4A-NA-C1A | 7.26 | 109.97 | 106.71 |
| 14 | b | 501 | CLA | C4A-NA-C1A | 7.26 | 109.97 | 106.71 |
| 14 | 3 | 509 | CLA | C4A-NA-C1A | 7.25 | 109.97 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | L | 1502 | CLA | C4A-NA-C1A | 7.25 | 109.97 | 106.71 |
| 14 | A | 1126 | CLA | C4A-NA-C1A | 7.25 | 109.96 | 106.71 |
| 14 | c | 504 | CLA | C4A-NA-C1A | 7.25 | 109.96 | 106.71 |
| 14 | Y | 505 | CLA | C4A-NA-C1A | 7.24 | 109.96 | 106.71 |
| 14 | H | 1204 | CLA | C4A-NA-C1A | 7.24 | 109.96 | 106.71 |
| 14 | 2 | 517 | CLA | C4A-NA-C1A | 7.23 | 109.96 | 106.71 |
| 14 | 5 | 507 | CLA | C4A-NA-C1A | 7.23 | 109.96 | 106.71 |
| 17 | n | 4019 | BCR | C24-C23-C22 | -7.23 | 115.31 | 126.23 |
| 14 | B | 1204 | CLA | C4A-NA-C1A | 7.23 | 109.95 | 106.71 |
| 14 | A | 1128 | CLA | CMB-C2B-C1B | -7.22 | 117.37 | 128.46 |
| 14 | Z | 519 | CLA | C4A-NA-C1A | 7.21 | 109.95 | 106.71 |
| 17 | L | 4019 | BCR | C24-C23-C22 | -7.20 | 115.35 | 126.23 |
| 17 | V | 4019 | BCR | C24-C23-C22 | -7.20 | 115.35 | 126.23 |
| 14 | e | 1128 | CLA | CMB-C2B-C1B | -7.20 | 117.39 | 128.46 |
| 14 | u | 504 | CLA | C4A-NA-C1A | 7.20 | 109.94 | 106.71 |
| 14 | s | 509 | CLA | C4A-NA-C1A | 7.20 | 109.94 | 106.71 |
| 14 | t | 509 | CLA | C4A-NA-C1A | 7.20 | 109.94 | 106.71 |
| 14 | G | 1128 | CLA | CMB-C2B-C1B | -7.19 | 117.41 | 128.46 |
| 14 | 1 | 505 | CLA | C4A-NA-C1A | 7.19 | 109.94 | 106.71 |
| 14 | Z | 517 | CLA | C4A-NA-C1A | 7.19 | 109.94 | 106.71 |
| 14 | u | 507 | CLA | C4A-NA-C1A | 7.18 | 109.93 | 106.71 |
| 14 | b | 509 | CLA | C4A-NA-C1A | 7.18 | 109.93 | 106.71 |
| 14 | r | 503 | CLA | C4A-NA-C1A | 7.18 | 109.93 | 106.71 |
| 14 | Z | 503 | CLA | C4A-NA-C1A | 7.17 | 109.93 | 106.71 |
| 14 | 2 | 519 | CLA | C4A-NA-C1A | 7.17 | 109.93 | 106.71 |
| 14 | V | 1502 | CLA | C4A-NA-C1A | 7.16 | 109.92 | 106.71 |
| 14 | u | 503 | CLA | C4A-NA-C1A | 7.15 | 109.92 | 106.71 |
| 14 | 4 | 513 | CLA | C4A-NA-C1A | 7.15 | 109.92 | 106.71 |
| 14 | r | 506 | CLA | C4A-NA-C1A | 7.15 | 109.92 | 106.71 |
| 14 | a | 506 | CLA | C4A-NA-C1A | 7.14 | 109.92 | 106.71 |
| 14 | c | 507 | CLA | C4A-NA-C1A | 7.14 | 109.92 | 106.71 |
| 14 | t | 519 | CLA | C4A-NA-C1A | 7.14 | 109.92 | 106.71 |
| 14 | 2 | 503 | CLA | C4A-NA-C1A | 7.13 | 109.91 | 106.71 |
| 14 | b | 518 | CLA | C4A-NA-C1A | 7.13 | 109.91 | 106.71 |
| 14 | 4 | 519 | CLA | C4A-NA-C1A | 7.13 | 109.91 | 106.71 |
| 14 | Y | 507 | CLA | C4A-NA-C1A | 7.13 | 109.91 | 106.71 |
| 14 | c | 519 | CLA | C4A-NA-C1A | 7.12 | 109.91 | 106.71 |
| 14 | d | 506 | CLA | C4A-NA-C1A | 7.12 | 109.91 | 106.71 |
| 14 | 4 | 506 | CLA | C4A-NA-C1A | 7.12 | 109.91 | 106.71 |
| 14 | f | 1206 | CLA | C4A-NA-C1A | 7.12 | 109.91 | 106.71 |
| 14 | t | 518 | CLA | C4A-NA-C1A | 7.12 | 109.91 | 106.71 |
| 14 | s | 519 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14 | c | 503 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |
| 14 | e | 1113 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |
| 14 | A | 1113 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |
| 14 | 4 | 518 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |
| 14 | a | 513 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |
| 14 | b | 513 | CLA | C4A-NA-C1A | 7.11 | 109.90 | 106.71 |
| 14 | r | 519 | CLA | C4A-NA-C1A | 7.10 | 109.90 | 106.71 |
| 14 | H | 1206 | CLA | C4A-NA-C1A | 7.10 | 109.90 | 106.71 |
| 14 | q | 505 | CLA | C4A-NA-C1A | 7.10 | 109.90 | 106.71 |
| 14 | e | 1013 | CLA | C4A-NA-C1A | 7.10 | 109.90 | 106.71 |
| 14 | B | 1206 | CLA | C4A-NA-C1A | 7.10 | 109.90 | 106.71 |
| 14 | a | 501 | CLA | C4A-NA-C1A | 7.09 | 109.89 | 106.71 |
| 14 | q | 507 | CLA | C4A-NA-C1A | 7.09 | 109.89 | 106.71 |
| 14 | 2 | 506 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | b | 506 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | e | 1108 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | e | 1125 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | s | 501 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | G | 1013 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | t | 513 | CLA | C4A-NA-C1A | 7.08 | 109.89 | 106.71 |
| 14 | A | 1125 | CLA | C4A-NA-C1A | 7.07 | 109.89 | 106.71 |
| 14 | b | 519 | CLA | C4A-NA-C1A | 7.07 | 109.89 | 106.71 |
| 14 | c | 505 | CLA | C4A-NA-C1A | 7.07 | 109.89 | 106.71 |
| 14 | s | 504 | CLA | C4A-NA-C1A | 7.07 | 109.89 | 106.71 |
| 14 | H | 1238 | CLA | C4A-NA-C1A | 7.07 | 109.88 | 106.71 |
| 14 | e | 1111 | CLA | C4A-NA-C1A | 7.06 | 109.88 | 106.71 |
| 14 | 5 | 503 | CLA | C4A-NA-C1A | 7.06 | 109.88 | 106.71 |
| 14 | 6 | 506 | CLA | C4A-NA-C1A | 7.06 | 109.88 | 106.71 |
| 14 | A | 1111 | CLA | C4A-NA-C1A | 7.06 | 109.88 | 106.71 |
| 14 | B | 1202 | CLA | C4A-NA-C1A | 7.05 | 109.88 | 106.71 |
| 14 | 3 | 519 | CLA | C4A-NA-C1A | 7.05 | 109.88 | 106.71 |
| 14 | 3 | 504 | CLA | C4A-NA-C1A | 7.05 | 109.88 | 106.71 |
| 14 | 3 | 513 | CLA | C4A-NA-C1A | 7.05 | 109.88 | 106.71 |
| 14 | d | 511 | CLA | C4A-NA-C1A | 7.05 | 109.88 | 106.71 |
| 14 | 1 | 507 | CLA | C4A-NA-C1A | 7.05 | 109.87 | 106.71 |
| 14 | 3 | 506 | CLA | C4A-NA-C1A | 7.05 | 109.87 | 106.71 |
| 14 | 5 | 519 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | Z | 505 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | a | 507 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | f | 1202 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | 4 | 503 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | t | 510 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14 | G | 1113 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | t | 503 | CLA | C4A-NA-C1A | 7.04 | 109.87 | 106.71 |
| 14 | A | 1013 | CLA | C4A-NA-C1A | 7.03 | 109.87 | 106.71 |
| 14 | A | 1138 | CLA | C4A-NA-C1A | 7.03 | 109.87 | 106.71 |
| 14 | b | 503 | CLA | C4A-NA-C1A | 7.03 | 109.87 | 106.71 |
| 14 | A | 1108 | CLA | C4A-NA-C1A | 7.02 | 109.86 | 106.71 |
| 14 | G | 1138 | CLA | C4A-NA-C1A | 7.02 | 109.86 | 106.71 |
| 14 | 6 | 511 | CLA | C4A-NA-C1A | 7.02 | 109.86 | 106.71 |
| 14 | a | 519 | CLA | C4A-NA-C1A | 7.02 | 109.86 | 106.71 |
| 14 | B | 1217 | CLA | C4A-NA-C1A | 7.02 | 109.86 | 106.71 |
| 14 | G | 1111 | CLA | C4A-NA-C1A | 7.02 | 109.86 | 106.71 |
| 14 | Z | 506 | CLA | C4A-NA-C1A | 7.01 | 109.86 | 106.71 |
| 14 | v | 506 | CLA | C4A-NA-C1A | 7.01 | 109.86 | 106.71 |
| 14 | v | 511 | CLA | C4A-NA-C1A | 7.01 | 109.86 | 106.71 |
| 14 | 5 | 505 | CLA | C4A-NA-C1A | 7.00 | 109.86 | 106.71 |
| 14 | G | 1125 | CLA | C4A-NA-C1A | 7.00 | 109.85 | 106.71 |
| 14 | s | 506 | CLA | C4A-NA-C1A | 7.00 | 109.85 | 106.71 |
| 14 | u | 519 | CLA | C4A-NA-C1A | 7.00 | 109.85 | 106.71 |
| 14 | t | 507 | CLA | C4A-NA-C1A | 7.00 | 109.85 | 106.71 |
| 14 | t | 506 | CLA | C4A-NA-C1A | 6.99 | 109.85 | 106.71 |
| 14 | f | 1238 | CLA | C4A-NA-C1A | 6.99 | 109.85 | 106.71 |
| 14 | Z | 504 | CLA | C4A-NA-C1A | 6.99 | 109.85 | 106.71 |
| 14 | K | 1103 | CLA | C4A-NA-C1A | 6.99 | 109.85 | 106.71 |
| 14 | 3 | 501 | CLA | C4A-NA-C1A | 6.99 | 109.85 | 106.71 |
| 14 | 2 | 505 | CLA | C4A-NA-C1A | 6.98 | 109.85 | 106.71 |
| 14 | Y | 504 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | Y | 511 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | a | 504 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | 3 | 507 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | U | 1103 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | d | 518 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | f | 1217 | CLA | C4A-NA-C1A | 6.98 | 109.84 | 106.71 |
| 14 | q | 504 | CLA | C4A-NA-C1A | 6.97 | 109.84 | 106.71 |
| 14 | s | 513 | CLA | C4A-NA-C1A | 6.97 | 109.84 | 106.71 |
| 14 | d | 509 | CLA | C4A-NA-C1A | 6.97 | 109.84 | 106.71 |
| 14 | 6 | 509 | CLA | C4A-NA-C1A | 6.96 | 109.84 | 106.71 |
| 14 | s | 511 | CLA | C4A-NA-C1A | 6.96 | 109.84 | 106.71 |
| 14 | H | 1217 | CLA | C4A-NA-C1A | 6.96 | 109.83 | 106.71 |
| 14 | r | 518 | CLA | C4A-NA-C1A | 6.96 | 109.83 | 106.71 |
| 14 | 3 | 511 | CLA | C4A-NA-C1A | 6.96 | 109.83 | 106.71 |
| 14 | s | 507 | CLA | C4A-NA-C1A | 6.96 | 109.83 | 106.71 |
| 14 | H | 1202 | CLA | C4A-NA-C1A | 6.95 | 109.83 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1231 | CLA | C4A-NA-C1A | 6.95 | 109.83 | 106.71 |
| 14 | G | 1108 | CLA | C4A-NA-C1A | 6.95 | 109.83 | 106.71 |
| 14 | Y | 517 | CLA | C4A-NA-C1A | 6.94 | 109.83 | 106.71 |
| 14 | v | 508 | CLA | C4A-NA-C1A | 6.94 | 109.83 | 106.71 |
| 14 | a | 511 | CLA | C4A-NA-C1A | 6.94 | 109.83 | 106.71 |
| 14 | b | 507 | CLA | C4A-NA-C1A | 6.94 | 109.83 | 106.71 |
| 14 | u | 506 | CLA | C4A-NA-C1A | 6.94 | 109.83 | 106.71 |
| 14 | B | 1238 | CLA | C4A-NA-C1A | 6.94 | 109.82 | 106.71 |
| 14 | r | 504 | CLA | C4A-NA-C1A | 6.93 | 109.82 | 106.71 |
| 14 | G | 1130 | CLA | CMB-C2B-C1B | -6.93 | 117.81 | 128.46 |
| 14 | 1 | 504 | CLA | C4A-NA-C1A | 6.93 | 109.82 | 106.71 |
| 14 | 4 | 510 | CLA | C4A-NA-C1A | 6.93 | 109.82 | 106.71 |
| 14 | 6 | 508 | CLA | C4A-NA-C1A | 6.93 | 109.82 | 106.71 |
| 14 | f | 1235 | CLA | C4A-NA-C1A | 6.93 | 109.82 | 106.71 |
| 14 | B | 1231 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 14 | 3 | 518 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 14 | G | 1110 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 14 | 1 | 511 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 14 | Z | 518 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 14 | 2 | 518 | CLA | C4A-NA-C1A | 6.92 | 109.82 | 106.71 |
| 14 | A | 1130 | CLA | CMB-C2B-C1B | -6.91 | 117.84 | 128.46 |
| 14 | e | 1130 | CLA | CMB-C2B-C1B | -6.91 | 117.84 | 128.46 |
| 14 | m | 1103 | CLA | C4A-NA-C1A | 6.91 | 109.81 | 106.71 |
| 14 | 4 | 507 | CLA | C4A-NA-C1A | 6.91 | 109.81 | 106.71 |
| 14 | t | 512 | CLA | C4A-NA-C1A | 6.90 | 109.81 | 106.71 |
| 14 | d | 508 | CLA | C4A-NA-C1A | 6.90 | 109.81 | 106.71 |
| 14 | u | 509 | CLA | C4A-NA-C1A | 6.90 | 109.81 | 106.71 |
| 14 | b | 512 | CLA | C4A-NA-C1A | 6.90 | 109.81 | 106.71 |
| 14 | 6 | 518 | CLA | C4A-NA-C1A | 6.90 | 109.81 | 106.71 |
| 14 | e | 1138 | CLA | C4A-NA-C1A | 6.90 | 109.81 | 106.71 |
| 14 | s | 505 | CLA | C4A-NA-C1A | 6.89 | 109.80 | 106.71 |
| 14 | u | 505 | CLA | C4A-NA-C1A | 6.89 | 109.80 | 106.71 |
| 14 | 2 | 504 | CLA | C4A-NA-C1A | 6.88 | 109.80 | 106.71 |
| 14 | 6 | 504 | CLA | C4A-NA-C1A | 6.88 | 109.80 | 106.71 |
| 14 | f | 1231 | CLA | C4A-NA-C1A | 6.88 | 109.80 | 106.71 |
| 14 | B | 1235 | CLA | C4A-NA-C1A | 6.88 | 109.80 | 106.71 |
| 14 | 5 | 506 | CLA | C4A-NA-C1A | 6.88 | 109.80 | 106.71 |
| 14 | Z | 509 | CLA | C4A-NA-C1A | 6.87 | 109.80 | 106.71 |
| 14 | v | 509 | CLA | C4A-NA-C1A | 6.87 | 109.80 | 106.71 |
| 14 | a | 505 | CLA | C4A-NA-C1A | 6.86 | 109.79 | 106.71 |
| 14 | f | 1209 | CLA | C4A-NA-C1A | 6.86 | 109.79 | 106.71 |
| 14 | r | 505 | CLA | C4A-NA-C1A | 6.86 | 109.79 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14 | b | 510 | CLA | C4A-NA-C1A | 6.86 | 109.79 | 106.71 |
| 14 | v | 518 | CLA | C4A-NA-C1A | 6.85 | 109.79 | 106.71 |
| 14 | 4 | 512 | CLA | C4A-NA-C1A | 6.85 | 109.79 | 106.71 |
| 14 | a | 518 | CLA | C4A-NA-C1A | 6.85 | 109.79 | 106.71 |
| 14 | 3 | 505 | CLA | C4A-NA-C1A | 6.85 | 109.78 | 106.71 |
| 14 | q | 517 | CLA | C4A-NA-C1A | 6.85 | 109.78 | 106.71 |
| 14 | B | 1224 | CLA | C4A-NA-C1A | 6.85 | 109.78 | 106.71 |
| 14 | 4 | 504 | CLA | C4A-NA-C1A | 6.85 | 109.78 | 106.71 |
| 14 | 6 | 513 | CLA | C4A-NA-C1A | 6.84 | 109.78 | 106.71 |
| 14 | d | 504 | CLA | C4A-NA-C1A | 6.84 | 109.78 | 106.71 |
| 14 | f | 1229 | CLA | C4A-NA-C1A | 6.84 | 109.78 | 106.71 |
| 14 | d | 507 | CLA | C4A-NA-C1A | 6.84 | 109.78 | 106.71 |
| 14 | v | 504 | CLA | C4A-NA-C1A | 6.83 | 109.78 | 106.71 |
| 14 | v | 517 | CLA | C4A-NA-C1A | 6.83 | 109.78 | 106.71 |
| 14 | 1 | 517 | CLA | C4A-NA-C1A | 6.83 | 109.78 | 106.71 |
| 14 | 6 | 517 | CLA | C4A-NA-C1A | 6.83 | 109.78 | 106.71 |
| 14 | B | 1229 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | H | 1221 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | u | 510 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | 2 | 509 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | Y | 503 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | s | 518 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | A | 1110 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | 5 | 509 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | 1 | 503 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | H | 1235 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | q | 511 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | v | 513 | CLA | C4A-NA-C1A | 6.82 | 109.77 | 106.71 |
| 14 | B | 1209 | CLA | C4A-NA-C1A | 6.81 | 109.77 | 106.71 |
| 14 | d | 517 | CLA | C4A-NA-C1A | 6.81 | 109.77 | 106.71 |
| 14 | H | 1229 | CLA | C4A-NA-C1A | 6.81 | 109.77 | 106.71 |
| 14 | c | 506 | CLA | C4A-NA-C1A | 6.81 | 109.77 | 106.71 |
| 14 | H | 1240 | CLA | C4A-NA-C1A | 6.80 | 109.76 | 106.71 |
| 14 | t | 504 | CLA | C4A-NA-C1A | 6.80 | 109.76 | 106.71 |
| 14 | Z | 516 | CLA | C4A-NA-C1A | 6.80 | 109.76 | 106.71 |
| 14 | r | 509 | CLA | C4A-NA-C1A | 6.79 | 109.76 | 106.71 |
| 14 | a | 516 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |
| 14 | 6 | 507 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |
| 14 | B | 1221 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |
| 14 | e | 1110 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |
| 14 | f | 1224 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |
| 14 | q | 503 | CLA | C4A-NA-C1A | 6.78 | 109.75 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14 | Y | 510 | CLA | C4A-NA-C1A | 6.77 | 109.75 | 106.71 |
| 14 | c | 510 | CLA | C4A-NA-C1A | 6.77 | 109.75 | 106.71 |
| 14 | q | 513 | CLA | C4A-NA-C1A | 6.77 | 109.75 | 106.71 |
| 14 | Y | 513 | CLA | C4A-NA-C1A | 6.77 | 109.75 | 106.71 |
| 14 | c | 509 | CLA | C4A-NA-C1A | 6.77 | 109.75 | 106.71 |
| 14 | B | 1240 | CLA | C4A-NA-C1A | 6.76 | 109.75 | 106.71 |
| 14 | 6 | 505 | CLA | C4A-NA-C1A | 6.76 | 109.75 | 106.71 |
| 14 | Z | 508 | CLA | C4A-NA-C1A | 6.76 | 109.75 | 106.71 |
| 14 | b | 504 | CLA | C4A-NA-C1A | 6.76 | 109.75 | 106.71 |
| 14 | v | 519 | CLA | C4A-NA-C1A | 6.76 | 109.74 | 106.71 |
| 14 | H | 1209 | CLA | C4A-NA-C1A | 6.76 | 109.74 | 106.71 |
| 14 | f | 1221 | CLA | C4A-NA-C1A | 6.75 | 109.74 | 106.71 |
| 14 | v | 507 | CLA | C4A-NA-C1A | 6.75 | 109.74 | 106.71 |
| 14 | H | 1224 | CLA | C4A-NA-C1A | 6.75 | 109.74 | 106.71 |
| 14 | B | 1230 | CLA | C4A-NA-C1A | 6.75 | 109.74 | 106.71 |
| 14 | 1 | 513 | CLA | C4A-NA-C1A | 6.75 | 109.74 | 106.71 |
| 14 | 2 | 508 | CLA | C4A-NA-C1A | 6.74 | 109.74 | 106.71 |
| 14 | d | 505 | CLA | C4A-NA-C1A | 6.74 | 109.74 | 106.71 |
| 14 | 5 | 510 | CLA | C4A-NA-C1A | 6.74 | 109.74 | 106.71 |
| 14 | R | 1302 | CLA | C4A-NA-C1A | 6.74 | 109.73 | 106.71 |
| 14 | V | 1501 | CLA | C4A-NA-C1A | 6.73 | 109.73 | 106.71 |
| 14 | d | 513 | CLA | C4A-NA-C1A | 6.72 | 109.73 | 106.71 |
| 14 | 1 | 510 | CLA | C4A-NA-C1A | 6.72 | 109.73 | 106.71 |
| 14 | u | 518 | CLA | C4A-NA-C1A | 6.72 | 109.73 | 106.71 |
| 14 | f | 1240 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | v | 505 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | 2 | 516 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | 6 | 519 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | d | 519 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | f | 1236 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | Y | 509 | CLA | C4A-NA-C1A | 6.71 | 109.72 | 106.71 |
| 14 | 3 | 516 | CLA | C4A-NA-C1A | 6.70 | 109.72 | 106.71 |
| 14 | G | 1121 | CLA | C4A-NA-C1A | 6.70 | 109.72 | 106.71 |
| 14 | A | 1136 | CLA | C4A-NA-C1A | 6.70 | 109.72 | 106.71 |
| 14 | e | 1132 | CLA | C4A-NA-C1A | 6.70 | 109.72 | 106.71 |
| 14 | s | 516 | CLA | C4A-NA-C1A | 6.70 | 109.72 | 106.71 |
| 14 | n | 1501 | CLA | C4A-NA-C1A | 6.69 | 109.71 | 106.71 |
| 14 | G | 1132 | CLA | C4A-NA-C1A | 6.69 | 109.71 | 106.71 |
| 14 | A | 1121 | CLA | C4A-NA-C1A | 6.68 | 109.71 | 106.71 |
| 14 | f | 1230 | CLA | C4A-NA-C1A | 6.68 | 109.71 | 106.71 |
| 14 | L | 1501 | CLA | C4A-NA-C1A | 6.68 | 109.71 | 106.71 |
| 14 | q | 516 | CLA | C4A-NA-C1A | 6.68 | 109.71 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 14 | q | 510 | CLA | C4A-NA-C1A | 6.67 | 109.71 | 106.71 |
| 14 | v | 510 | CLA | C4A-NA-C1A | 6.67 | 109.70 | 106.71 |
| 14 | r | 508 | CLA | C4A-NA-C1A | 6.67 | 109.70 | 106.71 |
| 14 | G | 1106 | CLA | C4A-NA-C1A | 6.67 | 109.70 | 106.71 |
| 14 | U | 1105 | CLA | C4A-NA-C1A | 6.67 | 109.70 | 106.71 |
| 14 | A | 1106 | CLA | C4A-NA-C1A | 6.66 | 109.70 | 106.71 |
| 14 | e | 1136 | CLA | C4A-NA-C1A | 6.66 | 109.70 | 106.71 |
| 14 | 2 | 507 | CLA | C4A-NA-C1A | 6.66 | 109.70 | 106.71 |
| 14 | A | 1132 | CLA | C4A-NA-C1A | 6.66 | 109.70 | 106.71 |
| 14 | Y | 516 | CLA | C4A-NA-C1A | 6.65 | 109.70 | 106.71 |
| 14 | K | 1105 | CLA | C4A-NA-C1A | 6.65 | 109.69 | 106.71 |
| 14 | 6 | 510 | CLA | C4A-NA-C1A | 6.65 | 109.69 | 106.71 |
| 14 | H | 1230 | CLA | C4A-NA-C1A | 6.64 | 109.69 | 106.71 |
| 14 | B | 1236 | CLA | C4A-NA-C1A | 6.64 | 109.69 | 106.71 |
| 14 | F | 1302 | CLA | C4A-NA-C1A | 6.64 | 109.69 | 106.71 |
| 14 | H | 1236 | CLA | C4A-NA-C1A | 6.63 | 109.69 | 106.71 |
| 14 | 1 | 506 | CLA | C4A-NA-C1A | 6.63 | 109.69 | 106.71 |
| 14 | q | 509 | CLA | C4A-NA-C1A | 6.63 | 109.69 | 106.71 |
| 14 | 3 | 503 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | B | 1021 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | f | 1021 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | j | 1302 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | m | 1105 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | r | 516 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | q | 506 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | G | 1136 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | b | 508 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | d | 510 | CLA | C4A-NA-C1A | 6.62 | 109.68 | 106.71 |
| 14 | a | 510 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 14 | e | 1106 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 14 | e | 1121 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 14 | r | 507 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 14 | 5 | 518 | CLA | C4A-NA-C1A | 6.61 | 109.68 | 106.71 |
| 14 | r | 511 | CLA | C4A-NA-C1A | 6.60 | 109.67 | 106.71 |
| 14 | H | 1207 | CLA | C4A-NA-C1A | 6.60 | 109.67 | 106.71 |
| 14 | a | 503 | CLA | C4A-NA-C1A | 6.60 | 109.67 | 106.71 |
| 14 | c | 518 | CLA | C4A-NA-C1A | 6.60 | 109.67 | 106.71 |
| 14 | s | 503 | CLA | C4A-NA-C1A | 6.60 | 109.67 | 106.71 |
| 17 | f | 4006 | BCR | C7-C8-C9 | -6.59 | 116.27 | 126.23 |
| 14 | 1 | 509 | CLA | C4A-NA-C1A | 6.59 | 109.67 | 106.71 |
| 14 | Y | 506 | CLA | C4A-NA-C1A | 6.59 | 109.67 | 106.71 |
| 17 | V | 4022 | BCR | C7-C8-C9 | -6.59 | 116.28 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 14 | Z | 507 | CLA | C4A-NA-C1A | 6.59 | 109.67 | 106.71 |
| 14 | e | 1123 | CLA | C4A-NA-C1A | 6.59 | 109.67 | 106.71 |
| 14 | f | 1207 | CLA | C4A-NA-C1A | 6.59 | 109.67 | 106.71 |
| 14 | 2 | 511 | CLA | C4A-NA-C1A | 6.59 | 109.67 | 106.71 |
| 17 | L | 4022 | BCR | C7-C8-C9 | -6.59 | 116.28 | 126.23 |
| 14 | H | 1021 | CLA | C4A-NA-C1A | 6.58 | 109.67 | 106.71 |
| 14 | 1 | 516 | CLA | C4A-NA-C1A | 6.58 | 109.66 | 106.71 |
| 14 | 4 | 508 | CLA | C4A-NA-C1A | 6.57 | 109.66 | 106.71 |
| 14 | Z | 511 | CLA | C4A-NA-C1A | 6.57 | 109.66 | 106.71 |
| 14 | A | 1123 | CLA | C4A-NA-C1A | 6.57 | 109.66 | 106.71 |
| 14 | B | 1207 | CLA | C4A-NA-C1A | 6.57 | 109.66 | 106.71 |
| 17 | H | 4006 | BCR | C7-C8-C9 | -6.57 | 116.31 | 126.23 |
| 14 | 5 | 516 | CLA | C4A-NA-C1A | 6.56 | 109.66 | 106.71 |
| 14 | c | 516 | CLA | C4A-NA-C1A | 6.56 | 109.66 | 106.71 |
| 17 | B | 4006 | BCR | C7-C8-C9 | -6.56 | 116.32 | 126.23 |
| 17 | n | 4022 | BCR | C7-C8-C9 | -6.56 | 116.32 | 126.23 |
| 14 | 3 | 508 | CLA | C4A-NA-C1A | 6.56 | 109.65 | 106.71 |
| 14 | f | 1203 | CLA | C4A-NA-C1A | 6.56 | 109.65 | 106.71 |
| 14 | 3 | 510 | CLA | C4A-NA-C1A | 6.55 | 109.65 | 106.71 |
| 14 | H | 1203 | CLA | C4A-NA-C1A | 6.55 | 109.65 | 106.71 |
| 14 | a | 508 | CLA | C4A-NA-C1A | 6.55 | 109.65 | 106.71 |
| 14 | t | 508 | CLA | C4A-NA-C1A | 6.54 | 109.65 | 106.71 |
| 14 | f | 1227 | CLA | C4A-NA-C1A | 6.54 | 109.65 | 106.71 |
| 14 | B | 1203 | CLA | C4A-NA-C1A | 6.54 | 109.64 | 106.71 |
| 14 | q | 519 | CLA | C4A-NA-C1A | 6.52 | 109.64 | 106.71 |
| 14 | G | 1123 | CLA | C4A-NA-C1A | 6.52 | 109.64 | 106.71 |
| 14 | u | 516 | CLA | C4A-NA-C1A | 6.51 | 109.64 | 106.71 |
| 14 | G | 1114 | CLA | C4A-NA-C1A | 6.51 | 109.63 | 106.71 |
| 14 | c | 511 | CLA | C4A-NA-C1A | 6.51 | 109.63 | 106.71 |
| 14 | u | 511 | CLA | C4A-NA-C1A | 6.51 | 109.63 | 106.71 |
| 14 | c | 513 | CLA | C4A-NA-C1A | 6.51 | 109.63 | 106.71 |
| 14 | 5 | 511 | CLA | C4A-NA-C1A | 6.51 | 109.63 | 106.71 |
| 14 | s | 510 | CLA | C4A-NA-C1A | 6.50 | 109.63 | 106.71 |
| 14 | t | 516 | CLA | C4A-NA-C1A | 6.50 | 109.63 | 106.71 |
| 14 | s | 508 | CLA | C4A-NA-C1A | 6.49 | 109.63 | 106.71 |
| 14 | B | 1227 | CLA | C4A-NA-C1A | 6.49 | 109.62 | 106.71 |
| 14 | 4 | 516 | CLA | C4A-NA-C1A | 6.49 | 109.62 | 106.71 |
| 14 | e | 1105 | CLA | C4A-NA-C1A | 6.49 | 109.62 | 106.71 |
| 14 | b | 516 | CLA | C4A-NA-C1A | 6.48 | 109.62 | 106.71 |
| 14 | A | 1114 | CLA | C4A-NA-C1A | 6.48 | 109.62 | 106.71 |
| 14 | s | 517 | CLA | C4A-NA-C1A | 6.47 | 109.61 | 106.71 |
| 14 | e | 1114 | CLA | C4A-NA-C1A | 6.47 | 109.61 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1801 | CLA | C4A-NA-C1A | 6.45 | 109.61 | 106.71 |
| 14 | A | 1105 | CLA | C4A-NA-C1A | 6.44 | 109.60 | 106.71 |
| 14 | 5 | 513 | CLA | C4A-NA-C1A | 6.44 | 109.60 | 106.71 |
| 14 | t | 505 | CLA | C4A-NA-C1A | 6.44 | 109.60 | 106.71 |
| 14 | 4 | 505 | CLA | C4A-NA-C1A | 6.43 | 109.60 | 106.71 |
| 14 | 6 | 516 | CLA | C4A-NA-C1A | 6.43 | 109.60 | 106.71 |
| 14 | l | 519 | CLA | C4A-NA-C1A | 6.43 | 109.60 | 106.71 |
| 14 | u | 517 | CLA | C4A-NA-C1A | 6.43 | 109.60 | 106.71 |
| 14 | d | 516 | CLA | C4A-NA-C1A | 6.42 | 109.59 | 106.71 |
| 14 | r | 513 | CLA | C4A-NA-C1A | 6.42 | 109.59 | 106.71 |
| 14 | H | 1227 | CLA | C4A-NA-C1A | 6.41 | 109.59 | 106.71 |
| 14 | B | 1232 | CLA | C4A-NA-C1A | 6.41 | 109.59 | 106.71 |
| 14 | f | 1232 | CLA | C4A-NA-C1A | 6.41 | 109.59 | 106.71 |
| 14 | b | 505 | CLA | C4A-NA-C1A | 6.41 | 109.59 | 106.71 |
| 14 | f | 1232 | CLA | CMB-C2B-C1B | -6.40 | 118.62 | 128.46 |
| 14 | G | 1105 | CLA | C4A-NA-C1A | 6.40 | 109.58 | 106.71 |
| 14 | a | 517 | CLA | C4A-NA-C1A | 6.40 | 109.58 | 106.71 |
| 14 | v | 516 | CLA | C4A-NA-C1A | 6.40 | 109.58 | 106.71 |
| 14 | 2 | 513 | CLA | C4A-NA-C1A | 6.40 | 109.58 | 106.71 |
| 14 | u | 513 | CLA | C4A-NA-C1A | 6.39 | 109.58 | 106.71 |
| 14 | A | 1801 | CLA | C4A-NA-C1A | 6.39 | 109.58 | 106.71 |
| 14 | H | 1232 | CLA | C4A-NA-C1A | 6.39 | 109.58 | 106.71 |
| 14 | 3 | 517 | CLA | C4A-NA-C1A | 6.39 | 109.58 | 106.71 |
| 14 | B | 1232 | CLA | CMB-C2B-C1B | -6.38 | 118.65 | 128.46 |
| 17 | A | 4007 | BCR | C3-C4-C5 | -6.38 | 102.68 | 114.08 |
| 17 | G | 4007 | BCR | C3-C4-C5 | -6.38 | 102.69 | 114.08 |
| 17 | e | 4007 | BCR | C3-C4-C5 | -6.37 | 102.69 | 114.08 |
| 14 | e | 1801 | CLA | C4A-NA-C1A | 6.37 | 109.57 | 106.71 |
| 14 | H | 1232 | CLA | CMB-C2B-C1B | -6.37 | 118.67 | 128.46 |
| 14 | A | 1131 | CLA | C4A-NA-C1A | 6.37 | 109.57 | 106.71 |
| 14 | Z | 513 | CLA | C4A-NA-C1A | 6.37 | 109.57 | 106.71 |
| 14 | H | 1234 | CLA | CMB-C2B-C1B | -6.37 | 118.68 | 128.46 |
| 14 | Y | 519 | CLA | C4A-NA-C1A | 6.36 | 109.57 | 106.71 |
| 14 | B | 1234 | CLA | CMB-C2B-C1B | -6.36 | 118.69 | 128.46 |
| 14 | c | 517 | CLA | C4A-NA-C1A | 6.36 | 109.56 | 106.71 |
| 14 | f | 1234 | CLA | CMB-C2B-C1B | -6.34 | 118.71 | 128.46 |
| 14 | 5 | 517 | CLA | C4A-NA-C1A | 6.34 | 109.56 | 106.71 |
| 14 | j | 1301 | CLA | C4A-NA-C1A | 6.34 | 109.56 | 106.71 |
| 14 | 6 | 512 | CLA | C4A-NA-C1A | 6.33 | 109.55 | 106.71 |
| 14 | G | 1131 | CLA | C4A-NA-C1A | 6.33 | 109.55 | 106.71 |
| 14 | r | 510 | CLA | C4A-NA-C1A | 6.31 | 109.54 | 106.71 |
| 14 | 2 | 510 | CLA | C4A-NA-C1A | 6.31 | 109.54 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1131 | CLA | C4A-NA-C1A | 6.31 | 109.54 | 106.71 |
| 14 | G | 1107 | CLA | C4A-NA-C1A | 6.29 | 109.54 | 106.71 |
| 14 | B | 1219 | CLA | C4A-NA-C1A | 6.28 | 109.53 | 106.71 |
| 14 | f | 1219 | CLA | C4A-NA-C1A | 6.28 | 109.53 | 106.71 |
| 14 | A | 1102 | CLA | C4A-NA-C1A | 6.28 | 109.53 | 106.71 |
| 14 | F | 1301 | CLA | C4A-NA-C1A | 6.26 | 109.52 | 106.71 |
| 14 | G | 1102 | CLA | C4A-NA-C1A | 6.25 | 109.52 | 106.71 |
| 14 | Z | 510 | CLA | C4A-NA-C1A | 6.25 | 109.52 | 106.71 |
| 14 | R | 1301 | CLA | C4A-NA-C1A | 6.25 | 109.52 | 106.71 |
| 14 | v | 512 | CLA | C4A-NA-C1A | 6.24 | 109.51 | 106.71 |
| 15 | A | 2001 | PQN | C15-C13-C12 | -6.24 | 108.50 | 121.12 |
| 15 | G | 2001 | PQN | C15-C13-C12 | -6.24 | 108.50 | 121.12 |
| 15 | e | 2001 | PQN | C15-C13-C12 | -6.23 | 108.51 | 121.12 |
| 14 | d | 512 | CLA | C4A-NA-C1A | 6.22 | 109.50 | 106.71 |
| 14 | H | 1208 | CLA | C4A-NA-C1A | 6.20 | 109.50 | 106.71 |
| 14 | e | 1102 | CLA | C4A-NA-C1A | 6.19 | 109.49 | 106.71 |
| 14 | A | 1107 | CLA | C4A-NA-C1A | 6.19 | 109.49 | 106.71 |
| 14 | e | 1107 | CLA | C4A-NA-C1A | 6.18 | 109.48 | 106.71 |
| 14 | e | 1127 | CLA | C4A-NA-C1A | 6.17 | 109.48 | 106.71 |
| 14 | H | 1219 | CLA | C4A-NA-C1A | 6.15 | 109.47 | 106.71 |
| 14 | H | 1210 | CLA | C4A-NA-C1A | 6.15 | 109.47 | 106.71 |
| 14 | f | 1208 | CLA | C4A-NA-C1A | 6.14 | 109.47 | 106.71 |
| 14 | c | 512 | CLA | C4A-NA-C1A | 6.12 | 109.46 | 106.71 |
| 14 | A | 1127 | CLA | C4A-NA-C1A | 6.12 | 109.46 | 106.71 |
| 14 | B | 1210 | CLA | C4A-NA-C1A | 6.12 | 109.46 | 106.71 |
| 17 | A | 4011 | BCR | C7-C8-C9 | -6.12 | 116.99 | 126.23 |
| 17 | G | 4011 | BCR | C7-C8-C9 | -6.12 | 116.99 | 126.23 |
| 14 | B | 1208 | CLA | C4A-NA-C1A | 6.11 | 109.45 | 106.71 |
| 14 | Y | 512 | CLA | C4A-NA-C1A | 6.11 | 109.45 | 106.71 |
| 14 | u | 512 | CLA | C4A-NA-C1A | 6.11 | 109.45 | 106.71 |
| 14 | l | 512 | CLA | C4A-NA-C1A | 6.11 | 109.45 | 106.71 |
| 14 | f | 1210 | CLA | C4A-NA-C1A | 6.09 | 109.44 | 106.71 |
| 17 | e | 4011 | BCR | C7-C8-C9 | -6.09 | 117.03 | 126.23 |
| 14 | r | 512 | CLA | C4A-NA-C1A | 6.08 | 109.44 | 106.71 |
| 14 | H | 1216 | CLA | C4A-NA-C1A | 6.07 | 109.44 | 106.71 |
| 14 | 5 | 512 | CLA | C4A-NA-C1A | 6.06 | 109.43 | 106.71 |
| 14 | G | 1116 | CLA | C4A-NA-C1A | 6.05 | 109.43 | 106.71 |
| 14 | G | 1127 | CLA | C4A-NA-C1A | 6.05 | 109.43 | 106.71 |
| 14 | 2 | 512 | CLA | C4A-NA-C1A | 6.03 | 109.42 | 106.71 |
| 14 | A | 1013 | CLA | CMB-C2B-C3B | 6.01 | 135.92 | 124.68 |
| 14 | G | 1013 | CLA | CMB-C2B-C3B | 6.01 | 135.92 | 124.68 |
| 14 | B | 1222 | CLA | C4A-NA-C1A | 6.01 | 109.41 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1013 | CLA | CMB-C2B-C3B | 6.00 | 135.90 | 124.68 |
| 14 | q | 512 | CLA | C4A-NA-C1A | 5.99 | 109.40 | 106.71 |
| 14 | f | 1222 | CLA | C4A-NA-C1A | 5.99 | 109.40 | 106.71 |
| 14 | A | 1116 | CLA | C4A-NA-C1A | 5.99 | 109.40 | 106.71 |
| 14 | A | 1135 | CLA | C4A-NA-C1A | 5.99 | 109.40 | 106.71 |
| 14 | H | 1222 | CLA | C4A-NA-C1A | 5.98 | 109.40 | 106.71 |
| 14 | G | 1135 | CLA | C4A-NA-C1A | 5.98 | 109.39 | 106.71 |
| 14 | b | 511 | CLA | C4A-NA-C1A | 5.97 | 109.39 | 106.71 |
| 14 | H | 1226 | CLA | C4A-NA-C1A | 5.97 | 109.39 | 106.71 |
| 14 | e | 1116 | CLA | C4A-NA-C1A | 5.95 | 109.38 | 106.71 |
| 14 | B | 1216 | CLA | C4A-NA-C1A | 5.94 | 109.38 | 106.71 |
| 14 | Z | 512 | CLA | C4A-NA-C1A | 5.91 | 109.36 | 106.71 |
| 14 | H | 1221 | CLA | CMB-C2B-C1B | -5.90 | 119.39 | 128.46 |
| 14 | B | 1221 | CLA | CMB-C2B-C1B | -5.89 | 119.41 | 128.46 |
| 14 | f | 1221 | CLA | CMB-C2B-C1B | -5.89 | 119.42 | 128.46 |
| 14 | 4 | 511 | CLA | C4A-NA-C1A | 5.88 | 109.35 | 106.71 |
| 17 | f | 4010 | BCR | C20-C21-C22 | -5.88 | 118.92 | 127.31 |
| 17 | H | 4010 | BCR | C20-C21-C22 | -5.88 | 118.92 | 127.31 |
| 17 | B | 4010 | BCR | C20-C21-C22 | -5.87 | 118.93 | 127.31 |
| 17 | V | 4219 | BCR | C15-C14-C13 | -5.87 | 118.93 | 127.31 |
| 17 | L | 4219 | BCR | C15-C14-C13 | -5.87 | 118.93 | 127.31 |
| 14 | f | 1216 | CLA | C4A-NA-C1A | 5.87 | 109.34 | 106.71 |
| 14 | e | 1135 | CLA | C4A-NA-C1A | 5.85 | 109.34 | 106.71 |
| 17 | n | 4219 | BCR | C15-C14-C13 | -5.85 | 118.97 | 127.31 |
| 14 | A | 1117 | CLA | C4A-NA-C1A | 5.84 | 109.33 | 106.71 |
| 14 | A | 1128 | CLA | C4A-NA-C1A | 5.84 | 109.33 | 106.71 |
| 17 | T | 4013 | BCR | C20-C21-C22 | -5.83 | 118.99 | 127.31 |
| 14 | t | 511 | CLA | C4A-NA-C1A | 5.83 | 109.33 | 106.71 |
| 17 | J | 4013 | BCR | C20-C21-C22 | -5.82 | 119.01 | 127.31 |
| 14 | B | 1226 | CLA | C4A-NA-C1A | 5.81 | 109.32 | 106.71 |
| 14 | e | 1128 | CLA | C4A-NA-C1A | 5.81 | 109.32 | 106.71 |
| 14 | e | 1117 | CLA | C4A-NA-C1A | 5.80 | 109.31 | 106.71 |
| 17 | l | 4013 | BCR | C20-C21-C22 | -5.79 | 119.04 | 127.31 |
| 14 | G | 1011 | CLA | C4A-NA-C1A | 5.79 | 109.31 | 106.71 |
| 14 | G | 1128 | CLA | C4A-NA-C1A | 5.79 | 109.31 | 106.71 |
| 14 | e | 1011 | CLA | C4A-NA-C1A | 5.79 | 109.31 | 106.71 |
| 14 | A | 1011 | CLA | C4A-NA-C1A | 5.78 | 109.30 | 106.71 |
| 14 | K | 1401 | CLA | C4A-NA-C1A | 5.77 | 109.30 | 106.71 |
| 14 | f | 1226 | CLA | C4A-NA-C1A | 5.76 | 109.30 | 106.71 |
| 17 | H | 4010 | BCR | C15-C14-C13 | -5.76 | 119.09 | 127.31 |
| 14 | G | 1117 | CLA | C4A-NA-C1A | 5.76 | 109.29 | 106.71 |
| 17 | f | 4010 | BCR | C15-C14-C13 | -5.75 | 119.10 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | B | 4010 | BCR | C15-C14-C13 | -5.75 | 119.11 | 127.31 |
| 14 | G | 1129 | CLA | C4A-NA-C1A | 5.74 | 109.29 | 106.71 |
| 14 | f | 1225 | CLA | C4A-NA-C1A | 5.74 | 109.28 | 106.71 |
| 14 | m | 1401 | CLA | C4A-NA-C1A | 5.72 | 109.28 | 106.71 |
| 14 | e | 1124 | CLA | C4A-NA-C1A | 5.70 | 109.27 | 106.71 |
| 14 | a | 512 | CLA | C4A-NA-C1A | 5.69 | 109.27 | 106.71 |
| 14 | A | 1124 | CLA | C4A-NA-C1A | 5.69 | 109.26 | 106.71 |
| 14 | A | 1129 | CLA | C4A-NA-C1A | 5.69 | 109.26 | 106.71 |
| 14 | G | 1124 | CLA | C4A-NA-C1A | 5.68 | 109.26 | 106.71 |
| 14 | U | 1401 | CLA | C4A-NA-C1A | 5.68 | 109.26 | 106.71 |
| 14 | B | 1225 | CLA | C4A-NA-C1A | 5.66 | 109.25 | 106.71 |
| 14 | A | 1130 | CLA | CMB-C2B-C3B | 5.65 | 135.26 | 124.68 |
| 14 | e | 1130 | CLA | CMB-C2B-C3B | 5.65 | 135.26 | 124.68 |
| 14 | G | 1130 | CLA | CMB-C2B-C3B | 5.65 | 135.26 | 124.68 |
| 14 | e | 1129 | CLA | C4A-NA-C1A | 5.62 | 109.23 | 106.71 |
| 14 | H | 1225 | CLA | C4A-NA-C1A | 5.60 | 109.22 | 106.71 |
| 14 | f | 1234 | CLA | C4A-NA-C1A | 5.60 | 109.22 | 106.71 |
| 17 | v | 524 | BCR | C7-C8-C9 | -5.58 | 117.80 | 126.23 |
| 17 | d | 524 | BCR | C7-C8-C9 | -5.58 | 117.81 | 126.23 |
| 17 | 6 | 524 | BCR | C7-C8-C9 | -5.57 | 117.81 | 126.23 |
| 14 | e | 1135 | CLA | CMB-C2B-C1B | -5.57 | 119.91 | 128.46 |
| 14 | 3 | 512 | CLA | C4A-NA-C1A | 5.57 | 109.21 | 106.71 |
| 14 | A | 1135 | CLA | CMB-C2B-C1B | -5.55 | 119.93 | 128.46 |
| 14 | G | 1135 | CLA | CMB-C2B-C1B | -5.54 | 119.95 | 128.46 |
| 14 | s | 512 | CLA | C4A-NA-C1A | 5.53 | 109.19 | 106.71 |
| 14 | H | 1206 | CLA | CMB-C2B-C1B | -5.50 | 120.02 | 128.46 |
| 14 | f | 1206 | CLA | CMB-C2B-C1B | -5.50 | 120.02 | 128.46 |
| 14 | B | 1206 | CLA | CMB-C2B-C1B | -5.50 | 120.02 | 128.46 |
| 14 | e | 1102 | CLA | CMB-C2B-C1B | -5.48 | 120.03 | 128.46 |
| 14 | B | 1234 | CLA | C4A-NA-C1A | 5.48 | 109.17 | 106.71 |
| 14 | H | 1234 | CLA | C4A-NA-C1A | 5.48 | 109.17 | 106.71 |
| 14 | A | 1102 | CLA | CMB-C2B-C1B | -5.45 | 120.09 | 128.46 |
| 17 | F | 4016 | BCR | C15-C14-C13 | -5.45 | 119.54 | 127.31 |
| 14 | q | 508 | CLA | CMB-C2B-C1B | -5.45 | 120.09 | 128.46 |
| 14 | G | 1102 | CLA | CMB-C2B-C1B | -5.44 | 120.10 | 128.46 |
| 14 | G | 1126 | CLA | CMB-C2B-C1B | -5.44 | 120.10 | 128.46 |
| 17 | R | 4016 | BCR | C15-C14-C13 | -5.44 | 119.55 | 127.31 |
| 14 | Y | 508 | CLA | CMB-C2B-C1B | -5.43 | 120.12 | 128.46 |
| 14 | G | 1116 | CLA | CMB-C2B-C1B | -5.43 | 120.12 | 128.46 |
| 14 | H | 1228 | CLA | CMB-C2B-C1B | -5.42 | 120.13 | 128.46 |
| 17 | j | 4016 | BCR | C15-C14-C13 | -5.42 | 119.57 | 127.31 |
| 14 | 1 | 508 | CLA | CMB-C2B-C1B | -5.42 | 120.13 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1011 | CLA | O2D-CGD-CBD | 5.42 | 120.90 | 111.27 |
| 14 | G | 1011 | CLA | O2D-CGD-CBD | 5.42 | 120.89 | 111.27 |
| 14 | A | 1126 | CLA | CMB-C2B-C1B | -5.41 | 120.14 | 128.46 |
| 14 | e | 1126 | CLA | CMB-C2B-C1B | -5.41 | 120.14 | 128.46 |
| 14 | A | 1011 | CLA | O2D-CGD-CBD | 5.41 | 120.89 | 111.27 |
| 14 | e | 1116 | CLA | CMB-C2B-C1B | -5.41 | 120.15 | 128.46 |
| 14 | f | 1238 | CLA | CMB-C2B-C1B | -5.41 | 120.15 | 128.46 |
| 14 | B | 1238 | CLA | CMB-C2B-C1B | -5.40 | 120.16 | 128.46 |
| 14 | H | 1238 | CLA | CMB-C2B-C1B | -5.40 | 120.16 | 128.46 |
| 21 | f | 1852 | SQD | O5-C5-C4 | 5.40 | 119.50 | 109.69 |
| 21 | B | 1852 | SQD | O5-C5-C4 | 5.40 | 119.49 | 109.69 |
| 14 | B | 1228 | CLA | CMB-C2B-C1B | -5.39 | 120.18 | 128.46 |
| 14 | e | 1117 | CLA | CMB-C2B-C1B | -5.39 | 120.19 | 128.46 |
| 14 | A | 1116 | CLA | CMB-C2B-C1B | -5.39 | 120.19 | 128.46 |
| 14 | B | 1012 | CLA | CMB-C2B-C1B | -5.39 | 120.19 | 128.46 |
| 15 | H | 2002 | PQN | C14-C13-C12 | -5.38 | 109.87 | 123.68 |
| 14 | A | 1139 | CLA | C4A-NA-C1A | 5.38 | 109.13 | 106.71 |
| 14 | f | 1228 | CLA | CMB-C2B-C1B | -5.38 | 120.19 | 128.46 |
| 14 | e | 1139 | CLA | C4A-NA-C1A | 5.38 | 109.12 | 106.71 |
| 15 | B | 2002 | PQN | C14-C13-C12 | -5.37 | 109.89 | 123.68 |
| 14 | H | 1234 | CLA | CMB-C2B-C3B | 5.37 | 134.73 | 124.68 |
| 14 | f | 1012 | CLA | CMB-C2B-C1B | -5.37 | 120.21 | 128.46 |
| 14 | H | 1226 | CLA | C2D-C1D-ND | -5.37 | 106.15 | 110.10 |
| 14 | B | 1234 | CLA | CMB-C2B-C3B | 5.37 | 134.72 | 124.68 |
| 14 | H | 1012 | CLA | CMB-C2B-C1B | -5.37 | 120.22 | 128.46 |
| 21 | H | 1852 | SQD | O5-C5-C4 | 5.37 | 119.44 | 109.69 |
| 15 | f | 2002 | PQN | C14-C13-C12 | -5.36 | 109.92 | 123.68 |
| 14 | f | 1229 | CLA | CMB-C2B-C1B | -5.36 | 120.22 | 128.46 |
| 14 | f | 1234 | CLA | CMB-C2B-C3B | 5.36 | 134.70 | 124.68 |
| 14 | f | 1226 | CLA | C2D-C1D-ND | -5.36 | 106.16 | 110.10 |
| 14 | A | 1117 | CLA | CMB-C2B-C1B | -5.36 | 120.23 | 128.46 |
| 14 | H | 1229 | CLA | CMB-C2B-C1B | -5.35 | 120.24 | 128.46 |
| 14 | B | 1229 | CLA | CMB-C2B-C1B | -5.35 | 120.25 | 128.46 |
| 14 | G | 1117 | CLA | CMB-C2B-C1B | -5.35 | 120.25 | 128.46 |
| 14 | B | 1226 | CLA | C2D-C1D-ND | -5.35 | 106.17 | 110.10 |
| 14 | G | 1139 | CLA | C4A-NA-C1A | 5.34 | 109.11 | 106.71 |
| 14 | H | 1215 | CLA | CMB-C2B-C1B | -5.33 | 120.28 | 128.46 |
| 14 | H | 1223 | CLA | CMB-C2B-C1B | -5.33 | 120.28 | 128.46 |
| 14 | f | 1215 | CLA | CMB-C2B-C1B | -5.33 | 120.28 | 128.46 |
| 14 | f | 1223 | CLA | CMB-C2B-C1B | -5.32 | 120.29 | 128.46 |
| 14 | B | 1215 | CLA | CMB-C2B-C1B | -5.31 | 120.31 | 128.46 |
| 14 | B | 1223 | CLA | CMB-C2B-C1B | -5.31 | 120.31 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1113 | CLA | CMB-C2B-C1B | -5.31 | 120.31 | 128.46 |
| 14 | e | 1113 | CLA | CMB-C2B-C1B | -5.30 | 120.32 | 128.46 |
| 14 | G | 1105 | CLA | CMB-C2B-C1B | -5.29 | 120.33 | 128.46 |
| 14 | A | 1113 | CLA | CMB-C2B-C1B | -5.29 | 120.33 | 128.46 |
| 14 | A | 1105 | CLA | CMB-C2B-C1B | -5.29 | 120.33 | 128.46 |
| 15 | G | 2001 | PQN | C14-C13-C12 | -5.28 | 110.12 | 123.68 |
| 17 | e | 4011 | BCR | C20-C21-C22 | -5.28 | 119.77 | 127.31 |
| 14 | e | 1119 | CLA | CMB-C2B-C1B | -5.28 | 120.35 | 128.46 |
| 15 | A | 2001 | PQN | C14-C13-C12 | -5.28 | 110.14 | 123.68 |
| 17 | A | 4011 | BCR | C20-C21-C22 | -5.27 | 119.78 | 127.31 |
| 14 | e | 1105 | CLA | CMB-C2B-C1B | -5.27 | 120.36 | 128.46 |
| 15 | e | 2001 | PQN | C14-C13-C12 | -5.27 | 110.15 | 123.68 |
| 14 | A | 1119 | CLA | CMB-C2B-C1B | -5.27 | 120.36 | 128.46 |
| 17 | G | 4011 | BCR | C20-C21-C22 | -5.27 | 119.79 | 127.31 |
| 14 | G | 1119 | CLA | CMB-C2B-C1B | -5.25 | 120.39 | 128.46 |
| 14 | e | 1127 | CLA | CMB-C2B-C1B | -5.24 | 120.41 | 128.46 |
| 14 | G | 1127 | CLA | CMB-C2B-C1B | -5.24 | 120.41 | 128.46 |
| 17 | s | 522 | BCR | C11-C10-C9 | -5.23 | 119.85 | 127.31 |
| 14 | A | 1127 | CLA | CMB-C2B-C1B | -5.23 | 120.43 | 128.46 |
| 14 | A | 1022 | CLA | CMB-C2B-C1B | -5.22 | 120.44 | 128.46 |
| 17 | 3 | 522 | BCR | C11-C10-C9 | -5.21 | 119.88 | 127.31 |
| 14 | e | 1022 | CLA | CMB-C2B-C1B | -5.19 | 120.48 | 128.46 |
| 14 | G | 1022 | CLA | CMB-C2B-C1B | -5.19 | 120.49 | 128.46 |
| 17 | a | 522 | BCR | C11-C10-C9 | -5.19 | 119.91 | 127.31 |
| 14 | f | 1232 | CLA | CMB-C2B-C3B | 5.18 | 134.38 | 124.68 |
| 14 | B | 1232 | CLA | CMB-C2B-C3B | 5.17 | 134.35 | 124.68 |
| 14 | H | 1232 | CLA | CMB-C2B-C3B | 5.17 | 134.35 | 124.68 |
| 14 | e | 1123 | CLA | CMB-C2B-C1B | -5.16 | 120.53 | 128.46 |
| 14 | A | 1123 | CLA | CMB-C2B-C1B | -5.15 | 120.56 | 128.46 |
| 14 | G | 1123 | CLA | CMB-C2B-C1B | -5.14 | 120.56 | 128.46 |
| 14 | G | 1801 | CLA | CMB-C2B-C1B | -5.13 | 120.58 | 128.46 |
| 17 | J | 4012 | BCR | C20-C21-C22 | -5.13 | 119.99 | 127.31 |
| 17 | T | 4012 | BCR | C20-C21-C22 | -5.12 | 120.00 | 127.31 |
| 14 | A | 1801 | CLA | CMB-C2B-C1B | -5.12 | 120.60 | 128.46 |
| 17 | l | 4012 | BCR | C20-C21-C22 | -5.11 | 120.01 | 127.31 |
| 14 | e | 1801 | CLA | CMB-C2B-C1B | -5.09 | 120.64 | 128.46 |
| 14 | H | 1201 | CLA | CMB-C2B-C1B | -5.08 | 120.65 | 128.46 |
| 17 | A | 4007 | BCR | C28-C27-C26 | -5.08 | 105.01 | 114.08 |
| 17 | G | 4007 | BCR | C28-C27-C26 | -5.07 | 105.02 | 114.08 |
| 17 | e | 4007 | BCR | C28-C27-C26 | -5.07 | 105.03 | 114.08 |
| 14 | f | 1012 | CLA | C4A-NA-C1A | 5.05 | 108.98 | 106.71 |
| 14 | B | 1201 | CLA | CMB-C2B-C1B | -5.05 | 120.70 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1135 | CLA | CMB-C2B-C3B | 5.05 | 134.12 | 124.68 |
| 14 | B | 1012 | CLA | C4A-NA-C1A | 5.05 | 108.97 | 106.71 |
| 14 | H | 1202 | CLA | CMB-C2B-C1B | -5.05 | 120.71 | 128.46 |
| 14 | e | 1022 | CLA | C4A-NA-C1A | 5.04 | 108.97 | 106.71 |
| 14 | G | 1124 | CLA | CMB-C2B-C1B | -5.04 | 120.72 | 128.46 |
| 14 | B | 1202 | CLA | CMB-C2B-C1B | -5.03 | 120.73 | 128.46 |
| 14 | A | 1135 | CLA | CMB-C2B-C3B | 5.03 | 134.08 | 124.68 |
| 14 | e | 1124 | CLA | CMB-C2B-C1B | -5.03 | 120.74 | 128.46 |
| 14 | f | 1201 | CLA | CMB-C2B-C1B | -5.03 | 120.74 | 128.46 |
| 14 | 3 | 516 | CLA | CAC-C3C-C4C | 5.03 | 131.33 | 124.81 |
| 14 | s | 516 | CLA | CAC-C3C-C4C | 5.02 | 131.33 | 124.81 |
| 14 | A | 1124 | CLA | CMB-C2B-C1B | -5.02 | 120.75 | 128.46 |
| 14 | e | 1107 | CLA | CMB-C2B-C1B | -5.02 | 120.75 | 128.46 |
| 14 | G | 1135 | CLA | CMB-C2B-C3B | 5.02 | 134.06 | 124.68 |
| 14 | G | 1107 | CLA | CMB-C2B-C1B | -5.01 | 120.76 | 128.46 |
| 14 | a | 516 | CLA | CAC-C3C-C4C | 5.01 | 131.31 | 124.81 |
| 14 | B | 1231 | CLA | CMB-C2B-C1B | -5.00 | 120.77 | 128.46 |
| 14 | t | 508 | CLA | CMB-C2B-C1B | -5.00 | 120.77 | 128.46 |
| 14 | Z | 508 | CLA | CMB-C2B-C1B | -5.00 | 120.79 | 128.46 |
| 14 | e | 1103 | CLA | CMB-C2B-C1B | -5.00 | 120.79 | 128.46 |
| 14 | A | 1103 | CLA | CMB-C2B-C1B | -4.99 | 120.79 | 128.46 |
| 14 | f | 1231 | CLA | CMB-C2B-C1B | -4.99 | 120.79 | 128.46 |
| 14 | A | 1022 | CLA | C4A-NA-C1A | 4.99 | 108.95 | 106.71 |
| 17 | 3 | 521 | BCR | C20-C21-C22 | -4.99 | 120.19 | 127.31 |
| 14 | f | 1202 | CLA | CMB-C2B-C1B | -4.99 | 120.79 | 128.46 |
| 14 | G | 1103 | CLA | CMB-C2B-C1B | -4.99 | 120.80 | 128.46 |
| 14 | A | 1107 | CLA | CMB-C2B-C1B | -4.99 | 120.80 | 128.46 |
| 17 | a | 521 | BCR | C20-C21-C22 | -4.98 | 120.20 | 127.31 |
| 14 | 4 | 508 | CLA | CMB-C2B-C1B | -4.98 | 120.81 | 128.46 |
| 14 | H | 1231 | CLA | CMB-C2B-C1B | -4.97 | 120.82 | 128.46 |
| 17 | j | 4016 | BCR | C11-C10-C9 | -4.97 | 120.22 | 127.31 |
| 14 | G | 1022 | CLA | C4A-NA-C1A | 4.97 | 108.94 | 106.71 |
| 14 | b | 508 | CLA | CMB-C2B-C1B | -4.97 | 120.83 | 128.46 |
| 14 | 3 | 508 | CLA | CMB-C2B-C1B | -4.97 | 120.83 | 128.46 |
| 14 | s | 508 | CLA | CMB-C2B-C1B | -4.97 | 120.83 | 128.46 |
| 17 | G | 4008 | BCR | C20-C21-C22 | -4.96 | 120.23 | 127.31 |
| 17 | e | 4008 | BCR | C20-C21-C22 | -4.96 | 120.23 | 127.31 |
| 17 | s | 521 | BCR | C20-C21-C22 | -4.96 | 120.23 | 127.31 |
| 17 | R | 4016 | BCR | C11-C10-C9 | -4.96 | 120.23 | 127.31 |
| 17 | F | 4016 | BCR | C11-C10-C9 | -4.96 | 120.24 | 127.31 |
| 17 | T | 4015 | BCR | C7-C8-C9 | -4.95 | 118.75 | 126.23 |
| 14 | u | 509 | CLA | CMB-C2B-C1B | -4.95 | 120.85 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | c | 509 | CLA | CMB-C2B-C1B | -4.95 | 120.85 | 128.46 |
| 17 | B | 4006 | BCR | C24-C23-C22 | -4.95 | 118.75 | 126.23 |
| 14 | r | 508 | CLA | CMB-C2B-C1B | -4.95 | 120.86 | 128.46 |
| 14 | 2 | 508 | CLA | CMB-C2B-C1B | -4.95 | 120.86 | 128.46 |
| 17 | A | 4008 | BCR | C20-C21-C22 | -4.95 | 120.25 | 127.31 |
| 17 | J | 4013 | BCR | C24-C23-C22 | -4.94 | 118.76 | 126.23 |
| 17 | l | 4013 | BCR | C24-C23-C22 | -4.94 | 118.76 | 126.23 |
| 17 | l | 4015 | BCR | C7-C8-C9 | -4.94 | 118.77 | 126.23 |
| 14 | a | 509 | CLA | CMB-C2B-C1B | -4.94 | 120.88 | 128.46 |
| 14 | 5 | 509 | CLA | CMB-C2B-C1B | -4.94 | 120.88 | 128.46 |
| 14 | H | 1012 | CLA | C4A-NA-C1A | 4.93 | 108.92 | 106.71 |
| 14 | H | 1211 | CLA | CMB-C2B-C1B | -4.93 | 120.88 | 128.46 |
| 14 | H | 1225 | CLA | CMB-C2B-C1B | -4.93 | 120.88 | 128.46 |
| 14 | a | 508 | CLA | CMB-C2B-C1B | -4.93 | 120.89 | 128.46 |
| 14 | G | 1130 | CLA | C4A-NA-C1A | 4.93 | 108.92 | 106.71 |
| 17 | H | 4006 | BCR | C24-C23-C22 | -4.93 | 118.79 | 126.23 |
| 17 | J | 4015 | BCR | C7-C8-C9 | -4.93 | 118.79 | 126.23 |
| 14 | H | 1222 | CLA | CMB-C2B-C1B | -4.92 | 120.89 | 128.46 |
| 17 | e | 4001 | BCR | C16-C17-C18 | -4.92 | 120.28 | 127.31 |
| 17 | T | 4013 | BCR | C24-C23-C22 | -4.92 | 118.79 | 126.23 |
| 17 | A | 4001 | BCR | C16-C17-C18 | -4.92 | 120.29 | 127.31 |
| 17 | f | 4006 | BCR | C24-C23-C22 | -4.92 | 118.81 | 126.23 |
| 14 | f | 1222 | CLA | CMB-C2B-C1B | -4.92 | 120.91 | 128.46 |
| 14 | B | 1225 | CLA | CMB-C2B-C1B | -4.91 | 120.91 | 128.46 |
| 14 | B | 1222 | CLA | CMB-C2B-C1B | -4.91 | 120.91 | 128.46 |
| 14 | s | 509 | CLA | CMB-C2B-C1B | -4.91 | 120.92 | 128.46 |
| 14 | 3 | 509 | CLA | CMB-C2B-C1B | -4.91 | 120.92 | 128.46 |
| 14 | f | 1226 | CLA | CMB-C2B-C3B | 4.91 | 133.86 | 124.68 |
| 14 | f | 1225 | CLA | CMB-C2B-C1B | -4.91 | 120.92 | 128.46 |
| 17 | G | 4001 | BCR | C16-C17-C18 | -4.90 | 120.31 | 127.31 |
| 14 | B | 1211 | CLA | CMB-C2B-C1B | -4.90 | 120.93 | 128.46 |
| 17 | n | 4219 | BCR | C1-C6-C5 | -4.90 | 115.72 | 122.61 |
| 14 | f | 1211 | CLA | CMB-C2B-C1B | -4.89 | 120.94 | 128.46 |
| 14 | B | 1226 | CLA | CMB-C2B-C3B | 4.89 | 133.83 | 124.68 |
| 17 | L | 4219 | BCR | C1-C6-C5 | -4.89 | 115.73 | 122.61 |
| 14 | H | 1226 | CLA | CMB-C2B-C3B | 4.89 | 133.82 | 124.68 |
| 14 | B | 1012 | CLA | CMB-C2B-C3B | 4.88 | 133.81 | 124.68 |
| 17 | e | 4002 | BCR | C16-C17-C18 | -4.88 | 120.34 | 127.31 |
| 17 | A | 4002 | BCR | C16-C17-C18 | -4.88 | 120.34 | 127.31 |
| 17 | V | 4219 | BCR | C1-C6-C5 | -4.88 | 115.74 | 122.61 |
| 17 | G | 4002 | BCR | C16-C17-C18 | -4.88 | 120.35 | 127.31 |
| 17 | e | 4002 | BCR | C7-C8-C9 | -4.87 | 118.87 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | c | 508 | CLA | CMB-C2B-C1B | -4.87 | 120.98 | 128.46 |
| 14 | f | 1012 | CLA | CMB-C2B-C3B | 4.87 | 133.79 | 124.68 |
| 14 | A | 1130 | CLA | C4A-NA-C1A | 4.87 | 108.89 | 106.71 |
| 14 | H | 1012 | CLA | CMB-C2B-C3B | 4.86 | 133.77 | 124.68 |
| 17 | A | 4002 | BCR | C7-C8-C9 | -4.85 | 118.91 | 126.23 |
| 14 | 5 | 508 | CLA | CMB-C2B-C1B | -4.85 | 121.02 | 128.46 |
| 17 | G | 4002 | BCR | C7-C8-C9 | -4.83 | 118.94 | 126.23 |
| 14 | u | 508 | CLA | CMB-C2B-C1B | -4.83 | 121.04 | 128.46 |
| 14 | f | 1221 | CLA | CMB-C2B-C3B | 4.82 | 133.70 | 124.68 |
| 14 | H | 1221 | CLA | CMB-C2B-C3B | 4.82 | 133.70 | 124.68 |
| 14 | B | 1221 | CLA | CMB-C2B-C3B | 4.82 | 133.69 | 124.68 |
| 17 | e | 4008 | BCR | C15-C14-C13 | -4.81 | 120.44 | 127.31 |
| 17 | A | 4008 | BCR | C15-C14-C13 | -4.81 | 120.44 | 127.31 |
| 14 | B | 1224 | CLA | CMB-C2B-C1B | -4.81 | 121.07 | 128.46 |
| 17 | s | 523 | BCR | C15-C14-C13 | -4.81 | 120.45 | 127.31 |
| 14 | H | 1224 | CLA | CMB-C2B-C1B | -4.80 | 121.08 | 128.46 |
| 17 | a | 523 | BCR | C15-C14-C13 | -4.80 | 120.45 | 127.31 |
| 17 | 3 | 523 | BCR | C15-C14-C13 | -4.80 | 120.46 | 127.31 |
| 17 | H | 4004 | BCR | C20-C21-C22 | -4.80 | 120.46 | 127.31 |
| 14 | f | 1224 | CLA | CMB-C2B-C1B | -4.79 | 121.10 | 128.46 |
| 17 | B | 4004 | BCR | C20-C21-C22 | -4.79 | 120.47 | 127.31 |
| 14 | 2 | 509 | CLA | CMB-C2B-C1B | -4.78 | 121.11 | 128.46 |
| 14 | B | 1229 | CLA | CMB-C2B-C3B | 4.78 | 133.63 | 124.68 |
| 17 | G | 4008 | BCR | C15-C14-C13 | -4.78 | 120.49 | 127.31 |
| 14 | H | 1229 | CLA | CMB-C2B-C3B | 4.78 | 133.62 | 124.68 |
| 14 | r | 509 | CLA | CMB-C2B-C1B | -4.78 | 121.12 | 128.46 |
| 17 | f | 4004 | BCR | C20-C21-C22 | -4.77 | 120.50 | 127.31 |
| 21 | f | 1852 | SQD | O7-S-C6 | 4.77 | 112.61 | 106.94 |
| 21 | B | 1852 | SQD | O7-S-C6 | 4.77 | 112.61 | 106.94 |
| 14 | f | 1229 | CLA | CMB-C2B-C3B | 4.77 | 133.59 | 124.68 |
| 14 | Z | 509 | CLA | CMB-C2B-C1B | -4.76 | 121.15 | 128.46 |
| 14 | e | 1130 | CLA | C4A-NA-C1A | 4.75 | 108.84 | 106.71 |
| 14 | G | 1126 | CLA | CMB-C2B-C3B | 4.75 | 133.57 | 124.68 |
| 21 | H | 1852 | SQD | O7-S-C6 | 4.74 | 112.57 | 106.94 |
| 14 | e | 1126 | CLA | CMB-C2B-C3B | 4.73 | 133.53 | 124.68 |
| 14 | A | 1126 | CLA | CMB-C2B-C3B | 4.73 | 133.52 | 124.68 |
| 17 | B | 4017 | BCR | C15-C14-C13 | -4.73 | 120.56 | 127.31 |
| 17 | H | 4017 | BCR | C15-C14-C13 | -4.72 | 120.58 | 127.31 |
| 14 | H | 1228 | CLA | CMB-C2B-C3B | 4.72 | 133.50 | 124.68 |
| 21 | Y | 822 | SQD | O5-C5-C4 | 4.71 | 118.25 | 109.69 |
| 14 | d | 508 | CLA | CMB-C2B-C1B | -4.71 | 121.22 | 128.46 |
| 17 | b | 522 | BCR | C15-C16-C17 | -4.71 | 113.82 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1228 | CLA | CMB-C2B-C3B | 4.71 | 133.49 | 124.68 |
| 21 | 1 | 822 | SQD | O5-C5-C4 | 4.71 | 118.24 | 109.69 |
| 17 | l | 4013 | BCR | C16-C17-C18 | -4.71 | 120.59 | 127.31 |
| 14 | f | 1228 | CLA | CMB-C2B-C3B | 4.70 | 133.48 | 124.68 |
| 17 | f | 4017 | BCR | C15-C14-C13 | -4.70 | 120.60 | 127.31 |
| 17 | t | 522 | BCR | C15-C16-C17 | -4.70 | 113.84 | 123.47 |
| 17 | 4 | 522 | BCR | C15-C16-C17 | -4.70 | 113.85 | 123.47 |
| 21 | q | 822 | SQD | O5-C5-C4 | 4.70 | 118.23 | 109.69 |
| 14 | 6 | 508 | CLA | CMB-C2B-C1B | -4.70 | 121.25 | 128.46 |
| 14 | v | 508 | CLA | CMB-C2B-C1B | -4.69 | 121.26 | 128.46 |
| 14 | f | 1023 | CLA | CMB-C2B-C1B | -4.69 | 121.26 | 128.46 |
| 14 | B | 1023 | CLA | CMB-C2B-C1B | -4.68 | 121.27 | 128.46 |
| 17 | J | 4013 | BCR | C16-C17-C18 | -4.67 | 120.64 | 127.31 |
| 17 | s | 522 | BCR | C3-C4-C5 | -4.67 | 105.74 | 114.08 |
| 14 | H | 1023 | CLA | CMB-C2B-C1B | -4.67 | 121.29 | 128.46 |
| 14 | G | 1116 | CLA | CMB-C2B-C3B | 4.66 | 133.41 | 124.68 |
| 17 | 3 | 522 | BCR | C3-C4-C5 | -4.66 | 105.75 | 114.08 |
| 14 | K | 1401 | CLA | CAA-C2A-C3A | -4.66 | 100.02 | 112.78 |
| 17 | a | 522 | BCR | C3-C4-C5 | -4.66 | 105.76 | 114.08 |
| 14 | U | 1401 | CLA | CAA-C2A-C3A | -4.66 | 100.02 | 112.78 |
| 17 | T | 4013 | BCR | C16-C17-C18 | -4.66 | 120.66 | 127.31 |
| 14 | m | 1401 | CLA | CAA-C2A-C3A | -4.66 | 100.03 | 112.78 |
| 14 | e | 1102 | CLA | CMB-C2B-C3B | 4.65 | 133.38 | 124.68 |
| 14 | e | 1116 | CLA | CMB-C2B-C3B | 4.65 | 133.38 | 124.68 |
| 14 | A | 1102 | CLA | CMB-C2B-C3B | 4.64 | 133.36 | 124.68 |
| 14 | A | 1116 | CLA | CMB-C2B-C3B | 4.64 | 133.36 | 124.68 |
| 17 | V | 4219 | BCR | C16-C17-C18 | -4.64 | 120.69 | 127.31 |
| 17 | t | 523 | BCR | C15-C14-C13 | -4.63 | 120.70 | 127.31 |
| 17 | b | 523 | BCR | C15-C14-C13 | -4.63 | 120.70 | 127.31 |
| 17 | d | 522 | BCR | C15-C14-C13 | -4.63 | 120.70 | 127.31 |
| 17 | L | 4219 | BCR | C16-C17-C18 | -4.63 | 120.71 | 127.31 |
| 14 | G | 1102 | CLA | CMB-C2B-C3B | 4.63 | 133.33 | 124.68 |
| 17 | 5 | 522 | BCR | C15-C14-C13 | -4.62 | 120.71 | 127.31 |
| 17 | 3 | 524 | BCR | C15-C14-C13 | -4.62 | 120.72 | 127.31 |
| 17 | e | 4008 | BCR | C16-C17-C18 | -4.62 | 120.72 | 127.31 |
| 14 | e | 1104 | CLA | CMB-C2B-C1B | -4.62 | 121.37 | 128.46 |
| 17 | n | 4219 | BCR | C16-C17-C18 | -4.62 | 120.72 | 127.31 |
| 17 | B | 4010 | BCR | C15-C16-C17 | -4.61 | 114.02 | 123.47 |
| 17 | a | 524 | BCR | C15-C14-C13 | -4.61 | 120.73 | 127.31 |
| 17 | f | 4010 | BCR | C15-C16-C17 | -4.61 | 114.03 | 123.47 |
| 17 | H | 4010 | BCR | C15-C16-C17 | -4.61 | 114.03 | 123.47 |
| 17 | 4 | 523 | BCR | C15-C14-C13 | -4.61 | 120.73 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | H | 4004 | BCR | C16-C17-C18 | -4.61 | 120.74 | 127.31 |
| 17 | s | 524 | BCR | C15-C14-C13 | -4.61 | 120.74 | 127.31 |
| 14 | A | 1104 | CLA | CMB-C2B-C1B | -4.61 | 121.39 | 128.46 |
| 17 | u | 522 | BCR | C15-C14-C13 | -4.60 | 120.74 | 127.31 |
| 17 | c | 522 | BCR | C15-C14-C13 | -4.60 | 120.75 | 127.31 |
| 17 | f | 4004 | BCR | C16-C17-C18 | -4.60 | 120.75 | 127.31 |
| 17 | G | 4008 | BCR | C16-C17-C18 | -4.59 | 120.76 | 127.31 |
| 14 | G | 1113 | CLA | CMB-C2B-C3B | 4.59 | 133.27 | 124.68 |
| 17 | B | 4004 | BCR | C16-C17-C18 | -4.59 | 120.76 | 127.31 |
| 17 | L | 4219 | BCR | C15-C16-C17 | -4.59 | 114.07 | 123.47 |
| 14 | e | 1113 | CLA | CMB-C2B-C3B | 4.59 | 133.26 | 124.68 |
| 17 | V | 4219 | BCR | C15-C16-C17 | -4.59 | 114.08 | 123.47 |
| 14 | A | 1113 | CLA | CMB-C2B-C3B | 4.59 | 133.26 | 124.68 |
| 17 | 6 | 522 | BCR | C15-C14-C13 | -4.59 | 120.77 | 127.31 |
| 17 | A | 4008 | BCR | C16-C17-C18 | -4.59 | 120.77 | 127.31 |
| 14 | G | 1104 | CLA | CMB-C2B-C1B | -4.58 | 121.42 | 128.46 |
| 17 | v | 522 | BCR | C15-C14-C13 | -4.58 | 120.77 | 127.31 |
| 17 | 5 | 522 | BCR | C11-C10-C9 | -4.58 | 120.77 | 127.31 |
| 14 | A | 1105 | CLA | CMB-C2B-C3B | 4.58 | 133.25 | 124.68 |
| 17 | n | 4219 | BCR | C15-C16-C17 | -4.58 | 114.09 | 123.47 |
| 14 | G | 1105 | CLA | CMB-C2B-C3B | 4.58 | 133.24 | 124.68 |
| 14 | e | 1105 | CLA | CMB-C2B-C3B | 4.58 | 133.24 | 124.68 |
| 17 | u | 522 | BCR | C11-C10-C9 | -4.58 | 120.78 | 127.31 |
| 17 | Z | 522 | BCR | C15-C14-C13 | -4.57 | 120.78 | 127.31 |
| 17 | c | 522 | BCR | C11-C10-C9 | -4.57 | 120.79 | 127.31 |
| 14 | f | 1223 | CLA | CMB-C2B-C3B | 4.57 | 133.22 | 124.68 |
| 14 | B | 1223 | CLA | CMB-C2B-C3B | 4.57 | 133.22 | 124.68 |
| 14 | H | 1223 | CLA | CMB-C2B-C3B | 4.56 | 133.22 | 124.68 |
| 17 | B | 4010 | BCR | C3-C4-C5 | -4.56 | 105.94 | 114.08 |
| 17 | f | 4010 | BCR | C3-C4-C5 | -4.55 | 105.96 | 114.08 |
| 14 | e | 1127 | CLA | CMB-C2B-C3B | 4.54 | 133.17 | 124.68 |
| 14 | A | 1127 | CLA | CMB-C2B-C3B | 4.54 | 133.17 | 124.68 |
| 14 | G | 1127 | CLA | CMB-C2B-C3B | 4.54 | 133.17 | 124.68 |
| 14 | G | 1801 | CLA | CMB-C2B-C3B | 4.54 | 133.17 | 124.68 |
| 17 | H | 4010 | BCR | C3-C4-C5 | -4.54 | 105.98 | 114.08 |
| 17 | 2 | 522 | BCR | C15-C14-C13 | -4.53 | 120.84 | 127.31 |
| 14 | 5 | 511 | CLA | CMB-C2B-C1B | -4.53 | 121.50 | 128.46 |
| 14 | A | 1801 | CLA | CMB-C2B-C3B | 4.53 | 133.15 | 124.68 |
| 17 | 5 | 521 | BCR | C15-C14-C13 | -4.52 | 120.85 | 127.31 |
| 14 | u | 511 | CLA | CMB-C2B-C1B | -4.52 | 121.52 | 128.46 |
| 14 | d | 509 | CLA | CMB-C2B-C1B | -4.52 | 121.52 | 128.46 |
| 17 | f | 4017 | BCR | C16-C17-C18 | -4.51 | 120.87 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | q | 522 | BCR | C11-C10-C9 | -4.51 | 120.87 | 127.31 |
| 17 | c | 521 | BCR | C15-C14-C13 | -4.51 | 120.87 | 127.31 |
| 14 | c | 511 | CLA | CMB-C2B-C1B | -4.51 | 121.53 | 128.46 |
| 17 | Y | 522 | BCR | C11-C10-C9 | -4.51 | 120.88 | 127.31 |
| 17 | u | 521 | BCR | C15-C14-C13 | -4.51 | 120.88 | 127.31 |
| 14 | A | 1022 | CLA | CMB-C2B-C3B | 4.51 | 133.11 | 124.68 |
| 14 | v | 509 | CLA | CMB-C2B-C1B | -4.50 | 121.54 | 128.46 |
| 14 | e | 1801 | CLA | CMB-C2B-C3B | 4.50 | 133.10 | 124.68 |
| 14 | 6 | 509 | CLA | CMB-C2B-C1B | -4.50 | 121.54 | 128.46 |
| 17 | Y | 524 | BCR | C16-C17-C18 | -4.50 | 120.89 | 127.31 |
| 17 | q | 524 | BCR | C16-C17-C18 | -4.50 | 120.89 | 127.31 |
| 17 | r | 522 | BCR | C15-C14-C13 | -4.50 | 120.89 | 127.31 |
| 17 | l | 524 | BCR | C16-C17-C18 | -4.50 | 120.89 | 127.31 |
| 17 | H | 4017 | BCR | C16-C17-C18 | -4.50 | 120.89 | 127.31 |
| 17 | a | 522 | BCR | C15-C14-C13 | -4.50 | 120.89 | 127.31 |
| 14 | f | 1238 | CLA | CMB-C2B-C3B | 4.49 | 133.09 | 124.68 |
| 17 | l | 522 | BCR | C11-C10-C9 | -4.49 | 120.90 | 127.31 |
| 17 | v | 524 | BCR | C15-C14-C13 | -4.49 | 120.90 | 127.31 |
| 17 | B | 4017 | BCR | C16-C17-C18 | -4.49 | 120.90 | 127.31 |
| 14 | H | 1238 | CLA | CMB-C2B-C3B | 4.49 | 133.08 | 124.68 |
| 14 | e | 1022 | CLA | CMB-C2B-C3B | 4.48 | 133.07 | 124.68 |
| 14 | B | 1023 | CLA | CAC-C3C-C4C | 4.48 | 130.63 | 124.81 |
| 14 | G | 1022 | CLA | CMB-C2B-C3B | 4.48 | 133.06 | 124.68 |
| 17 | d | 524 | BCR | C15-C14-C13 | -4.48 | 120.92 | 127.31 |
| 14 | B | 1238 | CLA | CMB-C2B-C3B | 4.48 | 133.05 | 124.68 |
| 17 | 3 | 522 | BCR | C15-C14-C13 | -4.47 | 120.93 | 127.31 |
| 17 | s | 522 | BCR | C15-C14-C13 | -4.47 | 120.93 | 127.31 |
| 14 | H | 1023 | CLA | CAC-C3C-C4C | 4.47 | 130.60 | 124.81 |
| 14 | 3 | 506 | CLA | CMB-C2B-C1B | -4.46 | 121.61 | 128.46 |
| 17 | 6 | 524 | BCR | C15-C14-C13 | -4.46 | 120.94 | 127.31 |
| 14 | f | 1023 | CLA | CAC-C3C-C4C | 4.46 | 130.59 | 124.81 |
| 14 | B | 1213 | CLA | CMB-C2B-C1B | -4.46 | 121.62 | 128.46 |
| 14 | H | 1213 | CLA | CMB-C2B-C1B | -4.45 | 121.62 | 128.46 |
| 14 | t | 511 | CLA | CMB-C2B-C1B | -4.45 | 121.62 | 128.46 |
| 14 | e | 1129 | CLA | CMB-C2B-C1B | -4.45 | 121.63 | 128.46 |
| 14 | a | 506 | CLA | CMB-C2B-C1B | -4.45 | 121.63 | 128.46 |
| 17 | 3 | 521 | BCR | C15-C14-C13 | -4.45 | 120.97 | 127.31 |
| 17 | a | 521 | BCR | C15-C14-C13 | -4.44 | 120.97 | 127.31 |
| 14 | 4 | 511 | CLA | CMB-C2B-C1B | -4.44 | 121.63 | 128.46 |
| 14 | s | 506 | CLA | CMB-C2B-C1B | -4.44 | 121.64 | 128.46 |
| 17 | r | 521 | BCR | C28-C27-C26 | -4.44 | 106.15 | 114.08 |
| 17 | R | 4016 | BCR | C7-C8-C9 | -4.44 | 119.53 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | b | 511 | CLA | CMB-C2B-C1B | -4.44 | 121.65 | 128.46 |
| 17 | s | 521 | BCR | C15-C14-C13 | -4.43 | 120.99 | 127.31 |
| 21 | c | 822 | SQD | O7-S-C6 | 4.43 | 112.20 | 106.94 |
| 14 | f | 1213 | CLA | CMB-C2B-C1B | -4.43 | 121.66 | 128.46 |
| 14 | A | 1129 | CLA | CMB-C2B-C1B | -4.43 | 121.66 | 128.46 |
| 17 | 2 | 521 | BCR | C28-C27-C26 | -4.42 | 106.18 | 114.08 |
| 21 | 5 | 822 | SQD | O7-S-C6 | 4.42 | 112.19 | 106.94 |
| 14 | G | 1129 | CLA | CMB-C2B-C1B | -4.42 | 121.67 | 128.46 |
| 17 | Z | 521 | BCR | C28-C27-C26 | -4.42 | 106.19 | 114.08 |
| 14 | A | 1106 | CLA | CMB-C2B-C1B | -4.41 | 121.68 | 128.46 |
| 17 | j | 4016 | BCR | C7-C8-C9 | -4.41 | 119.56 | 126.23 |
| 17 | F | 4016 | BCR | C7-C8-C9 | -4.41 | 119.57 | 126.23 |
| 21 | u | 822 | SQD | O7-S-C6 | 4.41 | 112.18 | 106.94 |
| 21 | b | 822 | SQD | O47-C7-C8 | 4.41 | 119.20 | 111.09 |
| 14 | e | 1106 | CLA | CMB-C2B-C1B | -4.41 | 121.69 | 128.46 |
| 21 | 4 | 822 | SQD | O47-C7-C8 | 4.41 | 119.20 | 111.09 |
| 21 | t | 822 | SQD | O47-C7-C8 | 4.41 | 119.20 | 111.09 |
| 14 | G | 1106 | CLA | CMB-C2B-C1B | -4.41 | 121.69 | 128.46 |
| 14 | H | 1202 | CLA | CMB-C2B-C3B | 4.41 | 132.92 | 124.68 |
| 14 | H | 1222 | CLA | CMB-C2B-C3B | 4.40 | 132.91 | 124.68 |
| 18 | B | 1842 | LHG | O4-P-O5 | 4.40 | 134.00 | 112.24 |
| 18 | H | 1842 | LHG | O4-P-O5 | 4.40 | 134.00 | 112.24 |
| 14 | B | 1202 | CLA | CMB-C2B-C3B | 4.40 | 132.91 | 124.68 |
| 14 | f | 1222 | CLA | CMB-C2B-C3B | 4.40 | 132.91 | 124.68 |
| 18 | f | 1842 | LHG | O4-P-O5 | 4.40 | 133.99 | 112.24 |
| 14 | B | 1222 | CLA | CMB-C2B-C3B | 4.40 | 132.91 | 124.68 |
| 14 | A | 1120 | CLA | CMB-C2B-C1B | -4.39 | 121.71 | 128.46 |
| 14 | r | 511 | CLA | CMB-C2B-C1B | -4.39 | 121.71 | 128.46 |
| 14 | 2 | 511 | CLA | CMB-C2B-C1B | -4.38 | 121.73 | 128.46 |
| 14 | H | 1210 | CLA | CMB-C2B-C1B | -4.38 | 121.73 | 128.46 |
| 14 | Z | 511 | CLA | CMB-C2B-C1B | -4.38 | 121.73 | 128.46 |
| 14 | 3 | 511 | CLA | CMB-C2B-C1B | -4.38 | 121.73 | 128.46 |
| 14 | e | 1120 | CLA | CMB-C2B-C1B | -4.38 | 121.73 | 128.46 |
| 17 | r | 524 | BCR | C15-C14-C13 | -4.38 | 121.06 | 127.31 |
| 14 | f | 1202 | CLA | CMB-C2B-C3B | 4.37 | 132.86 | 124.68 |
| 17 | 5 | 524 | BCR | C15-C14-C13 | -4.37 | 121.07 | 127.31 |
| 14 | a | 511 | CLA | CMB-C2B-C1B | -4.37 | 121.74 | 128.46 |
| 14 | s | 511 | CLA | CMB-C2B-C1B | -4.37 | 121.74 | 128.46 |
| 14 | G | 1120 | CLA | CMB-C2B-C1B | -4.37 | 121.75 | 128.46 |
| 14 | f | 1210 | CLA | CMB-C2B-C1B | -4.36 | 121.76 | 128.46 |
| 14 | H | 1201 | CLA | CMB-C2B-C3B | 4.36 | 132.84 | 124.68 |
| 17 | 2 | 524 | BCR | C15-C14-C13 | -4.36 | 121.09 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | u | 524 | BCR | C15-C14-C13 | -4.35 | 121.10 | 127.31 |
| 14 | n | 1501 | CLA | CMB-C2B-C1B | -4.35 | 121.78 | 128.46 |
| 14 | B | 1210 | CLA | CMB-C2B-C1B | -4.35 | 121.78 | 128.46 |
| 17 | t | 524 | BCR | C16-C17-C18 | -4.35 | 121.11 | 127.31 |
| 14 | B | 1201 | CLA | CMB-C2B-C3B | 4.35 | 132.81 | 124.68 |
| 14 | V | 1501 | CLA | CMB-C2B-C1B | -4.34 | 121.79 | 128.46 |
| 14 | L | 1501 | CLA | CMB-C2B-C1B | -4.34 | 121.79 | 128.46 |
| 17 | c | 524 | BCR | C15-C14-C13 | -4.34 | 121.11 | 127.31 |
| 14 | f | 1201 | CLA | CMB-C2B-C3B | 4.34 | 132.79 | 124.68 |
| 17 | 4 | 524 | BCR | C16-C17-C18 | -4.34 | 121.12 | 127.31 |
| 17 | b | 524 | BCR | C16-C17-C18 | -4.33 | 121.13 | 127.31 |
| 14 | f | 1203 | CLA | CMB-C2B-C1B | -4.33 | 121.81 | 128.46 |
| 17 | Z | 524 | BCR | C15-C14-C13 | -4.33 | 121.13 | 127.31 |
| 17 | 2 | 521 | BCR | C24-C23-C22 | -4.33 | 119.69 | 126.23 |
| 17 | t | 521 | BCR | C7-C8-C9 | -4.33 | 119.69 | 126.23 |
| 14 | B | 1203 | CLA | CMB-C2B-C1B | -4.33 | 121.81 | 128.46 |
| 14 | H | 1203 | CLA | CMB-C2B-C1B | -4.33 | 121.81 | 128.46 |
| 14 | 3 | 504 | CLA | CMB-C2B-C1B | -4.33 | 121.81 | 128.46 |
| 17 | r | 521 | BCR | C24-C23-C22 | -4.33 | 119.70 | 126.23 |
| 17 | Z | 521 | BCR | C24-C23-C22 | -4.33 | 119.70 | 126.23 |
| 14 | H | 1212 | CLA | CMB-C2B-C1B | -4.32 | 121.82 | 128.46 |
| 14 | s | 504 | CLA | CMB-C2B-C1B | -4.32 | 121.82 | 128.46 |
| 17 | f | 4004 | BCR | C24-C23-C22 | -4.32 | 119.71 | 126.23 |
| 14 | G | 1111 | CLA | CMB-C2B-C1B | -4.32 | 121.83 | 128.46 |
| 17 | Y | 524 | BCR | C15-C14-C13 | -4.32 | 121.15 | 127.31 |
| 17 | 4 | 521 | BCR | C7-C8-C9 | -4.32 | 119.71 | 126.23 |
| 17 | s | 522 | BCR | C7-C8-C9 | -4.32 | 119.71 | 126.23 |
| 17 | K | 4104 | BCR | C7-C8-C9 | -4.31 | 119.72 | 126.23 |
| 17 | n | 4022 | BCR | C11-C10-C9 | -4.31 | 121.16 | 127.31 |
| 14 | Y | 506 | CLA | CMB-C2B-C1B | -4.31 | 121.84 | 128.46 |
| 14 | q | 506 | CLA | CMB-C2B-C1B | -4.31 | 121.84 | 128.46 |
| 14 | f | 1212 | CLA | CMB-C2B-C1B | -4.31 | 121.84 | 128.46 |
| 14 | e | 1111 | CLA | CMB-C2B-C1B | -4.31 | 121.84 | 128.46 |
| 17 | r | 521 | BCR | C20-C21-C22 | -4.31 | 121.16 | 127.31 |
| 14 | a | 504 | CLA | CMB-C2B-C1B | -4.31 | 121.85 | 128.46 |
| 17 | 1 | 524 | BCR | C15-C14-C13 | -4.30 | 121.17 | 127.31 |
| 14 | B | 1212 | CLA | CMB-C2B-C1B | -4.30 | 121.85 | 128.46 |
| 14 | A | 1111 | CLA | CMB-C2B-C1B | -4.30 | 121.85 | 128.46 |
| 14 | 1 | 506 | CLA | CMB-C2B-C1B | -4.30 | 121.86 | 128.46 |
| 17 | 3 | 522 | BCR | C7-C8-C9 | -4.30 | 119.74 | 126.23 |
| 14 | n | 1502 | CLA | CMB-C2B-C1B | -4.30 | 121.86 | 128.46 |
| 17 | U | 4104 | BCR | C7-C8-C9 | -4.30 | 119.74 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 2 | 521 | BCR | C20-C21-C22 | -4.30 | 121.18 | 127.31 |
| 17 | t | 524 | BCR | C11-C10-C9 | -4.29 | 121.18 | 127.31 |
| 17 | B | 4004 | BCR | C24-C23-C22 | -4.29 | 119.75 | 126.23 |
| 17 | H | 4004 | BCR | C24-C23-C22 | -4.29 | 119.75 | 126.23 |
| 14 | A | 1128 | CLA | CMB-C2B-C3B | 4.29 | 132.71 | 124.68 |
| 14 | B | 1231 | CLA | CMB-C2B-C3B | 4.29 | 132.71 | 124.68 |
| 14 | H | 1225 | CLA | CMB-C2B-C3B | 4.29 | 132.71 | 124.68 |
| 14 | L | 1502 | CLA | CMB-C2B-C1B | -4.29 | 121.87 | 128.46 |
| 17 | b | 524 | BCR | C11-C10-C9 | -4.29 | 121.18 | 127.31 |
| 14 | H | 1231 | CLA | CMB-C2B-C3B | 4.29 | 132.71 | 124.68 |
| 14 | f | 1231 | CLA | CMB-C2B-C3B | 4.29 | 132.71 | 124.68 |
| 14 | e | 1128 | CLA | CMB-C2B-C3B | 4.29 | 132.70 | 124.68 |
| 17 | m | 4104 | BCR | C7-C8-C9 | -4.29 | 119.76 | 126.23 |
| 17 | Z | 523 | BCR | C15-C14-C13 | -4.29 | 121.19 | 127.31 |
| 17 | q | 524 | BCR | C15-C14-C13 | -4.29 | 121.19 | 127.31 |
| 17 | 4 | 524 | BCR | C11-C10-C9 | -4.29 | 121.19 | 127.31 |
| 14 | G | 1114 | CLA | CMB-C2B-C1B | -4.28 | 121.88 | 128.46 |
| 21 | Y | 822 | SQD | O7-S-C6 | 4.28 | 112.03 | 106.94 |
| 14 | H | 1211 | CLA | CMB-C2B-C3B | 4.28 | 132.69 | 124.68 |
| 17 | r | 523 | BCR | C15-C14-C13 | -4.27 | 121.21 | 127.31 |
| 14 | A | 1114 | CLA | CMB-C2B-C1B | -4.27 | 121.90 | 128.46 |
| 17 | Z | 521 | BCR | C20-C21-C22 | -4.27 | 121.21 | 127.31 |
| 14 | A | 1109 | CLA | CMB-C2B-C1B | -4.27 | 121.90 | 128.46 |
| 14 | e | 1114 | CLA | CMB-C2B-C1B | -4.27 | 121.90 | 128.46 |
| 14 | B | 1211 | CLA | CMB-C2B-C3B | 4.27 | 132.67 | 124.68 |
| 14 | f | 1211 | CLA | CMB-C2B-C3B | 4.27 | 132.66 | 124.68 |
| 17 | b | 521 | BCR | C7-C8-C9 | -4.27 | 119.79 | 126.23 |
| 17 | a | 522 | BCR | C7-C8-C9 | -4.27 | 119.79 | 126.23 |
| 21 | v | 822 | SQD | O47-C7-C8 | 4.27 | 118.94 | 111.09 |
| 14 | 4 | 509 | CLA | CMB-C2B-C1B | -4.27 | 121.91 | 128.46 |
| 17 | L | 4022 | BCR | C11-C10-C9 | -4.27 | 121.22 | 127.31 |
| 14 | G | 1128 | CLA | CMB-C2B-C3B | 4.27 | 132.66 | 124.68 |
| 17 | 2 | 523 | BCR | C15-C14-C13 | -4.27 | 121.22 | 127.31 |
| 14 | e | 1125 | CLA | CMB-C2B-C1B | -4.26 | 121.91 | 128.46 |
| 14 | B | 1225 | CLA | CMB-C2B-C3B | 4.26 | 132.66 | 124.68 |
| 14 | V | 1502 | CLA | CMB-C2B-C1B | -4.26 | 121.91 | 128.46 |
| 14 | f | 1215 | CLA | CMB-C2B-C3B | 4.26 | 132.65 | 124.68 |
| 18 | e | 5008 | LHG | O4-P-O5 | 4.26 | 133.31 | 112.24 |
| 14 | Y | 504 | CLA | O2D-CGD-O1D | -4.26 | 115.50 | 123.84 |
| 17 | V | 4022 | BCR | C11-C10-C9 | -4.26 | 121.23 | 127.31 |
| 14 | f | 1225 | CLA | CMB-C2B-C3B | 4.26 | 132.65 | 124.68 |
| 21 | 1 | 822 | SQD | O7-S-C6 | 4.26 | 112.00 | 106.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | A | 5008 | LHG | O4-P-O5 | 4.26 | 133.29 | 112.24 |
| 14 | G | 1109 | CLA | CMB-C2B-C1B | -4.26 | 121.92 | 128.46 |
| 14 | H | 1215 | CLA | CMB-C2B-C3B | 4.26 | 132.64 | 124.68 |
| 18 | e | 5002 | LHG | O4-P-O5 | 4.26 | 133.28 | 112.24 |
| 17 | u | 523 | BCR | C15-C14-C13 | -4.26 | 121.24 | 127.31 |
| 14 | A | 1123 | CLA | CMB-C2B-C3B | 4.25 | 132.64 | 124.68 |
| 17 | S | 4018 | BCR | C16-C17-C18 | -4.25 | 121.24 | 127.31 |
| 21 | 6 | 822 | SQD | O47-C7-C8 | 4.25 | 118.91 | 111.09 |
| 14 | e | 1123 | CLA | CMB-C2B-C3B | 4.25 | 132.63 | 124.68 |
| 14 | e | 1133 | CLA | CMB-C2B-C1B | -4.25 | 121.93 | 128.46 |
| 18 | A | 5004 | LHG | O4-P-O5 | 4.25 | 133.25 | 112.24 |
| 18 | G | 5002 | LHG | O4-P-O5 | 4.25 | 133.25 | 112.24 |
| 18 | A | 5002 | LHG | O4-P-O5 | 4.25 | 133.25 | 112.24 |
| 18 | G | 5008 | LHG | O4-P-O5 | 4.25 | 133.25 | 112.24 |
| 14 | b | 509 | CLA | CMB-C2B-C1B | -4.25 | 121.93 | 128.46 |
| 18 | G | 5004 | LHG | O4-P-O5 | 4.25 | 133.24 | 112.24 |
| 21 | q | 822 | SQD | O7-S-C6 | 4.25 | 111.99 | 106.94 |
| 17 | k | 4018 | BCR | C16-C17-C18 | -4.25 | 121.25 | 127.31 |
| 14 | G | 1123 | CLA | CMB-C2B-C3B | 4.25 | 132.62 | 124.68 |
| 14 | q | 504 | CLA | O2D-CGD-O1D | -4.25 | 115.54 | 123.84 |
| 14 | e | 1109 | CLA | CMB-C2B-C1B | -4.24 | 121.94 | 128.46 |
| 14 | A | 1125 | CLA | CMB-C2B-C1B | -4.24 | 121.94 | 128.46 |
| 17 | W | 4021 | BCR | C24-C23-C22 | -4.24 | 119.82 | 126.23 |
| 14 | A | 1115 | CLA | CMB-C2B-C1B | -4.24 | 121.94 | 128.46 |
| 14 | l | 504 | CLA | O2D-CGD-O1D | -4.24 | 115.54 | 123.84 |
| 14 | G | 1115 | CLA | CMB-C2B-C1B | -4.24 | 121.94 | 128.46 |
| 21 | d | 822 | SQD | O47-C7-C8 | 4.24 | 118.89 | 111.09 |
| 14 | B | 1215 | CLA | CMB-C2B-C3B | 4.24 | 132.61 | 124.68 |
| 18 | e | 5004 | LHG | O4-P-O5 | 4.24 | 133.20 | 112.24 |
| 14 | t | 509 | CLA | CMB-C2B-C1B | -4.24 | 121.95 | 128.46 |
| 17 | M | 4021 | BCR | C24-C23-C22 | -4.23 | 119.84 | 126.23 |
| 17 | l | 521 | BCR | C24-C23-C22 | -4.23 | 119.84 | 126.23 |
| 14 | G | 1125 | CLA | CMB-C2B-C1B | -4.23 | 121.97 | 128.46 |
| 17 | q | 521 | BCR | C24-C23-C22 | -4.22 | 119.85 | 126.23 |
| 18 | k | 5001 | LHG | O4-P-O5 | 4.22 | 133.11 | 112.24 |
| 17 | I | 4018 | BCR | C16-C17-C18 | -4.22 | 121.29 | 127.31 |
| 14 | e | 1115 | CLA | CMB-C2B-C1B | -4.22 | 121.98 | 128.46 |
| 14 | A | 1133 | CLA | CMB-C2B-C1B | -4.22 | 121.98 | 128.46 |
| 17 | o | 4021 | BCR | C24-C23-C22 | -4.22 | 119.86 | 126.23 |
| 18 | S | 5001 | LHG | O4-P-O5 | 4.22 | 133.10 | 112.24 |
| 17 | l | 522 | BCR | C15-C14-C13 | -4.22 | 121.29 | 127.31 |
| 18 | I | 5001 | LHG | O4-P-O5 | 4.22 | 133.09 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1133 | CLA | CMB-C2B-C1B | -4.22 | 121.98 | 128.46 |
| 17 | q | 522 | BCR | C15-C14-C13 | -4.22 | 121.29 | 127.31 |
| 14 | d | 504 | CLA | CMB-C2B-C1B | -4.21 | 121.99 | 128.46 |
| 17 | s | 521 | BCR | C16-C17-C18 | -4.21 | 121.30 | 127.31 |
| 17 | Y | 521 | BCR | C24-C23-C22 | -4.21 | 119.87 | 126.23 |
| 18 | G | 5003 | LHG | O4-P-O5 | 4.21 | 133.06 | 112.24 |
| 18 | A | 5003 | LHG | O4-P-O5 | 4.21 | 133.03 | 112.24 |
| 17 | 3 | 521 | BCR | C16-C17-C18 | -4.20 | 121.31 | 127.31 |
| 17 | Y | 522 | BCR | C15-C14-C13 | -4.20 | 121.31 | 127.31 |
| 17 | 5 | 523 | BCR | C15-C14-C13 | -4.20 | 121.31 | 127.31 |
| 18 | e | 5003 | LHG | O4-P-O5 | 4.20 | 133.02 | 112.24 |
| 17 | S | 4018 | BCR | C15-C16-C17 | -4.20 | 114.87 | 123.47 |
| 17 | a | 521 | BCR | C16-C17-C18 | -4.20 | 121.32 | 127.31 |
| 17 | c | 523 | BCR | C15-C14-C13 | -4.20 | 121.32 | 127.31 |
| 18 | e | 5006 | LHG | O4-P-O5 | 4.19 | 132.97 | 112.24 |
| 17 | S | 4018 | BCR | C24-C23-C22 | -4.19 | 119.90 | 126.23 |
| 14 | v | 504 | CLA | CMB-C2B-C1B | -4.19 | 122.02 | 128.46 |
| 17 | k | 4018 | BCR | C15-C16-C17 | -4.19 | 114.89 | 123.47 |
| 14 | 6 | 504 | CLA | CMB-C2B-C1B | -4.19 | 122.02 | 128.46 |
| 18 | G | 5006 | LHG | O4-P-O5 | 4.19 | 132.96 | 112.24 |
| 18 | A | 5006 | LHG | O4-P-O5 | 4.19 | 132.95 | 112.24 |
| 17 | k | 4018 | BCR | C24-C23-C22 | -4.19 | 119.91 | 126.23 |
| 17 | I | 4018 | BCR | C15-C16-C17 | -4.19 | 114.90 | 123.47 |
| 14 | G | 1139 | CLA | CMB-C2B-C1B | -4.18 | 122.04 | 128.46 |
| 14 | G | 1011 | CLA | C1D-ND-C4D | -4.18 | 103.37 | 106.33 |
| 17 | I | 4018 | BCR | C24-C23-C22 | -4.18 | 119.92 | 126.23 |
| 14 | A | 1139 | CLA | CMB-C2B-C1B | -4.18 | 122.05 | 128.46 |
| 14 | e | 1139 | CLA | CMB-C2B-C1B | -4.17 | 122.05 | 128.46 |
| 18 | G | 5007 | LHG | O4-P-O5 | 4.17 | 132.86 | 112.24 |
| 18 | n | 5221 | LHG | O4-P-O5 | 4.17 | 132.86 | 112.24 |
| 18 | L | 5221 | LHG | O4-P-O5 | 4.17 | 132.84 | 112.24 |
| 18 | A | 5007 | LHG | O4-P-O5 | 4.17 | 132.84 | 112.24 |
| 18 | V | 5221 | LHG | O4-P-O5 | 4.17 | 132.83 | 112.24 |
| 14 | A | 1134 | CLA | CAA-C2A-C3A | -4.17 | 101.37 | 112.78 |
| 14 | e | 1134 | CLA | CAA-C2A-C3A | -4.16 | 101.38 | 112.78 |
| 17 | H | 4010 | BCR | C11-C10-C9 | -4.16 | 121.37 | 127.31 |
| 18 | n | 5220 | LHG | O4-P-O5 | 4.16 | 132.82 | 112.24 |
| 18 | e | 5007 | LHG | O4-P-O5 | 4.16 | 132.81 | 112.24 |
| 18 | V | 5220 | LHG | O4-P-O5 | 4.16 | 132.80 | 112.24 |
| 18 | L | 5220 | LHG | O4-P-O5 | 4.16 | 132.79 | 112.24 |
| 14 | r | 510 | CLA | CMB-C2B-C1B | -4.16 | 122.08 | 128.46 |
| 14 | 2 | 510 | CLA | CMB-C2B-C1B | -4.15 | 122.08 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1023 | CLA | CMB-C2B-C3B | 4.15 | 132.44 | 124.68 |
| 17 | e | 4001 | BCR | C3-C4-C5 | -4.15 | 106.67 | 114.08 |
| 17 | n | 4019 | BCR | C7-C8-C9 | -4.15 | 119.96 | 126.23 |
| 18 | G | 5001 | LHG | O4-P-O5 | 4.15 | 132.75 | 112.24 |
| 18 | e | 5001 | LHG | O4-P-O5 | 4.15 | 132.75 | 112.24 |
| 18 | G | 5009 | LHG | O4-P-O5 | 4.15 | 132.75 | 112.24 |
| 14 | G | 1134 | CLA | CAA-C2A-C3A | -4.15 | 101.42 | 112.78 |
| 14 | H | 1208 | CLA | CMB-C2B-C1B | -4.15 | 122.09 | 128.46 |
| 18 | A | 5001 | LHG | O4-P-O5 | 4.15 | 132.74 | 112.24 |
| 14 | e | 1011 | CLA | C1D-ND-C4D | -4.15 | 103.39 | 106.33 |
| 14 | f | 1208 | CLA | CMB-C2B-C1B | -4.14 | 122.09 | 128.46 |
| 18 | e | 5009 | LHG | O4-P-O5 | 4.14 | 132.73 | 112.24 |
| 14 | A | 1011 | CLA | CGD-CBD-CAD | 4.14 | 124.16 | 110.73 |
| 18 | A | 5009 | LHG | O4-P-O5 | 4.14 | 132.72 | 112.24 |
| 14 | B | 1023 | CLA | CMB-C2B-C3B | 4.14 | 132.43 | 124.68 |
| 17 | A | 4001 | BCR | C3-C4-C5 | -4.14 | 106.68 | 114.08 |
| 14 | Z | 510 | CLA | CMB-C2B-C1B | -4.14 | 122.10 | 128.46 |
| 17 | B | 4010 | BCR | C11-C10-C9 | -4.14 | 121.40 | 127.31 |
| 17 | L | 4019 | BCR | C7-C8-C9 | -4.14 | 119.98 | 126.23 |
| 14 | H | 1023 | CLA | CMB-C2B-C3B | 4.14 | 132.43 | 124.68 |
| 18 | n | 5218 | LHG | O4-P-O5 | 4.14 | 132.71 | 112.24 |
| 14 | e | 1011 | CLA | CGD-CBD-CAD | 4.14 | 124.14 | 110.73 |
| 18 | V | 5218 | LHG | O4-P-O5 | 4.14 | 132.70 | 112.24 |
| 17 | Z | 521 | BCR | C16-C17-C18 | -4.14 | 121.41 | 127.31 |
| 18 | L | 5218 | LHG | O4-P-O5 | 4.14 | 132.69 | 112.24 |
| 17 | V | 4019 | BCR | C7-C8-C9 | -4.14 | 119.99 | 126.23 |
| 14 | B | 1208 | CLA | CMB-C2B-C1B | -4.13 | 122.11 | 128.46 |
| 17 | G | 4001 | BCR | C3-C4-C5 | -4.13 | 106.70 | 114.08 |
| 14 | G | 1011 | CLA | CGD-CBD-CAD | 4.13 | 124.11 | 110.73 |
| 14 | m | 1401 | CLA | CMB-C2B-C1B | -4.12 | 122.13 | 128.46 |
| 17 | f | 4010 | BCR | C11-C10-C9 | -4.12 | 121.43 | 127.31 |
| 17 | e | 4003 | BCR | C3-C4-C5 | -4.12 | 106.72 | 114.08 |
| 17 | 2 | 521 | BCR | C16-C17-C18 | -4.12 | 121.44 | 127.31 |
| 14 | K | 1401 | CLA | CMB-C2B-C1B | -4.11 | 122.14 | 128.46 |
| 18 | e | 5005 | LHG | O4-P-O5 | 4.11 | 132.57 | 112.24 |
| 14 | A | 1011 | CLA | C1D-ND-C4D | -4.11 | 103.42 | 106.33 |
| 17 | s | 523 | BCR | C11-C10-C9 | -4.11 | 121.45 | 127.31 |
| 18 | A | 5005 | LHG | O4-P-O5 | 4.11 | 132.54 | 112.24 |
| 17 | A | 4003 | BCR | C3-C4-C5 | -4.10 | 106.75 | 114.08 |
| 14 | c | 509 | CLA | CMB-C2B-C3B | 4.10 | 132.36 | 124.68 |
| 18 | G | 5005 | LHG | O4-P-O5 | 4.10 | 132.53 | 112.24 |
| 14 | G | 1103 | CLA | CMB-C2B-C3B | 4.10 | 132.35 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1224 | CLA | CMB-C2B-C3B | 4.10 | 132.35 | 124.68 |
| 14 | A | 1103 | CLA | CMB-C2B-C3B | 4.10 | 132.35 | 124.68 |
| 14 | e | 1103 | CLA | CMB-C2B-C3B | 4.10 | 132.34 | 124.68 |
| 14 | H | 1209 | CLA | CMB-C2B-C1B | -4.09 | 122.17 | 128.46 |
| 14 | A | 1117 | CLA | CMB-C2B-C3B | 4.09 | 132.33 | 124.68 |
| 14 | B | 1224 | CLA | CMB-C2B-C3B | 4.09 | 132.33 | 124.68 |
| 14 | 5 | 509 | CLA | CMB-C2B-C3B | 4.09 | 132.33 | 124.68 |
| 17 | r | 521 | BCR | C16-C17-C18 | -4.09 | 121.47 | 127.31 |
| 14 | u | 509 | CLA | CMB-C2B-C3B | 4.09 | 132.33 | 124.68 |
| 14 | U | 1401 | CLA | CMB-C2B-C1B | -4.09 | 122.18 | 128.46 |
| 14 | e | 1117 | CLA | CMB-C2B-C3B | 4.09 | 132.32 | 124.68 |
| 17 | a | 523 | BCR | C11-C10-C9 | -4.09 | 121.48 | 127.31 |
| 14 | A | 1108 | CLA | CMB-C2B-C1B | -4.08 | 122.19 | 128.46 |
| 21 | c | 822 | SQD | O47-C7-C8 | 4.08 | 118.60 | 111.09 |
| 14 | G | 1117 | CLA | CMB-C2B-C3B | 4.08 | 132.32 | 124.68 |
| 17 | G | 4003 | BCR | C3-C4-C5 | -4.08 | 106.79 | 114.08 |
| 14 | e | 1108 | CLA | CMB-C2B-C1B | -4.08 | 122.19 | 128.46 |
| 14 | G | 1108 | CLA | CMB-C2B-C1B | -4.08 | 122.20 | 128.46 |
| 17 | 3 | 523 | BCR | C11-C10-C9 | -4.07 | 121.50 | 127.31 |
| 21 | u | 822 | SQD | O47-C7-C8 | 4.07 | 118.58 | 111.09 |
| 14 | f | 1224 | CLA | CMB-C2B-C3B | 4.07 | 132.29 | 124.68 |
| 14 | f | 1209 | CLA | O2D-CGD-CBD | 4.07 | 118.50 | 111.27 |
| 21 | 5 | 822 | SQD | O47-C7-C8 | 4.07 | 118.57 | 111.09 |
| 17 | j | 4016 | BCR | C24-C23-C22 | -4.07 | 120.09 | 126.23 |
| 17 | q | 522 | BCR | C7-C8-C9 | -4.06 | 120.10 | 126.23 |
| 21 | n | 5216 | SQD | O7-S-C6 | 4.06 | 111.77 | 106.94 |
| 21 | L | 5216 | SQD | O7-S-C6 | 4.06 | 111.77 | 106.94 |
| 14 | f | 1209 | CLA | CMB-C2B-C1B | -4.06 | 122.22 | 128.46 |
| 14 | B | 1209 | CLA | CMB-C2B-C1B | -4.06 | 122.23 | 128.46 |
| 14 | 2 | 505 | CLA | CMB-C2B-C1B | -4.06 | 122.23 | 128.46 |
| 17 | L | 4022 | BCR | C20-C21-C22 | -4.06 | 121.52 | 127.31 |
| 14 | Z | 505 | CLA | CMB-C2B-C1B | -4.06 | 122.23 | 128.46 |
| 17 | W | 4021 | BCR | C15-C14-C13 | -4.06 | 121.52 | 127.31 |
| 14 | Y | 511 | CLA | CMB-C2B-C1B | -4.06 | 122.23 | 128.46 |
| 14 | a | 509 | CLA | CMB-C2B-C3B | 4.05 | 132.26 | 124.68 |
| 14 | B | 1209 | CLA | O2D-CGD-CBD | 4.05 | 118.47 | 111.27 |
| 14 | r | 505 | CLA | CMB-C2B-C1B | -4.05 | 122.24 | 128.46 |
| 17 | 1 | 522 | BCR | C7-C8-C9 | -4.04 | 120.12 | 126.23 |
| 21 | V | 5216 | SQD | O7-S-C6 | 4.04 | 111.75 | 106.94 |
| 18 | f | 1855 | LHG | O4-P-O5 | 4.04 | 132.23 | 112.24 |
| 14 | s | 509 | CLA | CMB-C2B-C3B | 4.04 | 132.24 | 124.68 |
| 14 | H | 1209 | CLA | O2D-CGD-CBD | 4.04 | 118.45 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | B | 1855 | LHG | O4-P-O5 | 4.04 | 132.22 | 112.24 |
| 17 | Y | 522 | BCR | C7-C8-C9 | -4.04 | 120.13 | 126.23 |
| 17 | V | 4022 | BCR | C20-C21-C22 | -4.04 | 121.55 | 127.31 |
| 17 | F | 4016 | BCR | C24-C23-C22 | -4.04 | 120.13 | 126.23 |
| 14 | l | 511 | CLA | CMB-C2B-C1B | -4.04 | 122.26 | 128.46 |
| 17 | n | 4022 | BCR | C20-C21-C22 | -4.03 | 121.55 | 127.31 |
| 18 | H | 1855 | LHG | O4-P-O5 | 4.03 | 132.18 | 112.24 |
| 17 | t | 521 | BCR | C20-C21-C22 | -4.03 | 121.55 | 127.31 |
| 14 | L | 1503 | CLA | CMB-C2B-C1B | -4.03 | 122.26 | 128.46 |
| 14 | 3 | 509 | CLA | CMB-C2B-C3B | 4.03 | 132.22 | 124.68 |
| 17 | Z | 522 | BCR | C11-C10-C9 | -4.03 | 121.56 | 127.31 |
| 17 | 6 | 523 | BCR | C15-C14-C13 | -4.03 | 121.56 | 127.31 |
| 17 | v | 523 | BCR | C15-C14-C13 | -4.03 | 121.56 | 127.31 |
| 14 | V | 1503 | CLA | CMB-C2B-C1B | -4.03 | 122.27 | 128.46 |
| 14 | n | 1503 | CLA | CMB-C2B-C1B | -4.03 | 122.27 | 128.46 |
| 17 | R | 4016 | BCR | C24-C23-C22 | -4.03 | 120.15 | 126.23 |
| 17 | 4 | 521 | BCR | C20-C21-C22 | -4.03 | 121.56 | 127.31 |
| 17 | e | 4003 | BCR | C20-C21-C22 | -4.03 | 121.56 | 127.31 |
| 14 | d | 506 | CLA | CMB-C2B-C1B | -4.03 | 122.27 | 128.46 |
| 17 | o | 4021 | BCR | C15-C14-C13 | -4.03 | 121.56 | 127.31 |
| 14 | q | 511 | CLA | CMB-C2B-C1B | -4.03 | 122.28 | 128.46 |
| 14 | v | 506 | CLA | CMB-C2B-C1B | -4.03 | 122.28 | 128.46 |
| 17 | b | 521 | BCR | C20-C21-C22 | -4.03 | 121.56 | 127.31 |
| 17 | M | 4021 | BCR | C15-C14-C13 | -4.02 | 121.57 | 127.31 |
| 14 | 6 | 506 | CLA | CMB-C2B-C1B | -4.02 | 122.28 | 128.46 |
| 21 | q | 822 | SQD | C1-O5-C5 | 4.02 | 121.58 | 113.69 |
| 17 | b | 524 | BCR | C15-C14-C13 | -4.02 | 121.58 | 127.31 |
| 17 | m | 4104 | BCR | C20-C21-C22 | -4.02 | 121.58 | 127.31 |
| 14 | H | 1240 | CLA | CMB-C2B-C1B | -4.02 | 122.29 | 128.46 |
| 21 | Y | 822 | SQD | C1-O5-C5 | 4.02 | 121.57 | 113.69 |
| 17 | 2 | 522 | BCR | C11-C10-C9 | -4.01 | 121.58 | 127.31 |
| 17 | d | 523 | BCR | C15-C14-C13 | -4.01 | 121.58 | 127.31 |
| 21 | l | 822 | SQD | C1-O5-C5 | 4.01 | 121.56 | 113.69 |
| 17 | e | 4003 | BCR | C16-C17-C18 | -4.01 | 121.59 | 127.31 |
| 17 | t | 524 | BCR | C15-C14-C13 | -4.01 | 121.59 | 127.31 |
| 17 | 4 | 524 | BCR | C15-C14-C13 | -4.01 | 121.59 | 127.31 |
| 17 | 6 | 524 | BCR | C16-C17-C18 | -4.01 | 121.59 | 127.31 |
| 14 | r | 503 | CLA | CMB-C2B-C1B | -4.01 | 122.30 | 128.46 |
| 17 | A | 4003 | BCR | C20-C21-C22 | -4.01 | 121.59 | 127.31 |
| 14 | f | 1240 | CLA | CMB-C2B-C1B | -4.00 | 122.31 | 128.46 |
| 17 | G | 4003 | BCR | C16-C17-C18 | -4.00 | 121.60 | 127.31 |
| 14 | B | 1240 | CLA | CMB-C2B-C1B | -4.00 | 122.32 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | U | 4104 | BCR | C20-C21-C22 | -4.00 | 121.60 | 127.31 |
| 17 | b | 522 | BCR | C15-C14-C13 | -4.00 | 121.61 | 127.31 |
| 17 | M | 4021 | BCR | C20-C21-C22 | -4.00 | 121.61 | 127.31 |
| 17 | 4 | 522 | BCR | C15-C14-C13 | -4.00 | 121.61 | 127.31 |
| 17 | K | 4104 | BCR | C20-C21-C22 | -3.99 | 121.62 | 127.31 |
| 17 | H | 4005 | BCR | C7-C8-C9 | -3.99 | 120.21 | 126.23 |
| 14 | Z | 503 | CLA | CMB-C2B-C1B | -3.99 | 122.34 | 128.46 |
| 14 | s | 501 | CLA | CMB-C2B-C1B | -3.99 | 122.34 | 128.46 |
| 17 | d | 524 | BCR | C16-C17-C18 | -3.99 | 121.62 | 127.31 |
| 17 | o | 4021 | BCR | C20-C21-C22 | -3.99 | 121.62 | 127.31 |
| 14 | a | 501 | CLA | CMB-C2B-C1B | -3.99 | 122.34 | 128.46 |
| 14 | d | 505 | CLA | CMB-C2B-C1B | -3.99 | 122.34 | 128.46 |
| 14 | 2 | 503 | CLA | CMB-C2B-C1B | -3.99 | 122.34 | 128.46 |
| 17 | A | 4003 | BCR | C16-C17-C18 | -3.98 | 121.63 | 127.31 |
| 17 | 5 | 521 | BCR | C20-C21-C22 | -3.98 | 121.63 | 127.31 |
| 17 | c | 521 | BCR | C20-C21-C22 | -3.98 | 121.63 | 127.31 |
| 17 | t | 522 | BCR | C15-C14-C13 | -3.98 | 121.63 | 127.31 |
| 14 | B | 1204 | CLA | CMB-C2B-C1B | -3.98 | 122.35 | 128.46 |
| 14 | f | 1204 | CLA | CMB-C2B-C1B | -3.98 | 122.35 | 128.46 |
| 17 | v | 524 | BCR | C16-C17-C18 | -3.98 | 121.64 | 127.31 |
| 14 | 3 | 501 | CLA | CMB-C2B-C1B | -3.97 | 122.36 | 128.46 |
| 17 | r | 522 | BCR | C11-C10-C9 | -3.97 | 121.64 | 127.31 |
| 17 | u | 521 | BCR | C20-C21-C22 | -3.97 | 121.64 | 127.31 |
| 14 | 6 | 505 | CLA | CMB-C2B-C1B | -3.97 | 122.36 | 128.46 |
| 17 | V | 4019 | BCR | C11-C10-C9 | -3.97 | 121.65 | 127.31 |
| 17 | f | 4014 | BCR | C16-C17-C18 | -3.97 | 121.65 | 127.31 |
| 14 | v | 505 | CLA | CMB-C2B-C1B | -3.97 | 122.36 | 128.46 |
| 17 | G | 4003 | BCR | C20-C21-C22 | -3.97 | 121.65 | 127.31 |
| 17 | W | 4021 | BCR | C20-C21-C22 | -3.97 | 121.65 | 127.31 |
| 17 | B | 4005 | BCR | C7-C8-C9 | -3.97 | 120.24 | 126.23 |
| 17 | r | 521 | BCR | C15-C14-C13 | -3.97 | 121.65 | 127.31 |
| 17 | B | 4009 | BCR | C11-C10-C9 | -3.96 | 121.65 | 127.31 |
| 14 | H | 1204 | CLA | CMB-C2B-C1B | -3.96 | 122.37 | 128.46 |
| 17 | L | 4019 | BCR | C11-C10-C9 | -3.96 | 121.65 | 127.31 |
| 17 | 1 | 523 | BCR | C15-C14-C13 | -3.96 | 121.66 | 127.31 |
| 17 | U | 4104 | BCR | C16-C17-C18 | -3.96 | 121.66 | 127.31 |
| 17 | B | 4014 | BCR | C16-C17-C18 | -3.96 | 121.66 | 127.31 |
| 17 | B | 4017 | BCR | C24-C23-C22 | -3.96 | 120.26 | 126.23 |
| 17 | 1 | 521 | BCR | C20-C21-C22 | -3.96 | 121.66 | 127.31 |
| 17 | H | 4017 | BCR | C24-C23-C22 | -3.95 | 120.26 | 126.23 |
| 17 | q | 523 | BCR | C15-C14-C13 | -3.95 | 121.67 | 127.31 |
| 17 | Y | 521 | BCR | C3-C4-C5 | -3.95 | 107.02 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | f | 4005 | BCR | C7-C8-C9 | -3.95 | 120.26 | 126.23 |
| 17 | 2 | 521 | BCR | C15-C14-C13 | -3.95 | 121.67 | 127.31 |
| 17 | H | 4014 | BCR | C16-C17-C18 | -3.95 | 121.67 | 127.31 |
| 14 | G | 1138 | CLA | CMB-C2B-C1B | -3.95 | 122.39 | 128.46 |
| 14 | G | 1136 | CLA | CMB-C2B-C1B | -3.95 | 122.40 | 128.46 |
| 17 | m | 4104 | BCR | C16-C17-C18 | -3.95 | 121.68 | 127.31 |
| 17 | K | 4104 | BCR | C16-C17-C18 | -3.95 | 121.68 | 127.31 |
| 14 | A | 1138 | CLA | CMB-C2B-C1B | -3.95 | 122.40 | 128.46 |
| 17 | l | 521 | BCR | C3-C4-C5 | -3.95 | 107.03 | 114.08 |
| 17 | q | 521 | BCR | C3-C4-C5 | -3.94 | 107.03 | 114.08 |
| 17 | Y | 521 | BCR | C20-C21-C22 | -3.94 | 121.68 | 127.31 |
| 17 | f | 4006 | BCR | C15-C14-C13 | -3.94 | 121.68 | 127.31 |
| 17 | n | 4019 | BCR | C11-C10-C9 | -3.94 | 121.68 | 127.31 |
| 17 | f | 4017 | BCR | C24-C23-C22 | -3.94 | 120.28 | 126.23 |
| 17 | H | 4006 | BCR | C15-C14-C13 | -3.94 | 121.69 | 127.31 |
| 17 | H | 4009 | BCR | C11-C10-C9 | -3.94 | 121.69 | 127.31 |
| 17 | q | 521 | BCR | C20-C21-C22 | -3.94 | 121.69 | 127.31 |
| 14 | G | 1140 | CLA | CMB-C2B-C1B | -3.94 | 122.41 | 128.46 |
| 17 | v | 522 | BCR | C11-C10-C9 | -3.94 | 121.69 | 127.31 |
| 14 | q | 508 | CLA | CMB-C2B-C3B | 3.94 | 132.04 | 124.68 |
| 17 | M | 4021 | BCR | C15-C16-C17 | -3.94 | 115.41 | 123.47 |
| 17 | Y | 523 | BCR | C15-C14-C13 | -3.94 | 121.69 | 127.31 |
| 17 | f | 4009 | BCR | C11-C10-C9 | -3.94 | 121.69 | 127.31 |
| 17 | Z | 521 | BCR | C15-C14-C13 | -3.93 | 121.70 | 127.31 |
| 17 | B | 4006 | BCR | C15-C14-C13 | -3.93 | 121.70 | 127.31 |
| 17 | 6 | 522 | BCR | C11-C10-C9 | -3.93 | 121.70 | 127.31 |
| 17 | G | 4002 | BCR | C20-C21-C22 | -3.93 | 121.70 | 127.31 |
| 14 | l | 508 | CLA | CMB-C2B-C3B | 3.93 | 132.03 | 124.68 |
| 14 | e | 1140 | CLA | CMB-C2B-C1B | -3.93 | 122.43 | 128.46 |
| 14 | Y | 508 | CLA | CMB-C2B-C3B | 3.93 | 132.02 | 124.68 |
| 14 | e | 1138 | CLA | CMB-C2B-C1B | -3.92 | 122.43 | 128.46 |
| 14 | A | 1140 | CLA | CMB-C2B-C1B | -3.92 | 122.43 | 128.46 |
| 17 | d | 522 | BCR | C11-C10-C9 | -3.92 | 121.71 | 127.31 |
| 17 | B | 4014 | BCR | C20-C19-C18 | -3.92 | 115.40 | 126.42 |
| 21 | s | 822 | SQD | O7-S-C6 | 3.92 | 111.60 | 106.94 |
| 17 | W | 4021 | BCR | C15-C16-C17 | -3.92 | 115.45 | 123.47 |
| 17 | A | 4002 | BCR | C20-C21-C22 | -3.92 | 121.72 | 127.31 |
| 17 | f | 4014 | BCR | C20-C19-C18 | -3.92 | 115.41 | 126.42 |
| 14 | b | 506 | CLA | CMB-C2B-C1B | -3.92 | 122.44 | 128.46 |
| 14 | A | 1136 | CLA | CMB-C2B-C1B | -3.92 | 122.45 | 128.46 |
| 14 | v | 510 | CLA | CMB-C2B-C1B | -3.91 | 122.45 | 128.46 |
| 14 | 6 | 510 | CLA | CMB-C2B-C1B | -3.91 | 122.45 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | o | 4021 | BCR | C15-C16-C17 | -3.91 | 115.46 | 123.47 |
| 17 | 5 | 521 | BCR | C16-C17-C18 | -3.91 | 121.73 | 127.31 |
| 14 | d | 510 | CLA | CMB-C2B-C1B | -3.91 | 122.45 | 128.46 |
| 14 | e | 1136 | CLA | CMB-C2B-C1B | -3.91 | 122.46 | 128.46 |
| 17 | H | 4014 | BCR | C20-C19-C18 | -3.91 | 115.44 | 126.42 |
| 14 | H | 1235 | CLA | CMB-C2B-C1B | -3.91 | 122.46 | 128.46 |
| 17 | c | 521 | BCR | C16-C17-C18 | -3.91 | 121.73 | 127.31 |
| 14 | B | 1235 | CLA | CMB-C2B-C1B | -3.91 | 122.46 | 128.46 |
| 14 | 4 | 506 | CLA | CMB-C2B-C1B | -3.91 | 122.46 | 128.46 |
| 17 | u | 521 | BCR | C16-C17-C18 | -3.90 | 121.74 | 127.31 |
| 14 | r | 507 | CLA | CMB-C2B-C1B | -3.90 | 122.47 | 128.46 |
| 14 | B | 1209 | CLA | O2D-CGD-O1D | -3.90 | 116.21 | 123.84 |
| 14 | H | 1209 | CLA | O2D-CGD-O1D | -3.90 | 116.21 | 123.84 |
| 21 | 3 | 822 | SQD | O7-S-C6 | 3.90 | 111.57 | 106.94 |
| 17 | e | 4002 | BCR | C20-C21-C22 | -3.90 | 121.75 | 127.31 |
| 14 | f | 1209 | CLA | O2D-CGD-O1D | -3.90 | 116.22 | 123.84 |
| 14 | 1 | 509 | CLA | CMB-C2B-C1B | -3.89 | 122.48 | 128.46 |
| 14 | 2 | 507 | CLA | CMB-C2B-C1B | -3.89 | 122.48 | 128.46 |
| 17 | G | 4003 | BCR | C15-C14-C13 | -3.89 | 121.76 | 127.31 |
| 17 | T | 4012 | BCR | C3-C4-C5 | -3.89 | 107.13 | 114.08 |
| 14 | Y | 513 | CLA | CMB-C2B-C1B | -3.89 | 122.49 | 128.46 |
| 14 | Y | 509 | CLA | CMB-C2B-C1B | -3.89 | 122.49 | 128.46 |
| 14 | f | 1235 | CLA | CMB-C2B-C1B | -3.89 | 122.49 | 128.46 |
| 17 | H | 4006 | BCR | C34-C9-C10 | -3.89 | 117.48 | 122.92 |
| 17 | U | 4104 | BCR | C38-C26-C25 | -3.89 | 120.17 | 124.53 |
| 21 | a | 822 | SQD | O7-S-C6 | 3.88 | 111.56 | 106.94 |
| 14 | q | 509 | CLA | CMB-C2B-C1B | -3.88 | 122.49 | 128.46 |
| 14 | t | 506 | CLA | CMB-C2B-C1B | -3.88 | 122.50 | 128.46 |
| 17 | 3 | 524 | BCR | C16-C17-C18 | -3.88 | 121.77 | 127.31 |
| 14 | Z | 507 | CLA | CMB-C2B-C1B | -3.88 | 122.50 | 128.46 |
| 17 | G | 4007 | BCR | C15-C14-C13 | -3.88 | 121.78 | 127.31 |
| 14 | e | 1011 | CLA | O2D-CGD-O1D | -3.88 | 116.26 | 123.84 |
| 17 | m | 4104 | BCR | C38-C26-C25 | -3.88 | 120.17 | 124.53 |
| 21 | Z | 822 | SQD | O7-S-C6 | 3.88 | 111.55 | 106.94 |
| 17 | e | 4003 | BCR | C15-C14-C13 | -3.88 | 121.78 | 127.31 |
| 14 | b | 504 | CLA | CMB-C2B-C1B | -3.88 | 122.51 | 128.46 |
| 17 | f | 4006 | BCR | C34-C9-C10 | -3.87 | 117.50 | 122.92 |
| 17 | a | 524 | BCR | C16-C17-C18 | -3.87 | 121.78 | 127.31 |
| 14 | a | 512 | CLA | CMB-C2B-C1B | -3.87 | 122.51 | 128.46 |
| 17 | J | 4012 | BCR | C3-C4-C5 | -3.87 | 107.16 | 114.08 |
| 14 | l | 513 | CLA | CMB-C2B-C1B | -3.87 | 122.51 | 128.46 |
| 17 | A | 4003 | BCR | C15-C14-C13 | -3.87 | 121.78 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | s | 524 | BCR | C16-C17-C18 | -3.87 | 121.78 | 127.31 |
| 14 | t | 504 | CLA | CMB-C2B-C1B | -3.87 | 122.52 | 128.46 |
| 14 | s | 512 | CLA | CMB-C2B-C1B | -3.87 | 122.52 | 128.46 |
| 14 | q | 513 | CLA | CMB-C2B-C1B | -3.87 | 122.52 | 128.46 |
| 17 | A | 4007 | BCR | C15-C14-C13 | -3.86 | 121.80 | 127.31 |
| 14 | A | 1011 | CLA | O2D-CGD-O1D | -3.86 | 116.28 | 123.84 |
| 14 | r | 509 | CLA | CMB-C2B-C3B | 3.86 | 131.90 | 124.68 |
| 14 | G | 1011 | CLA | O2D-CGD-O1D | -3.86 | 116.29 | 123.84 |
| 14 | d | 511 | CLA | CMB-C2B-C1B | -3.86 | 122.53 | 128.46 |
| 14 | 2 | 509 | CLA | CMB-C2B-C3B | 3.86 | 131.90 | 124.68 |
| 14 | A | 1120 | CLA | CMB-C2B-C3B | 3.86 | 131.90 | 124.68 |
| 17 | K | 4104 | BCR | C38-C26-C25 | -3.86 | 120.20 | 124.53 |
| 17 | B | 4006 | BCR | C34-C9-C10 | -3.86 | 117.52 | 122.92 |
| 21 | 2 | 822 | SQD | O7-S-C6 | 3.86 | 111.52 | 106.94 |
| 14 | G | 1120 | CLA | CMB-C2B-C3B | 3.86 | 131.89 | 124.68 |
| 14 | 4 | 504 | CLA | CMB-C2B-C1B | -3.85 | 122.54 | 128.46 |
| 14 | 3 | 512 | CLA | CMB-C2B-C1B | -3.85 | 122.54 | 128.46 |
| 17 | l | 4012 | BCR | C3-C4-C5 | -3.85 | 107.20 | 114.08 |
| 17 | e | 4001 | BCR | C20-C21-C22 | -3.85 | 121.81 | 127.31 |
| 14 | e | 1104 | CLA | CMB-C2B-C3B | 3.85 | 131.88 | 124.68 |
| 14 | e | 1120 | CLA | CMB-C2B-C3B | 3.85 | 131.88 | 124.68 |
| 17 | u | 523 | BCR | C7-C8-C9 | -3.85 | 120.42 | 126.23 |
| 14 | d | 512 | CLA | CMB-C2B-C1B | -3.85 | 122.55 | 128.46 |
| 14 | H | 1213 | CLA | CMB-C2B-C3B | 3.85 | 131.87 | 124.68 |
| 14 | 6 | 511 | CLA | CMB-C2B-C1B | -3.85 | 122.55 | 128.46 |
| 17 | A | 4001 | BCR | C20-C21-C22 | -3.84 | 121.82 | 127.31 |
| 17 | L | 4219 | BCR | C33-C5-C6 | -3.84 | 120.21 | 124.53 |
| 14 | A | 1104 | CLA | CMB-C2B-C3B | 3.84 | 131.87 | 124.68 |
| 14 | Z | 509 | CLA | CMB-C2B-C3B | 3.84 | 131.87 | 124.68 |
| 14 | f | 1213 | CLA | CMB-C2B-C3B | 3.84 | 131.87 | 124.68 |
| 14 | B | 1213 | CLA | CMB-C2B-C3B | 3.84 | 131.87 | 124.68 |
| 17 | n | 4219 | BCR | C33-C5-C6 | -3.84 | 120.21 | 124.53 |
| 17 | G | 4001 | BCR | C20-C21-C22 | -3.84 | 121.83 | 127.31 |
| 14 | G | 1104 | CLA | CMB-C2B-C3B | 3.84 | 131.86 | 124.68 |
| 21 | r | 822 | SQD | O7-S-C6 | 3.84 | 111.50 | 106.94 |
| 14 | v | 511 | CLA | CMB-C2B-C1B | -3.83 | 122.57 | 128.46 |
| 17 | H | 4006 | BCR | C33-C5-C6 | -3.83 | 120.22 | 124.53 |
| 17 | e | 4007 | BCR | C15-C14-C13 | -3.83 | 121.84 | 127.31 |
| 14 | 6 | 512 | CLA | CMB-C2B-C1B | -3.83 | 122.58 | 128.46 |
| 14 | 5 | 506 | CLA | CMB-C2B-C1B | -3.83 | 122.58 | 128.46 |
| 14 | c | 506 | CLA | CMB-C2B-C1B | -3.83 | 122.58 | 128.46 |
| 17 | B | 4006 | BCR | C33-C5-C6 | -3.82 | 120.23 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | T | 4015 | BCR | C15-C14-C13 | -3.82 | 121.85 | 127.31 |
| 17 | d | 523 | BCR | C16-C17-C18 | -3.82 | 121.85 | 127.31 |
| 17 | V | 4219 | BCR | C33-C5-C6 | -3.82 | 120.24 | 124.53 |
| 17 | 5 | 523 | BCR | C7-C8-C9 | -3.82 | 120.46 | 126.23 |
| 17 | B | 4017 | BCR | C10-C11-C12 | -3.82 | 111.30 | 123.22 |
| 17 | f | 4006 | BCR | C33-C5-C6 | -3.82 | 120.24 | 124.53 |
| 17 | H | 4017 | BCR | C10-C11-C12 | -3.82 | 111.30 | 123.22 |
| 17 | f | 4017 | BCR | C10-C11-C12 | -3.82 | 111.30 | 123.22 |
| 14 | u | 506 | CLA | CMB-C2B-C1B | -3.82 | 122.59 | 128.46 |
| 14 | v | 512 | CLA | CMB-C2B-C1B | -3.82 | 122.59 | 128.46 |
| 17 | l | 521 | BCR | C15-C14-C13 | -3.82 | 121.86 | 127.31 |
| 17 | 6 | 521 | BCR | C24-C23-C22 | -3.82 | 120.47 | 126.23 |
| 17 | q | 521 | BCR | C15-C14-C13 | -3.81 | 121.87 | 127.31 |
| 14 | c | 501 | CLA | CMB-C2B-C1B | -3.81 | 122.60 | 128.46 |
| 17 | Y | 521 | BCR | C15-C14-C13 | -3.81 | 121.87 | 127.31 |
| 14 | f | 1219 | CLA | CMB-C2B-C1B | -3.81 | 122.61 | 128.46 |
| 17 | J | 4015 | BCR | C15-C14-C13 | -3.80 | 121.88 | 127.31 |
| 17 | c | 523 | BCR | C7-C8-C9 | -3.80 | 120.49 | 126.23 |
| 14 | G | 1124 | CLA | CMB-C2B-C3B | 3.80 | 131.79 | 124.68 |
| 17 | d | 521 | BCR | C24-C23-C22 | -3.80 | 120.49 | 126.23 |
| 14 | e | 1124 | CLA | CMB-C2B-C3B | 3.80 | 131.79 | 124.68 |
| 21 | d | 822 | SQD | O9-S-O7 | -3.80 | 100.80 | 113.95 |
| 17 | v | 521 | BCR | C24-C23-C22 | -3.80 | 120.50 | 126.23 |
| 17 | f | 4010 | BCR | C8-C7-C6 | -3.80 | 116.54 | 127.20 |
| 17 | 6 | 523 | BCR | C16-C17-C18 | -3.80 | 121.89 | 127.31 |
| 21 | 6 | 822 | SQD | O9-S-O7 | -3.79 | 100.82 | 113.95 |
| 17 | l | 4015 | BCR | C15-C14-C13 | -3.79 | 121.90 | 127.31 |
| 21 | v | 822 | SQD | O9-S-O7 | -3.79 | 100.83 | 113.95 |
| 17 | b | 524 | BCR | C33-C5-C6 | -3.79 | 120.27 | 124.53 |
| 17 | B | 4010 | BCR | C8-C7-C6 | -3.79 | 116.56 | 127.20 |
| 14 | 4 | 510 | CLA | CMB-C2B-C1B | -3.79 | 122.64 | 128.46 |
| 14 | G | 1135 | CLA | C1-C2-C3 | -3.79 | 119.49 | 126.04 |
| 14 | e | 1135 | CLA | C1-C2-C3 | -3.79 | 119.49 | 126.04 |
| 14 | u | 501 | CLA | CMB-C2B-C1B | -3.79 | 122.64 | 128.46 |
| 14 | l | 506 | CLA | CMB-C2B-C3B | 3.78 | 131.76 | 124.68 |
| 14 | Y | 506 | CLA | CMB-C2B-C3B | 3.78 | 131.76 | 124.68 |
| 14 | A | 1124 | CLA | CMB-C2B-C3B | 3.78 | 131.76 | 124.68 |
| 14 | B | 1219 | CLA | CMB-C2B-C1B | -3.78 | 122.65 | 128.46 |
| 14 | 5 | 501 | CLA | CMB-C2B-C1B | -3.78 | 122.65 | 128.46 |
| 14 | H | 1219 | CLA | CMB-C2B-C1B | -3.78 | 122.65 | 128.46 |
| 17 | 4 | 524 | BCR | C33-C5-C6 | -3.78 | 120.28 | 124.53 |
| 14 | A | 1135 | CLA | C1-C2-C3 | -3.78 | 119.50 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | H | 4010 | BCR | C8-C7-C6 | -3.78 | 116.59 | 127.20 |
| 17 | d | 521 | BCR | C28-C27-C26 | -3.78 | 107.33 | 114.08 |
| 14 | F | 1301 | CLA | CMB-C2B-C1B | -3.78 | 122.66 | 128.46 |
| 17 | v | 521 | BCR | C16-C17-C18 | -3.78 | 121.92 | 127.31 |
| 17 | a | 522 | BCR | C24-C23-C22 | -3.77 | 120.53 | 126.23 |
| 17 | G | 4002 | BCR | C11-C10-C9 | -3.77 | 121.92 | 127.31 |
| 14 | e | 1112 | CLA | CMB-C2B-C1B | -3.77 | 122.67 | 128.46 |
| 14 | q | 506 | CLA | CMB-C2B-C3B | 3.77 | 131.74 | 124.68 |
| 14 | b | 510 | CLA | CMB-C2B-C1B | -3.77 | 122.67 | 128.46 |
| 14 | j | 1301 | CLA | CMB-C2B-C1B | -3.77 | 122.67 | 128.46 |
| 17 | 2 | 524 | BCR | C33-C5-C6 | -3.77 | 120.30 | 124.53 |
| 14 | R | 1301 | CLA | CMB-C2B-C1B | -3.77 | 122.67 | 128.46 |
| 14 | s | 516 | CLA | CMB-C2B-C1B | -3.77 | 122.67 | 128.46 |
| 17 | 6 | 521 | BCR | C28-C27-C26 | -3.77 | 107.35 | 114.08 |
| 14 | G | 1112 | CLA | CMB-C2B-C1B | -3.77 | 122.68 | 128.46 |
| 21 | 1 | 822 | SQD | O9-S-O7 | -3.76 | 100.92 | 113.95 |
| 17 | 6 | 521 | BCR | C16-C17-C18 | -3.76 | 121.94 | 127.31 |
| 14 | 5 | 512 | CLA | CMB-C2B-C1B | -3.76 | 122.68 | 128.46 |
| 17 | J | 4012 | BCR | C11-C10-C9 | -3.76 | 121.94 | 127.31 |
| 14 | u | 512 | CLA | CMB-C2B-C1B | -3.76 | 122.68 | 128.46 |
| 17 | f | 4004 | BCR | C11-C10-C9 | -3.76 | 121.94 | 127.31 |
| 14 | A | 1121 | CLA | CAA-C2A-C3A | -3.76 | 102.48 | 112.78 |
| 17 | r | 524 | BCR | C33-C5-C6 | -3.76 | 120.31 | 124.53 |
| 21 | Y | 822 | SQD | O9-S-O7 | -3.76 | 100.93 | 113.95 |
| 14 | A | 1112 | CLA | CMB-C2B-C1B | -3.76 | 122.69 | 128.46 |
| 17 | v | 521 | BCR | C28-C27-C26 | -3.76 | 107.36 | 114.08 |
| 21 | n | 5216 | SQD | O9-S-O7 | -3.76 | 100.94 | 113.95 |
| 14 | t | 510 | CLA | CMB-C2B-C1B | -3.76 | 122.69 | 128.46 |
| 14 | A | 1129 | CLA | CMB-C2B-C3B | 3.76 | 131.71 | 124.68 |
| 14 | e | 1129 | CLA | CMB-C2B-C3B | 3.76 | 131.71 | 124.68 |
| 17 | l | 4012 | BCR | C11-C10-C9 | -3.76 | 121.95 | 127.31 |
| 14 | a | 510 | CLA | CMB-C2B-C1B | -3.76 | 122.69 | 128.46 |
| 21 | u | 822 | SQD | O9-S-O7 | -3.76 | 100.95 | 113.95 |
| 17 | d | 521 | BCR | C16-C17-C18 | -3.76 | 121.95 | 127.31 |
| 17 | Z | 524 | BCR | C33-C5-C6 | -3.76 | 120.31 | 124.53 |
| 21 | L | 5216 | SQD | O6-C1-C2 | 3.75 | 114.17 | 108.30 |
| 21 | q | 822 | SQD | O9-S-O7 | -3.75 | 100.95 | 113.95 |
| 14 | G | 1121 | CLA | CAA-C2A-C3A | -3.75 | 102.50 | 112.78 |
| 14 | H | 1211 | CLA | CHB-C4A-NA | 3.75 | 129.70 | 124.51 |
| 17 | 3 | 522 | BCR | C24-C23-C22 | -3.75 | 120.56 | 126.23 |
| 21 | V | 5216 | SQD | O9-S-O7 | -3.75 | 100.96 | 113.95 |
| 21 | L | 5216 | SQD | O9-S-O7 | -3.75 | 100.97 | 113.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | H | 4004 | BCR | C11-C10-C9 | -3.75 | 121.96 | 127.31 |
| 14 | e | 1121 | CLA | CAA-C2A-C3A | -3.75 | 102.51 | 112.78 |
| 21 | b | 822 | SQD | O9-S-C6 | 3.75 | 111.40 | 106.94 |
| 17 | B | 4004 | BCR | C11-C10-C9 | -3.75 | 121.96 | 127.31 |
| 17 | T | 4012 | BCR | C11-C10-C9 | -3.75 | 121.96 | 127.31 |
| 17 | Z | 524 | BCR | C16-C17-C18 | -3.75 | 121.96 | 127.31 |
| 14 | 5 | 511 | CLA | CMB-C2B-C3B | 3.75 | 131.69 | 124.68 |
| 17 | A | 4002 | BCR | C11-C10-C9 | -3.75 | 121.96 | 127.31 |
| 14 | H | 1212 | CLA | CMB-C2B-C3B | 3.75 | 131.69 | 124.68 |
| 17 | B | 4009 | BCR | C21-C20-C19 | -3.75 | 111.52 | 123.22 |
| 21 | 5 | 822 | SQD | O9-S-O7 | -3.75 | 100.98 | 113.95 |
| 14 | u | 511 | CLA | CMB-C2B-C3B | 3.75 | 131.69 | 124.68 |
| 14 | f | 1211 | CLA | CHB-C4A-NA | 3.74 | 129.69 | 124.51 |
| 14 | L | 1502 | CLA | CMB-C2B-C3B | 3.74 | 131.68 | 124.68 |
| 14 | n | 1502 | CLA | CMB-C2B-C3B | 3.74 | 131.68 | 124.68 |
| 17 | H | 4009 | BCR | C21-C20-C19 | -3.74 | 111.53 | 123.22 |
| 17 | 2 | 524 | BCR | C16-C17-C18 | -3.74 | 121.97 | 127.31 |
| 14 | f | 1203 | CLA | CMB-C2B-C3B | 3.74 | 131.68 | 124.68 |
| 14 | f | 1212 | CLA | CMB-C2B-C3B | 3.74 | 131.68 | 124.68 |
| 14 | 3 | 510 | CLA | CMB-C2B-C1B | -3.74 | 122.71 | 128.46 |
| 17 | r | 524 | BCR | C16-C17-C18 | -3.74 | 121.97 | 127.31 |
| 14 | H | 1203 | CLA | CMB-C2B-C3B | 3.74 | 131.68 | 124.68 |
| 17 | v | 523 | BCR | C16-C17-C18 | -3.74 | 121.97 | 127.31 |
| 17 | t | 524 | BCR | C33-C5-C6 | -3.74 | 120.33 | 124.53 |
| 14 | B | 1212 | CLA | CMB-C2B-C3B | 3.74 | 131.68 | 124.68 |
| 21 | c | 822 | SQD | O9-S-O7 | -3.74 | 101.01 | 113.95 |
| 17 | f | 4009 | BCR | C21-C20-C19 | -3.74 | 111.55 | 123.22 |
| 14 | G | 1129 | CLA | CMB-C2B-C3B | 3.74 | 131.67 | 124.68 |
| 14 | 3 | 516 | CLA | CMB-C2B-C1B | -3.74 | 122.72 | 128.46 |
| 17 | e | 4002 | BCR | C11-C10-C9 | -3.74 | 121.98 | 127.31 |
| 14 | s | 510 | CLA | CMB-C2B-C1B | -3.74 | 122.72 | 128.46 |
| 17 | v | 523 | BCR | C7-C8-C9 | -3.74 | 120.59 | 126.23 |
| 21 | 4 | 822 | SQD | O9-S-C6 | 3.74 | 111.38 | 106.94 |
| 14 | v | 516 | CLA | CMB-C2B-C1B | -3.73 | 122.73 | 128.46 |
| 14 | B | 1203 | CLA | CMB-C2B-C3B | 3.73 | 131.66 | 124.68 |
| 17 | d | 523 | BCR | C7-C8-C9 | -3.73 | 120.60 | 126.23 |
| 14 | c | 512 | CLA | CMB-C2B-C1B | -3.73 | 122.73 | 128.46 |
| 14 | c | 511 | CLA | CMB-C2B-C3B | 3.73 | 131.66 | 124.68 |
| 17 | Z | 521 | BCR | C11-C10-C9 | -3.73 | 121.99 | 127.31 |
| 21 | t | 822 | SQD | O9-S-C6 | 3.73 | 111.37 | 106.94 |
| 21 | V | 5216 | SQD | C4-C3-C2 | 3.73 | 117.33 | 110.82 |
| 17 | s | 522 | BCR | C24-C23-C22 | -3.73 | 120.60 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1210 | CLA | CMB-C2B-C3B | 3.73 | 131.65 | 124.68 |
| 17 | 2 | 521 | BCR | C11-C10-C9 | -3.72 | 122.00 | 127.31 |
| 14 | 1 | 507 | CLA | CMB-C2B-C1B | -3.72 | 122.74 | 128.46 |
| 14 | d | 516 | CLA | CMB-C2B-C1B | -3.72 | 122.74 | 128.46 |
| 21 | b | 822 | SQD | O9-S-O7 | -3.72 | 101.06 | 113.95 |
| 14 | A | 1119 | CLA | CMB-C2B-C3B | 3.72 | 131.64 | 124.68 |
| 17 | M | 4021 | BCR | C28-C27-C26 | -3.72 | 107.43 | 114.08 |
| 17 | 6 | 523 | BCR | C7-C8-C9 | -3.72 | 120.61 | 126.23 |
| 19 | e | 1849 | LMU | O5'-C5'-C4' | 3.72 | 116.45 | 109.69 |
| 14 | e | 1119 | CLA | CMB-C2B-C3B | 3.72 | 131.64 | 124.68 |
| 21 | n | 5216 | SQD | O6-C1-C2 | 3.72 | 114.11 | 108.30 |
| 17 | W | 4021 | BCR | C28-C27-C26 | -3.72 | 107.43 | 114.08 |
| 14 | a | 516 | CLA | CMB-C2B-C1B | -3.72 | 122.75 | 128.46 |
| 21 | V | 5216 | SQD | O6-C1-C2 | 3.72 | 114.11 | 108.30 |
| 17 | t | 524 | BCR | C7-C8-C9 | -3.72 | 120.61 | 126.23 |
| 14 | 6 | 516 | CLA | CMB-C2B-C1B | -3.72 | 122.75 | 128.46 |
| 17 | H | 4010 | BCR | C24-C23-C22 | -3.72 | 120.62 | 126.23 |
| 14 | f | 1021 | CLA | O2D-CGD-O1D | -3.72 | 116.57 | 123.84 |
| 17 | r | 521 | BCR | C11-C10-C9 | -3.72 | 122.00 | 127.31 |
| 14 | B | 1211 | CLA | CHB-C4A-NA | 3.72 | 129.65 | 124.51 |
| 21 | 4 | 822 | SQD | O9-S-O7 | -3.72 | 101.09 | 113.95 |
| 17 | m | 4104 | BCR | C24-C23-C22 | -3.71 | 120.62 | 126.23 |
| 14 | q | 507 | CLA | CMB-C2B-C1B | -3.71 | 122.76 | 128.46 |
| 21 | t | 822 | SQD | O9-S-O7 | -3.71 | 101.10 | 113.95 |
| 14 | B | 1021 | CLA | O2D-CGD-O1D | -3.71 | 116.58 | 123.84 |
| 14 | G | 1119 | CLA | CMB-C2B-C3B | 3.71 | 131.62 | 124.68 |
| 14 | B | 1210 | CLA | CMB-C2B-C3B | 3.71 | 131.62 | 124.68 |
| 19 | A | 1849 | LMU | O5'-C5'-C4' | 3.71 | 116.43 | 109.69 |
| 14 | f | 1210 | CLA | CMB-C2B-C3B | 3.71 | 131.62 | 124.68 |
| 14 | V | 1502 | CLA | CMB-C2B-C3B | 3.71 | 131.62 | 124.68 |
| 17 | U | 4104 | BCR | C24-C23-C22 | -3.71 | 120.63 | 126.23 |
| 17 | f | 4010 | BCR | C24-C23-C22 | -3.71 | 120.63 | 126.23 |
| 17 | B | 4010 | BCR | C24-C23-C22 | -3.70 | 120.64 | 126.23 |
| 14 | b | 516 | CLA | CMB-C2B-C1B | -3.70 | 122.77 | 128.46 |
| 21 | L | 5216 | SQD | C4-C3-C2 | 3.70 | 117.29 | 110.82 |
| 14 | t | 516 | CLA | CMB-C2B-C1B | -3.70 | 122.78 | 128.46 |
| 17 | H | 4009 | BCR | C15-C14-C13 | -3.70 | 122.03 | 127.31 |
| 14 | l | 1302 | CLA | O2D-CGD-O1D | -3.70 | 116.60 | 123.84 |
| 17 | B | 4009 | BCR | C15-C14-C13 | -3.70 | 122.03 | 127.31 |
| 17 | t | 523 | BCR | C24-C23-C22 | -3.70 | 120.64 | 126.23 |
| 17 | o | 4021 | BCR | C28-C27-C26 | -3.70 | 107.47 | 114.08 |
| 14 | Y | 507 | CLA | CMB-C2B-C1B | -3.70 | 122.78 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | n | 5216 | SQD | C4-C3-C2 | 3.70 | 117.28 | 110.82 |
| 17 | l | 4015 | BCR | C16-C17-C18 | -3.70 | 122.03 | 127.31 |
| 17 | K | 4104 | BCR | C24-C23-C22 | -3.70 | 120.65 | 126.23 |
| 14 | H | 1021 | CLA | O2D-CGD-O1D | -3.70 | 116.61 | 123.84 |
| 17 | I | 4018 | BCR | C7-C8-C9 | -3.70 | 120.65 | 126.23 |
| 17 | 4 | 524 | BCR | C7-C8-C9 | -3.69 | 120.65 | 126.23 |
| 17 | 4 | 523 | BCR | C24-C23-C22 | -3.69 | 120.65 | 126.23 |
| 14 | J | 1302 | CLA | O2D-CGD-O1D | -3.69 | 116.62 | 123.84 |
| 17 | H | 4004 | BCR | C15-C14-C13 | -3.69 | 122.05 | 127.31 |
| 14 | Z | 518 | CLA | CMB-C2B-C1B | -3.69 | 122.79 | 128.46 |
| 17 | k | 4018 | BCR | C7-C8-C9 | -3.69 | 120.66 | 126.23 |
| 21 | 3 | 822 | SQD | O9-S-O7 | -3.69 | 101.19 | 113.95 |
| 19 | G | 1849 | LMU | O5'-C5'-C4' | 3.69 | 116.39 | 109.69 |
| 17 | S | 4018 | BCR | C7-C8-C9 | -3.69 | 120.66 | 126.23 |
| 14 | 4 | 516 | CLA | CMB-C2B-C1B | -3.69 | 122.80 | 128.46 |
| 17 | f | 4009 | BCR | C15-C14-C13 | -3.69 | 122.05 | 127.31 |
| 17 | b | 523 | BCR | C24-C23-C22 | -3.68 | 120.67 | 126.23 |
| 14 | 4 | 513 | CLA | CMB-C2B-C1B | -3.68 | 122.80 | 128.46 |
| 17 | t | 521 | BCR | C24-C23-C22 | -3.68 | 120.67 | 126.23 |
| 14 | 5 | 504 | CLA | CMB-C2B-C1B | -3.68 | 122.80 | 128.46 |
| 17 | b | 522 | BCR | C20-C21-C22 | -3.68 | 122.05 | 127.31 |
| 21 | s | 822 | SQD | O9-S-O7 | -3.68 | 101.20 | 113.95 |
| 14 | T | 1302 | CLA | O2D-CGD-O1D | -3.68 | 116.64 | 123.84 |
| 14 | t | 513 | CLA | CMB-C2B-C1B | -3.68 | 122.81 | 128.46 |
| 17 | Z | 523 | BCR | C16-C17-C18 | -3.68 | 122.06 | 127.31 |
| 17 | T | 4015 | BCR | C16-C17-C18 | -3.68 | 122.06 | 127.31 |
| 14 | u | 504 | CLA | CMB-C2B-C1B | -3.68 | 122.81 | 128.46 |
| 17 | t | 522 | BCR | C20-C21-C22 | -3.68 | 122.06 | 127.31 |
| 17 | J | 4015 | BCR | C16-C17-C18 | -3.68 | 122.06 | 127.31 |
| 17 | v | 521 | BCR | C15-C14-C13 | -3.67 | 122.07 | 127.31 |
| 17 | b | 524 | BCR | C7-C8-C9 | -3.67 | 120.68 | 126.23 |
| 17 | 4 | 521 | BCR | C24-C23-C22 | -3.67 | 120.68 | 126.23 |
| 21 | a | 822 | SQD | O9-S-O7 | -3.67 | 101.24 | 113.95 |
| 17 | 4 | 522 | BCR | C20-C21-C22 | -3.67 | 122.07 | 127.31 |
| 21 | H | 1852 | SQD | O48-C23-C24 | 3.67 | 123.43 | 111.91 |
| 14 | c | 504 | CLA | CMB-C2B-C1B | -3.67 | 122.83 | 128.46 |
| 17 | B | 4004 | BCR | C15-C14-C13 | -3.67 | 122.08 | 127.31 |
| 17 | q | 521 | BCR | C16-C17-C18 | -3.67 | 122.08 | 127.31 |
| 21 | Z | 822 | SQD | O47-C7-C8 | 3.67 | 119.40 | 111.50 |
| 17 | Z | 522 | BCR | C7-C8-C9 | -3.67 | 120.70 | 126.23 |
| 14 | 2 | 518 | CLA | CMB-C2B-C1B | -3.66 | 122.83 | 128.46 |
| 17 | 6 | 521 | BCR | C15-C14-C13 | -3.66 | 122.08 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 1 | 521 | BCR | C16-C17-C18 | -3.66 | 122.08 | 127.31 |
| 17 | r | 523 | BCR | C16-C17-C18 | -3.66 | 122.08 | 127.31 |
| 21 | 2 | 822 | SQD | O47-C7-C8 | 3.66 | 119.39 | 111.50 |
| 17 | 6 | 524 | BCR | C11-C10-C9 | -3.66 | 122.08 | 127.31 |
| 17 | W | 4021 | BCR | C10-C11-C12 | -3.66 | 111.80 | 123.22 |
| 14 | r | 518 | CLA | CMB-C2B-C1B | -3.66 | 122.84 | 128.46 |
| 17 | v | 524 | BCR | C11-C10-C9 | -3.66 | 122.09 | 127.31 |
| 21 | r | 822 | SQD | O47-C7-C8 | 3.66 | 119.39 | 111.50 |
| 17 | Y | 521 | BCR | C16-C17-C18 | -3.66 | 122.09 | 127.31 |
| 21 | Z | 822 | SQD | O9-S-O7 | -3.66 | 101.29 | 113.95 |
| 17 | 2 | 523 | BCR | C16-C17-C18 | -3.66 | 122.09 | 127.31 |
| 14 | d | 501 | CLA | CMB-C2B-C1B | -3.66 | 122.84 | 128.46 |
| 21 | B | 1852 | SQD | O48-C23-C24 | 3.66 | 123.38 | 111.91 |
| 17 | M | 4021 | BCR | C10-C11-C12 | -3.66 | 111.81 | 123.22 |
| 17 | f | 4004 | BCR | C15-C14-C13 | -3.66 | 122.09 | 127.31 |
| 21 | f | 1852 | SQD | O48-C23-C24 | 3.65 | 123.38 | 111.91 |
| 17 | I | 4018 | BCR | C27-C26-C25 | -3.65 | 117.42 | 122.73 |
| 14 | Y | 501 | CLA | CMB-C2B-C1B | -3.65 | 122.85 | 128.46 |
| 14 | G | 1137 | CLA | CMB-C2B-C1B | -3.65 | 122.85 | 128.46 |
| 21 | 2 | 822 | SQD | O9-S-O7 | -3.65 | 101.31 | 113.95 |
| 17 | d | 521 | BCR | C15-C14-C13 | -3.65 | 122.10 | 127.31 |
| 17 | b | 521 | BCR | C24-C23-C22 | -3.65 | 120.72 | 126.23 |
| 14 | d | 517 | CLA | CMB-C2B-C1B | -3.65 | 122.86 | 128.46 |
| 14 | B | 1206 | CLA | CMB-C2B-C3B | 3.65 | 131.50 | 124.68 |
| 14 | f | 1206 | CLA | CMB-C2B-C3B | 3.65 | 131.50 | 124.68 |
| 17 | B | 4006 | BCR | C20-C21-C22 | -3.65 | 122.11 | 127.31 |
| 14 | b | 513 | CLA | CMB-C2B-C1B | -3.65 | 122.86 | 128.46 |
| 21 | r | 822 | SQD | O9-S-O7 | -3.65 | 101.33 | 113.95 |
| 14 | s | 506 | CLA | CMB-C2B-C3B | 3.65 | 131.50 | 124.68 |
| 17 | d | 524 | BCR | C11-C10-C9 | -3.65 | 122.11 | 127.31 |
| 21 | B | 1852 | SQD | O9-S-O7 | -3.65 | 101.33 | 113.95 |
| 21 | H | 1852 | SQD | C1-O5-C5 | 3.64 | 120.84 | 113.69 |
| 14 | q | 501 | CLA | CMB-C2B-C1B | -3.64 | 122.86 | 128.46 |
| 14 | 3 | 506 | CLA | CMB-C2B-C3B | 3.64 | 131.50 | 124.68 |
| 14 | Z | 501 | CLA | CMB-C2B-C1B | -3.64 | 122.86 | 128.46 |
| 14 | u | 507 | CLA | CMB-C2B-C1B | -3.64 | 122.87 | 128.46 |
| 14 | 6 | 501 | CLA | CMB-C2B-C1B | -3.64 | 122.87 | 128.46 |
| 17 | k | 4018 | BCR | C27-C26-C25 | -3.64 | 117.44 | 122.73 |
| 14 | 1 | 501 | CLA | CMB-C2B-C1B | -3.64 | 122.87 | 128.46 |
| 14 | K | 1105 | CLA | CBC-CAC-C3C | 3.64 | 122.47 | 112.43 |
| 14 | a | 506 | CLA | CMB-C2B-C3B | 3.64 | 131.49 | 124.68 |
| 17 | b | 521 | BCR | C11-C10-C9 | -3.64 | 122.12 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | o | 4021 | BCR | C10-C11-C12 | -3.64 | 111.86 | 123.22 |
| 17 | a | 521 | BCR | C28-C27-C26 | -3.64 | 107.58 | 114.08 |
| 14 | e | 1022 | CLA | C1B-CHB-C4A | -3.64 | 122.92 | 130.12 |
| 14 | 5 | 507 | CLA | CMB-C2B-C1B | -3.64 | 122.88 | 128.46 |
| 17 | s | 521 | BCR | C28-C27-C26 | -3.64 | 107.59 | 114.08 |
| 17 | 1 | 524 | BCR | C33-C5-C6 | -3.63 | 120.45 | 124.53 |
| 14 | c | 507 | CLA | CMB-C2B-C1B | -3.63 | 122.88 | 128.46 |
| 21 | H | 1852 | SQD | O9-S-O7 | -3.63 | 101.38 | 113.95 |
| 21 | f | 1852 | SQD | O9-S-O7 | -3.63 | 101.38 | 113.95 |
| 14 | U | 1105 | CLA | CBC-CAC-C3C | 3.63 | 122.44 | 112.43 |
| 14 | G | 1022 | CLA | C1B-CHB-C4A | -3.63 | 122.93 | 130.12 |
| 17 | 2 | 522 | BCR | C7-C8-C9 | -3.63 | 120.75 | 126.23 |
| 14 | m | 1105 | CLA | CBC-CAC-C3C | 3.63 | 122.44 | 112.43 |
| 14 | A | 1022 | CLA | C1B-CHB-C4A | -3.63 | 122.93 | 130.12 |
| 17 | S | 4018 | BCR | C27-C26-C25 | -3.63 | 117.46 | 122.73 |
| 17 | Y | 523 | BCR | C16-C17-C18 | -3.63 | 122.13 | 127.31 |
| 17 | f | 4006 | BCR | C20-C21-C22 | -3.63 | 122.13 | 127.31 |
| 14 | H | 1206 | CLA | CMB-C2B-C3B | 3.63 | 131.47 | 124.68 |
| 14 | G | 1132 | CLA | O2D-CGD-O1D | -3.62 | 116.75 | 123.84 |
| 14 | e | 1125 | CLA | CMB-C2B-C3B | 3.62 | 131.46 | 124.68 |
| 14 | 6 | 517 | CLA | CMB-C2B-C1B | -3.62 | 122.89 | 128.46 |
| 17 | 3 | 521 | BCR | C28-C27-C26 | -3.62 | 107.61 | 114.08 |
| 14 | A | 1106 | CLA | CMB-C2B-C3B | 3.62 | 131.46 | 124.68 |
| 17 | H | 4005 | BCR | C15-C14-C13 | -3.62 | 122.14 | 127.31 |
| 17 | q | 524 | BCR | C33-C5-C6 | -3.62 | 120.46 | 124.53 |
| 17 | H | 4006 | BCR | C20-C21-C22 | -3.62 | 122.14 | 127.31 |
| 17 | Y | 524 | BCR | C33-C5-C6 | -3.62 | 120.46 | 124.53 |
| 14 | A | 1132 | CLA | O2D-CGD-O1D | -3.62 | 116.76 | 123.84 |
| 14 | 3 | 508 | CLA | CMB-C2B-C3B | 3.62 | 131.45 | 124.68 |
| 14 | e | 1132 | CLA | O2D-CGD-O1D | -3.62 | 116.77 | 123.84 |
| 14 | v | 517 | CLA | CMB-C2B-C1B | -3.62 | 122.91 | 128.46 |
| 14 | c | 508 | CLA | CMB-C2B-C3B | 3.62 | 131.44 | 124.68 |
| 21 | B | 1852 | SQD | C1-O5-C5 | 3.62 | 120.78 | 113.69 |
| 17 | V | 4219 | BCR | C10-C11-C12 | -3.61 | 111.94 | 123.22 |
| 14 | u | 510 | CLA | CMB-C2B-C1B | -3.61 | 122.91 | 128.46 |
| 14 | 5 | 508 | CLA | CMB-C2B-C3B | 3.61 | 131.44 | 124.68 |
| 17 | L | 4219 | BCR | C10-C11-C12 | -3.61 | 111.94 | 123.22 |
| 14 | G | 1106 | CLA | CMB-C2B-C3B | 3.61 | 131.44 | 124.68 |
| 14 | c | 510 | CLA | CMB-C2B-C1B | -3.61 | 122.91 | 128.46 |
| 14 | A | 1111 | CLA | CMB-C2B-C3B | 3.61 | 131.44 | 124.68 |
| 14 | G | 1129 | CLA | O2D-CGD-O1D | -3.61 | 116.78 | 123.84 |
| 14 | v | 507 | CLA | CMB-C2B-C1B | -3.61 | 122.91 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | f | 1852 | SQD | C1-O5-C5 | 3.61 | 120.77 | 113.69 |
| 14 | r | 501 | CLA | CMB-C2B-C1B | -3.61 | 122.92 | 128.46 |
| 14 | 2 | 501 | CLA | CMB-C2B-C1B | -3.61 | 122.92 | 128.46 |
| 17 | H | 4017 | BCR | C34-C9-C8 | 3.61 | 123.76 | 118.08 |
| 17 | b | 522 | BCR | C24-C23-C22 | -3.61 | 120.78 | 126.23 |
| 17 | r | 522 | BCR | C7-C8-C9 | -3.61 | 120.78 | 126.23 |
| 14 | G | 1111 | CLA | CMB-C2B-C3B | 3.61 | 131.43 | 124.68 |
| 14 | v | 501 | CLA | CMB-C2B-C1B | -3.60 | 122.92 | 128.46 |
| 14 | e | 1106 | CLA | CMB-C2B-C3B | 3.60 | 131.42 | 124.68 |
| 14 | s | 508 | CLA | CMB-C2B-C3B | 3.60 | 131.42 | 124.68 |
| 17 | 4 | 521 | BCR | C11-C10-C9 | -3.60 | 122.17 | 127.31 |
| 14 | u | 508 | CLA | CMB-C2B-C3B | 3.60 | 131.42 | 124.68 |
| 14 | e | 1111 | CLA | CMB-C2B-C3B | 3.60 | 131.42 | 124.68 |
| 14 | A | 1129 | CLA | O2D-CGD-O1D | -3.60 | 116.80 | 123.84 |
| 14 | e | 1129 | CLA | O2D-CGD-O1D | -3.60 | 116.80 | 123.84 |
| 14 | s | 507 | CLA | CMB-C2B-C1B | -3.60 | 122.93 | 128.46 |
| 14 | 6 | 507 | CLA | CMB-C2B-C1B | -3.60 | 122.93 | 128.46 |
| 14 | G | 1125 | CLA | CMB-C2B-C3B | 3.60 | 131.41 | 124.68 |
| 14 | a | 508 | CLA | CMB-C2B-C3B | 3.60 | 131.41 | 124.68 |
| 17 | n | 4219 | BCR | C10-C11-C12 | -3.60 | 111.99 | 123.22 |
| 17 | 1 | 523 | BCR | C16-C17-C18 | -3.60 | 122.18 | 127.31 |
| 14 | 5 | 510 | CLA | CMB-C2B-C1B | -3.60 | 122.94 | 128.46 |
| 17 | 5 | 521 | BCR | C28-C27-C26 | -3.60 | 107.66 | 114.08 |
| 14 | A | 1137 | CLA | CMB-C2B-C1B | -3.60 | 122.94 | 128.46 |
| 14 | 3 | 507 | CLA | CMB-C2B-C1B | -3.59 | 122.94 | 128.46 |
| 14 | 4 | 517 | CLA | CMB-C2B-C1B | -3.59 | 122.94 | 128.46 |
| 17 | B | 4017 | BCR | C34-C9-C8 | 3.59 | 123.74 | 118.08 |
| 14 | d | 507 | CLA | CMB-C2B-C1B | -3.59 | 122.94 | 128.46 |
| 14 | A | 1115 | CLA | CMB-C2B-C3B | 3.59 | 131.40 | 124.68 |
| 14 | A | 1125 | CLA | CMB-C2B-C3B | 3.59 | 131.40 | 124.68 |
| 17 | f | 4017 | BCR | C34-C9-C8 | 3.59 | 123.73 | 118.08 |
| 17 | H | 4009 | BCR | C24-C23-C22 | -3.59 | 120.81 | 126.23 |
| 17 | f | 4009 | BCR | C24-C23-C22 | -3.59 | 120.81 | 126.23 |
| 17 | B | 4009 | BCR | C24-C23-C22 | -3.59 | 120.81 | 126.23 |
| 17 | B | 4005 | BCR | C15-C14-C13 | -3.59 | 122.19 | 127.31 |
| 17 | f | 4017 | BCR | C8-C9-C10 | -3.59 | 113.44 | 118.94 |
| 14 | b | 517 | CLA | CMB-C2B-C1B | -3.59 | 122.95 | 128.46 |
| 17 | c | 521 | BCR | C28-C27-C26 | -3.59 | 107.67 | 114.08 |
| 14 | A | 1011 | CLA | CMB-C2B-C1B | -3.58 | 122.95 | 128.46 |
| 14 | G | 1121 | CLA | CMB-C2B-C1B | -3.58 | 122.96 | 128.46 |
| 14 | e | 1011 | CLA | CMB-C2B-C1B | -3.58 | 122.96 | 128.46 |
| 14 | b | 511 | CLA | CMB-C2B-C3B | 3.58 | 131.38 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | d | 509 | CLA | CMB-C2B-C3B | 3.58 | 131.38 | 124.68 |
| 17 | 4 | 522 | BCR | C24-C23-C22 | -3.58 | 120.82 | 126.23 |
| 17 | t | 521 | BCR | C11-C10-C9 | -3.58 | 122.20 | 127.31 |
| 14 | a | 507 | CLA | CMB-C2B-C1B | -3.58 | 122.96 | 128.46 |
| 14 | e | 1137 | CLA | CMB-C2B-C1B | -3.58 | 122.96 | 128.46 |
| 14 | t | 517 | CLA | CMB-C2B-C1B | -3.58 | 122.96 | 128.46 |
| 17 | H | 4017 | BCR | C8-C9-C10 | -3.58 | 113.45 | 118.94 |
| 14 | G | 1115 | CLA | CMB-C2B-C3B | 3.58 | 131.37 | 124.68 |
| 17 | 5 | 524 | BCR | C33-C5-C6 | -3.58 | 120.51 | 124.53 |
| 17 | u | 524 | BCR | C33-C5-C6 | -3.58 | 120.51 | 124.53 |
| 17 | u | 521 | BCR | C28-C27-C26 | -3.58 | 107.69 | 114.08 |
| 14 | u | 505 | CLA | CMB-C2B-C1B | -3.57 | 122.97 | 128.46 |
| 14 | e | 1115 | CLA | CMB-C2B-C3B | 3.57 | 131.36 | 124.68 |
| 17 | f | 4005 | BCR | C15-C14-C13 | -3.57 | 122.21 | 127.31 |
| 14 | v | 504 | CLA | CMB-C2B-C3B | 3.57 | 131.36 | 124.68 |
| 14 | 4 | 511 | CLA | CMB-C2B-C3B | 3.57 | 131.35 | 124.68 |
| 14 | e | 1118 | CLA | CMB-C2B-C1B | -3.57 | 122.98 | 128.46 |
| 14 | e | 1121 | CLA | CMB-C2B-C1B | -3.57 | 122.98 | 128.46 |
| 17 | t | 522 | BCR | C24-C23-C22 | -3.57 | 120.85 | 126.23 |
| 14 | d | 504 | CLA | CMB-C2B-C3B | 3.57 | 131.35 | 124.68 |
| 14 | c | 505 | CLA | CMB-C2B-C1B | -3.57 | 122.98 | 128.46 |
| 14 | A | 1118 | CLA | CMB-C2B-C1B | -3.56 | 122.98 | 128.46 |
| 17 | v | 521 | BCR | C20-C21-C22 | -3.56 | 122.22 | 127.31 |
| 17 | q | 523 | BCR | C16-C17-C18 | -3.56 | 122.22 | 127.31 |
| 17 | c | 524 | BCR | C33-C5-C6 | -3.56 | 120.53 | 124.53 |
| 14 | 4 | 509 | CLA | CMB-C2B-C3B | 3.56 | 131.34 | 124.68 |
| 17 | L | 4219 | BCR | C28-C27-C26 | -3.56 | 107.72 | 114.08 |
| 17 | 6 | 521 | BCR | C20-C21-C22 | -3.56 | 122.23 | 127.31 |
| 14 | A | 1121 | CLA | CMB-C2B-C1B | -3.56 | 122.99 | 128.46 |
| 17 | V | 4219 | BCR | C28-C27-C26 | -3.56 | 107.72 | 114.08 |
| 17 | B | 4017 | BCR | C8-C9-C10 | -3.56 | 113.48 | 118.94 |
| 14 | A | 1109 | CLA | CMB-C2B-C3B | 3.56 | 131.34 | 124.68 |
| 14 | t | 511 | CLA | CMB-C2B-C3B | 3.56 | 131.34 | 124.68 |
| 14 | G | 1109 | CLA | CMB-C2B-C3B | 3.56 | 131.34 | 124.68 |
| 17 | 6 | 522 | BCR | C7-C8-C9 | -3.56 | 120.86 | 126.23 |
| 17 | H | 4010 | BCR | C38-C26-C25 | -3.56 | 120.53 | 124.53 |
| 14 | l | 1303 | CLA | CMB-C2B-C1B | -3.56 | 123.00 | 128.46 |
| 14 | H | 1220 | CLA | CAA-C2A-C1A | -3.56 | 100.32 | 111.97 |
| 14 | 2 | 507 | CLA | CMB-C2B-C3B | 3.56 | 131.33 | 124.68 |
| 14 | T | 1303 | CLA | CMB-C2B-C1B | -3.56 | 123.00 | 128.46 |
| 14 | s | 505 | CLA | CMB-C2B-C1B | -3.56 | 123.00 | 128.46 |
| 14 | u | 516 | CLA | CMB-C2B-C1B | -3.56 | 123.00 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | L | 4019 | BCR | C15-C14-C13 | -3.56 | 122.23 | 127.31 |
| 14 | 6 | 509 | CLA | CMB-C2B-C3B | 3.56 | 131.33 | 124.68 |
| 17 | v | 521 | BCR | C3-C4-C5 | -3.56 | 107.73 | 114.08 |
| 14 | 6 | 504 | CLA | CMB-C2B-C3B | 3.55 | 131.33 | 124.68 |
| 14 | r | 507 | CLA | CMB-C2B-C3B | 3.55 | 131.33 | 124.68 |
| 14 | v | 509 | CLA | CMB-C2B-C3B | 3.55 | 131.32 | 124.68 |
| 14 | J | 1303 | CLA | CMB-C2B-C1B | -3.55 | 123.01 | 128.46 |
| 14 | B | 1220 | CLA | CAA-C2A-C1A | -3.55 | 100.34 | 111.97 |
| 14 | G | 1011 | CLA | CMB-C2B-C1B | -3.55 | 123.01 | 128.46 |
| 14 | b | 509 | CLA | CMB-C2B-C3B | 3.55 | 131.32 | 124.68 |
| 17 | s | 523 | BCR | C7-C8-C9 | -3.55 | 120.87 | 126.23 |
| 14 | a | 505 | CLA | CMB-C2B-C1B | -3.55 | 123.01 | 128.46 |
| 14 | f | 1220 | CLA | CAA-C2A-C1A | -3.55 | 100.35 | 111.97 |
| 14 | Z | 507 | CLA | CMB-C2B-C3B | 3.55 | 131.31 | 124.68 |
| 17 | n | 4219 | BCR | C28-C27-C26 | -3.55 | 107.74 | 114.08 |
| 14 | 3 | 505 | CLA | CMB-C2B-C1B | -3.55 | 123.01 | 128.46 |
| 14 | 4 | 508 | CLA | CMB-C2B-C3B | 3.54 | 131.31 | 124.68 |
| 17 | B | 4009 | BCR | C7-C8-C9 | -3.54 | 120.88 | 126.23 |
| 14 | e | 1109 | CLA | CMB-C2B-C3B | 3.54 | 131.31 | 124.68 |
| 17 | V | 4019 | BCR | C15-C14-C13 | -3.54 | 122.25 | 127.31 |
| 14 | B | 1216 | CLA | O2A-CGA-O1A | -3.54 | 114.65 | 123.59 |
| 17 | d | 522 | BCR | C7-C8-C9 | -3.54 | 120.88 | 126.23 |
| 14 | t | 508 | CLA | CMB-C2B-C3B | 3.54 | 131.31 | 124.68 |
| 17 | v | 522 | BCR | C7-C8-C9 | -3.54 | 120.88 | 126.23 |
| 14 | f | 1216 | CLA | O2A-CGA-O1A | -3.54 | 114.65 | 123.59 |
| 14 | G | 1110 | CLA | CMB-C2B-C1B | -3.54 | 123.02 | 128.46 |
| 14 | H | 1216 | CLA | O2A-CGA-O1A | -3.54 | 114.66 | 123.59 |
| 14 | v | 518 | CLA | CMB-C2B-C1B | -3.54 | 123.02 | 128.46 |
| 17 | d | 521 | BCR | C20-C21-C22 | -3.54 | 122.26 | 127.31 |
| 17 | 6 | 521 | BCR | C3-C4-C5 | -3.54 | 107.76 | 114.08 |
| 17 | 3 | 523 | BCR | C7-C8-C9 | -3.54 | 120.89 | 126.23 |
| 14 | c | 516 | CLA | CMB-C2B-C1B | -3.54 | 123.03 | 128.46 |
| 14 | 5 | 505 | CLA | CMB-C2B-C1B | -3.54 | 123.03 | 128.46 |
| 14 | G | 1118 | CLA | CMB-C2B-C1B | -3.54 | 123.03 | 128.46 |
| 17 | f | 4009 | BCR | C7-C8-C9 | -3.54 | 120.89 | 126.23 |
| 14 | G | 1013 | CLA | CAA-C2A-C1A | -3.54 | 100.39 | 111.97 |
| 14 | e | 1013 | CLA | O2D-CGD-O1D | -3.54 | 116.92 | 123.84 |
| 17 | d | 521 | BCR | C3-C4-C5 | -3.54 | 107.76 | 114.08 |
| 17 | Z | 524 | BCR | C11-C10-C9 | -3.53 | 122.27 | 127.31 |
| 14 | 6 | 518 | CLA | CMB-C2B-C1B | -3.53 | 123.03 | 128.46 |
| 17 | n | 4019 | BCR | C15-C14-C13 | -3.53 | 122.27 | 127.31 |
| 14 | m | 1105 | CLA | O2D-CGD-O1D | -3.53 | 116.93 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | H | 4009 | BCR | C7-C8-C9 | -3.53 | 120.90 | 126.23 |
| 17 | f | 4010 | BCR | C38-C26-C25 | -3.53 | 120.56 | 124.53 |
| 14 | 5 | 516 | CLA | CMB-C2B-C1B | -3.53 | 123.04 | 128.46 |
| 14 | t | 509 | CLA | CMB-C2B-C3B | 3.53 | 131.28 | 124.68 |
| 14 | A | 1013 | CLA | O2D-CGD-O1D | -3.53 | 116.94 | 123.84 |
| 14 | l | 505 | CLA | CMB-C2B-C1B | -3.53 | 123.04 | 128.46 |
| 14 | A | 1013 | CLA | CAA-C2A-C1A | -3.53 | 100.41 | 111.97 |
| 14 | e | 1013 | CLA | CAA-C2A-C1A | -3.53 | 100.41 | 111.97 |
| 17 | l | 521 | BCR | C11-C10-C9 | -3.53 | 122.28 | 127.31 |
| 14 | r | 512 | CLA | CMB-C2B-C1B | -3.53 | 123.04 | 128.46 |
| 17 | r | 524 | BCR | C11-C10-C9 | -3.53 | 122.28 | 127.31 |
| 14 | e | 1107 | CLA | CMB-C2B-C3B | 3.53 | 131.27 | 124.68 |
| 14 | G | 1138 | CLA | CMB-C2B-C3B | 3.52 | 131.27 | 124.68 |
| 14 | G | 1013 | CLA | O2D-CGD-O1D | -3.52 | 116.95 | 123.84 |
| 14 | Y | 505 | CLA | CMB-C2B-C1B | -3.52 | 123.05 | 128.46 |
| 14 | b | 508 | CLA | CMB-C2B-C3B | 3.52 | 131.27 | 124.68 |
| 14 | b | 519 | CLA | CMB-C2B-C1B | -3.52 | 123.05 | 128.46 |
| 14 | d | 518 | CLA | CMB-C2B-C1B | -3.52 | 123.05 | 128.46 |
| 14 | q | 505 | CLA | CMB-C2B-C1B | -3.52 | 123.05 | 128.46 |
| 17 | B | 4010 | BCR | C38-C26-C25 | -3.52 | 120.57 | 124.53 |
| 14 | K | 1105 | CLA | O2D-CGD-O1D | -3.52 | 116.96 | 123.84 |
| 14 | G | 1123 | CLA | O2D-CGD-O1D | -3.52 | 116.96 | 123.84 |
| 14 | 2 | 512 | CLA | CMB-C2B-C1B | -3.52 | 123.06 | 128.46 |
| 14 | d | 505 | CLA | CMB-C2B-C3B | 3.52 | 131.26 | 124.68 |
| 14 | A | 1110 | CLA | CMB-C2B-C1B | -3.52 | 123.06 | 128.46 |
| 14 | A | 1123 | CLA | O2D-CGD-O1D | -3.52 | 116.97 | 123.84 |
| 14 | Z | 512 | CLA | CMB-C2B-C1B | -3.52 | 123.06 | 128.46 |
| 14 | e | 1110 | CLA | CMB-C2B-C1B | -3.52 | 123.06 | 128.46 |
| 14 | A | 1138 | CLA | CMB-C2B-C3B | 3.51 | 131.25 | 124.68 |
| 17 | a | 523 | BCR | C7-C8-C9 | -3.51 | 120.92 | 126.23 |
| 17 | c | 521 | BCR | C3-C4-C5 | -3.51 | 107.80 | 114.08 |
| 17 | 2 | 524 | BCR | C11-C10-C9 | -3.51 | 122.30 | 127.31 |
| 14 | Z | 508 | CLA | CMB-C2B-C3B | 3.51 | 131.25 | 124.68 |
| 14 | 4 | 519 | CLA | CMB-C2B-C1B | -3.51 | 123.07 | 128.46 |
| 14 | U | 1105 | CLA | O2D-CGD-O1D | -3.51 | 116.97 | 123.84 |
| 14 | 2 | 517 | CLA | CMB-C2B-C1B | -3.51 | 123.07 | 128.46 |
| 14 | a | 511 | CLA | CMB-C2B-C3B | 3.51 | 131.24 | 124.68 |
| 14 | 2 | 505 | CLA | CMB-C2B-C3B | 3.51 | 131.24 | 124.68 |
| 14 | s | 511 | CLA | CMB-C2B-C3B | 3.51 | 131.24 | 124.68 |
| 14 | r | 505 | CLA | CMB-C2B-C3B | 3.51 | 131.24 | 124.68 |
| 14 | e | 1123 | CLA | O2D-CGD-O1D | -3.50 | 116.99 | 123.84 |
| 14 | 3 | 511 | CLA | CMB-C2B-C3B | 3.50 | 131.24 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | r | 510 | CLA | CMB-C2B-C3B | 3.50 | 131.24 | 124.68 |
| 14 | e | 1138 | CLA | CMB-C2B-C3B | 3.50 | 131.23 | 124.68 |
| 14 | r | 508 | CLA | CMB-C2B-C3B | 3.50 | 131.23 | 124.68 |
| 21 | s | 822 | SQD | O9-S-C6 | 3.50 | 111.10 | 106.94 |
| 17 | 5 | 521 | BCR | C3-C4-C5 | -3.50 | 107.83 | 114.08 |
| 14 | Z | 505 | CLA | CMB-C2B-C3B | 3.50 | 131.23 | 124.68 |
| 14 | 2 | 508 | CLA | CMB-C2B-C3B | 3.50 | 131.23 | 124.68 |
| 14 | r | 517 | CLA | CMB-C2B-C1B | -3.50 | 123.09 | 128.46 |
| 14 | 2 | 506 | CLA | CMB-C2B-C1B | -3.50 | 123.09 | 128.46 |
| 17 | u | 521 | BCR | C3-C4-C5 | -3.50 | 107.83 | 114.08 |
| 14 | 2 | 510 | CLA | CMB-C2B-C3B | 3.50 | 131.22 | 124.68 |
| 17 | q | 521 | BCR | C11-C10-C9 | -3.50 | 122.32 | 127.31 |
| 21 | 3 | 822 | SQD | O9-S-C6 | 3.50 | 111.09 | 106.94 |
| 17 | f | 4014 | BCR | C16-C15-C14 | -3.49 | 116.31 | 123.47 |
| 17 | n | 4219 | BCR | C3-C4-C5 | -3.49 | 107.84 | 114.08 |
| 17 | Y | 521 | BCR | C11-C10-C9 | -3.49 | 122.32 | 127.31 |
| 17 | A | 4007 | BCR | C11-C10-C9 | -3.49 | 122.32 | 127.31 |
| 14 | Z | 517 | CLA | CMB-C2B-C1B | -3.49 | 123.10 | 128.46 |
| 17 | H | 4014 | BCR | C16-C15-C14 | -3.49 | 116.32 | 123.47 |
| 14 | d | 501 | CLA | O2D-CGD-O1D | -3.49 | 117.01 | 123.84 |
| 14 | 4 | 507 | CLA | CMB-C2B-C1B | -3.49 | 123.10 | 128.46 |
| 14 | A | 1107 | CLA | CMB-C2B-C3B | 3.49 | 131.21 | 124.68 |
| 17 | G | 4007 | BCR | C11-C10-C9 | -3.49 | 122.33 | 127.31 |
| 17 | t | 522 | BCR | C28-C27-C26 | -3.49 | 107.84 | 114.08 |
| 14 | G | 1107 | CLA | CMB-C2B-C3B | 3.49 | 131.21 | 124.68 |
| 14 | r | 511 | CLA | CMB-C2B-C3B | 3.49 | 131.21 | 124.68 |
| 17 | 4 | 523 | BCR | C15-C16-C17 | -3.49 | 116.33 | 123.47 |
| 14 | 2 | 511 | CLA | CMB-C2B-C3B | 3.49 | 131.21 | 124.68 |
| 15 | f | 2002 | PQN | C14-C13-C15 | -3.49 | 109.40 | 115.27 |
| 17 | b | 523 | BCR | C15-C16-C17 | -3.49 | 116.33 | 123.47 |
| 14 | 6 | 501 | CLA | O2D-CGD-O1D | -3.49 | 117.02 | 123.84 |
| 21 | d | 822 | SQD | O9-S-C6 | 3.49 | 111.08 | 106.94 |
| 14 | Z | 511 | CLA | CMB-C2B-C3B | 3.48 | 131.20 | 124.68 |
| 14 | 4 | 501 | CLA | CMB-C2B-C1B | -3.48 | 123.11 | 128.46 |
| 21 | a | 822 | SQD | O9-S-C6 | 3.48 | 111.08 | 106.94 |
| 21 | r | 822 | SQD | O9-S-C6 | 3.48 | 111.08 | 106.94 |
| 14 | v | 503 | CLA | CMB-C2B-C1B | -3.48 | 123.11 | 128.46 |
| 14 | v | 505 | CLA | CMB-C2B-C3B | 3.48 | 131.20 | 124.68 |
| 17 | 5 | 524 | BCR | C7-C8-C9 | -3.48 | 120.97 | 126.23 |
| 17 | H | 4005 | BCR | C24-C23-C22 | -3.48 | 120.97 | 126.23 |
| 17 | B | 4014 | BCR | C16-C15-C14 | -3.48 | 116.34 | 123.47 |
| 14 | d | 503 | CLA | CMB-C2B-C1B | -3.48 | 123.11 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1204 | CLA | CMB-C2B-C3B | 3.48 | 131.19 | 124.68 |
| 14 | r | 506 | CLA | CMB-C2B-C1B | -3.48 | 123.11 | 128.46 |
| 17 | 1 | 521 | BCR | C28-C27-C26 | -3.48 | 107.86 | 114.08 |
| 14 | 6 | 505 | CLA | CMB-C2B-C3B | 3.48 | 131.19 | 124.68 |
| 17 | c | 524 | BCR | C7-C8-C9 | -3.48 | 120.97 | 126.23 |
| 21 | Z | 822 | SQD | O9-S-C6 | 3.48 | 111.08 | 106.94 |
| 14 | t | 507 | CLA | CMB-C2B-C1B | -3.48 | 123.11 | 128.46 |
| 17 | t | 523 | BCR | C15-C16-C17 | -3.48 | 116.34 | 123.47 |
| 17 | q | 521 | BCR | C28-C27-C26 | -3.48 | 107.86 | 114.08 |
| 15 | B | 2002 | PQN | C14-C13-C15 | -3.48 | 109.42 | 115.27 |
| 14 | Z | 510 | CLA | CMB-C2B-C3B | 3.48 | 131.19 | 124.68 |
| 14 | 3 | 504 | CLA | CMB-C2B-C3B | 3.48 | 131.19 | 124.68 |
| 17 | e | 4007 | BCR | C16-C17-C18 | -3.48 | 122.34 | 127.31 |
| 21 | 6 | 822 | SQD | O9-S-C6 | 3.48 | 111.07 | 106.94 |
| 14 | Z | 506 | CLA | CMB-C2B-C1B | -3.48 | 123.12 | 128.46 |
| 14 | H | 1204 | CLA | CMB-C2B-C3B | 3.48 | 131.18 | 124.68 |
| 14 | H | 1021 | CLA | CMB-C2B-C1B | -3.48 | 123.12 | 128.46 |
| 14 | b | 507 | CLA | CMB-C2B-C1B | -3.48 | 123.12 | 128.46 |
| 15 | H | 2002 | PQN | C14-C13-C15 | -3.48 | 109.42 | 115.27 |
| 17 | G | 4007 | BCR | C16-C17-C18 | -3.47 | 122.35 | 127.31 |
| 14 | t | 501 | CLA | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 14 | v | 501 | CLA | O2D-CGD-O1D | -3.47 | 117.05 | 123.84 |
| 17 | b | 522 | BCR | C28-C27-C26 | -3.47 | 107.88 | 114.08 |
| 17 | Y | 521 | BCR | C28-C27-C26 | -3.47 | 107.88 | 114.08 |
| 14 | d | 506 | CLA | CMB-C2B-C3B | 3.47 | 131.17 | 124.68 |
| 17 | L | 4219 | BCR | C3-C4-C5 | -3.47 | 107.88 | 114.08 |
| 17 | B | 4005 | BCR | C24-C23-C22 | -3.47 | 120.99 | 126.23 |
| 14 | t | 519 | CLA | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 21 | v | 822 | SQD | O7-S-C6 | 3.47 | 111.06 | 106.94 |
| 14 | v | 506 | CLA | CMB-C2B-C3B | 3.47 | 131.17 | 124.68 |
| 21 | 2 | 822 | SQD | O9-S-C6 | 3.47 | 111.06 | 106.94 |
| 14 | b | 501 | CLA | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 14 | f | 1021 | CLA | CMB-C2B-C1B | -3.47 | 123.13 | 128.46 |
| 14 | s | 517 | CLA | CMB-C2B-C1B | -3.47 | 123.14 | 128.46 |
| 17 | Z | 523 | BCR | C7-C8-C9 | -3.47 | 121.00 | 126.23 |
| 14 | 6 | 503 | CLA | CMB-C2B-C1B | -3.47 | 123.14 | 128.46 |
| 17 | e | 4007 | BCR | C24-C23-C22 | -3.46 | 121.00 | 126.23 |
| 17 | A | 4002 | BCR | C24-C23-C22 | -3.46 | 121.00 | 126.23 |
| 14 | B | 1021 | CLA | CMB-C2B-C1B | -3.46 | 123.14 | 128.46 |
| 17 | u | 524 | BCR | C7-C8-C9 | -3.46 | 121.00 | 126.23 |
| 14 | a | 504 | CLA | CMB-C2B-C3B | 3.46 | 131.16 | 124.68 |
| 17 | A | 4007 | BCR | C24-C23-C22 | -3.46 | 121.00 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1204 | CLA | CMB-C2B-C3B | 3.46 | 131.16 | 124.68 |
| 17 | 6 | 524 | BCR | C33-C5-C6 | -3.46 | 120.64 | 124.53 |
| 17 | 2 | 523 | BCR | C7-C8-C9 | -3.46 | 121.01 | 126.23 |
| 21 | d | 822 | SQD | O7-S-C6 | 3.46 | 111.05 | 106.94 |
| 17 | 4 | 522 | BCR | C28-C27-C26 | -3.46 | 107.90 | 114.08 |
| 17 | A | 4007 | BCR | C16-C17-C18 | -3.46 | 122.37 | 127.31 |
| 17 | G | 4002 | BCR | C24-C23-C22 | -3.46 | 121.01 | 126.23 |
| 14 | H | 1240 | CLA | CMB-C2B-C3B | 3.46 | 131.15 | 124.68 |
| 21 | v | 822 | SQD | O9-S-C6 | 3.46 | 111.05 | 106.94 |
| 17 | e | 4007 | BCR | C11-C10-C9 | -3.46 | 122.38 | 127.31 |
| 17 | T | 4013 | BCR | C3-C4-C5 | -3.46 | 107.90 | 114.08 |
| 17 | f | 4005 | BCR | C24-C23-C22 | -3.46 | 121.01 | 126.23 |
| 14 | K | 1105 | CLA | CMB-C2B-C1B | -3.46 | 123.15 | 128.46 |
| 14 | 6 | 506 | CLA | CMB-C2B-C3B | 3.46 | 131.14 | 124.68 |
| 17 | V | 4219 | BCR | C3-C4-C5 | -3.45 | 107.91 | 114.08 |
| 14 | s | 504 | CLA | CMB-C2B-C3B | 3.45 | 131.14 | 124.68 |
| 17 | J | 4012 | BCR | C7-C8-C9 | -3.45 | 121.02 | 126.23 |
| 17 | T | 4012 | BCR | C7-C8-C9 | -3.45 | 121.02 | 126.23 |
| 14 | q | 504 | CLA | CMB-C2B-C1B | -3.45 | 123.16 | 128.46 |
| 17 | a | 524 | BCR | C11-C10-C9 | -3.45 | 122.39 | 127.31 |
| 17 | 3 | 522 | BCR | C28-C27-C26 | -3.45 | 107.92 | 114.08 |
| 14 | U | 1105 | CLA | CMB-C2B-C1B | -3.45 | 123.16 | 128.46 |
| 14 | t | 512 | CLA | CMB-C2B-C1B | -3.45 | 123.16 | 128.46 |
| 17 | V | 4219 | BCR | C33-C5-C4 | 3.45 | 120.24 | 113.62 |
| 17 | G | 4007 | BCR | C24-C23-C22 | -3.45 | 121.02 | 126.23 |
| 14 | 3 | 517 | CLA | CMB-C2B-C1B | -3.45 | 123.17 | 128.46 |
| 17 | a | 522 | BCR | C28-C27-C26 | -3.45 | 107.92 | 114.08 |
| 14 | m | 1401 | CLA | CMB-C2B-C3B | 3.45 | 131.13 | 124.68 |
| 21 | 1 | 822 | SQD | O47-C7-C8 | 3.45 | 118.93 | 111.50 |
| 14 | 4 | 512 | CLA | CMB-C2B-C1B | -3.45 | 123.17 | 128.46 |
| 14 | f | 1240 | CLA | CMB-C2B-C3B | 3.45 | 131.12 | 124.68 |
| 17 | s | 524 | BCR | C11-C10-C9 | -3.45 | 122.39 | 127.31 |
| 21 | 6 | 822 | SQD | O7-S-C6 | 3.44 | 111.03 | 106.94 |
| 17 | b | 522 | BCR | C7-C8-C9 | -3.44 | 121.03 | 126.23 |
| 17 | e | 4002 | BCR | C24-C23-C22 | -3.44 | 121.03 | 126.23 |
| 17 | J | 4013 | BCR | C3-C4-C5 | -3.44 | 107.93 | 114.08 |
| 14 | B | 1240 | CLA | CMB-C2B-C3B | 3.44 | 131.12 | 124.68 |
| 14 | v | 508 | CLA | CMB-C2B-C3B | 3.44 | 131.12 | 124.68 |
| 14 | H | 1220 | CLA | CAA-CBA-CGA | -3.44 | 103.19 | 113.25 |
| 14 | b | 512 | CLA | CMB-C2B-C1B | -3.44 | 123.17 | 128.46 |
| 17 | l | 4012 | BCR | C7-C8-C9 | -3.44 | 121.03 | 126.23 |
| 17 | L | 4219 | BCR | C33-C5-C4 | 3.44 | 120.23 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | u | 517 | CLA | CMB-C2B-C1B | -3.44 | 123.17 | 128.46 |
| 17 | e | 4001 | BCR | C15-C16-C17 | -3.44 | 116.42 | 123.47 |
| 17 | 3 | 524 | BCR | C11-C10-C9 | -3.44 | 122.40 | 127.31 |
| 14 | 5 | 517 | CLA | CMB-C2B-C1B | -3.44 | 123.18 | 128.46 |
| 14 | m | 1105 | CLA | CMB-C2B-C1B | -3.44 | 123.18 | 128.46 |
| 14 | 6 | 508 | CLA | CMB-C2B-C3B | 3.44 | 131.11 | 124.68 |
| 14 | d | 508 | CLA | CMB-C2B-C3B | 3.44 | 131.11 | 124.68 |
| 17 | L | 4020 | BCR | C16-C17-C18 | -3.44 | 122.41 | 127.31 |
| 17 | V | 4019 | BCR | C16-C17-C18 | -3.44 | 122.41 | 127.31 |
| 17 | A | 4001 | BCR | C15-C16-C17 | -3.44 | 116.44 | 123.47 |
| 17 | n | 4219 | BCR | C33-C5-C4 | 3.43 | 120.21 | 113.62 |
| 21 | Y | 822 | SQD | O47-C7-C8 | 3.43 | 118.90 | 111.50 |
| 17 | l | 4013 | BCR | C3-C4-C5 | -3.43 | 107.95 | 114.08 |
| 17 | J | 4015 | BCR | C11-C10-C9 | -3.43 | 122.41 | 127.31 |
| 17 | n | 4020 | BCR | C16-C17-C18 | -3.43 | 122.41 | 127.31 |
| 14 | B | 1220 | CLA | CAA-CBA-CGA | -3.43 | 103.22 | 113.25 |
| 14 | K | 1401 | CLA | CMB-C2B-C3B | 3.43 | 131.10 | 124.68 |
| 17 | d | 524 | BCR | C33-C5-C6 | -3.43 | 120.67 | 124.53 |
| 17 | G | 4007 | BCR | C27-C26-C25 | -3.43 | 117.75 | 122.73 |
| 21 | q | 822 | SQD | O47-C7-C8 | 3.43 | 118.89 | 111.50 |
| 17 | r | 523 | BCR | C7-C8-C9 | -3.43 | 121.05 | 126.23 |
| 17 | A | 4002 | BCR | C16-C15-C14 | -3.43 | 116.45 | 123.47 |
| 17 | G | 4002 | BCR | C16-C15-C14 | -3.43 | 116.45 | 123.47 |
| 14 | f | 1220 | CLA | CAA-CBA-CGA | -3.43 | 103.23 | 113.25 |
| 17 | T | 4015 | BCR | C11-C10-C9 | -3.43 | 122.42 | 127.31 |
| 14 | H | 1216 | CLA | CMB-C2B-C1B | -3.43 | 123.19 | 128.46 |
| 14 | Y | 513 | CLA | CMB-C2B-C3B | 3.43 | 131.09 | 124.68 |
| 14 | l | 504 | CLA | CMB-C2B-C1B | -3.43 | 123.19 | 128.46 |
| 14 | a | 517 | CLA | CMB-C2B-C1B | -3.43 | 123.20 | 128.46 |
| 17 | v | 524 | BCR | C33-C5-C6 | -3.43 | 120.68 | 124.53 |
| 17 | s | 522 | BCR | C28-C27-C26 | -3.42 | 107.96 | 114.08 |
| 14 | c | 517 | CLA | CMB-C2B-C1B | -3.42 | 123.20 | 128.46 |
| 17 | e | 4007 | BCR | C27-C26-C25 | -3.42 | 117.76 | 122.73 |
| 14 | U | 1401 | CLA | CMB-C2B-C3B | 3.42 | 131.08 | 124.68 |
| 17 | a | 524 | BCR | C33-C5-C6 | -3.42 | 120.69 | 124.53 |
| 17 | l | 4015 | BCR | C11-C10-C9 | -3.42 | 122.43 | 127.31 |
| 17 | V | 4020 | BCR | C16-C17-C18 | -3.42 | 122.43 | 127.31 |
| 17 | e | 4002 | BCR | C16-C15-C14 | -3.42 | 116.47 | 123.47 |
| 14 | s | 503 | CLA | CMB-C2B-C1B | -3.42 | 123.21 | 128.46 |
| 17 | 3 | 524 | BCR | C33-C5-C6 | -3.42 | 120.69 | 124.53 |
| 17 | G | 4001 | BCR | C15-C16-C17 | -3.41 | 116.48 | 123.47 |
| 14 | B | 1216 | CLA | CMB-C2B-C1B | -3.41 | 123.22 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | Y | 516 | CLA | CMB-C2B-C1B | -3.41 | 123.22 | 128.46 |
| 14 | t | 507 | CLA | O2D-CGD-O1D | -3.41 | 117.17 | 123.84 |
| 17 | 4 | 522 | BCR | C7-C8-C9 | -3.41 | 121.08 | 126.23 |
| 14 | 1 | 516 | CLA | CMB-C2B-C1B | -3.41 | 123.22 | 128.46 |
| 14 | H | 1204 | CLA | O2D-CGD-O1D | -3.41 | 117.17 | 123.84 |
| 17 | A | 4007 | BCR | C27-C26-C25 | -3.41 | 117.78 | 122.73 |
| 14 | q | 516 | CLA | CMB-C2B-C1B | -3.41 | 123.22 | 128.46 |
| 14 | Y | 504 | CLA | CMB-C2B-C1B | -3.41 | 123.23 | 128.46 |
| 17 | 3 | 524 | BCR | C24-C23-C22 | -3.41 | 121.09 | 126.23 |
| 14 | e | 1112 | CLA | CMB-C2B-C3B | 3.41 | 131.05 | 124.68 |
| 14 | H | 1218 | CLA | CMB-C2B-C1B | -3.41 | 123.23 | 128.46 |
| 21 | Y | 822 | SQD | C4-C3-C2 | 3.41 | 116.77 | 110.82 |
| 21 | 1 | 822 | SQD | C4-C3-C2 | 3.41 | 116.77 | 110.82 |
| 14 | r | 516 | CLA | CMB-C2B-C1B | -3.41 | 123.23 | 128.46 |
| 14 | A | 1112 | CLA | CMB-C2B-C3B | 3.41 | 131.05 | 124.68 |
| 17 | s | 524 | BCR | C24-C23-C22 | -3.40 | 121.09 | 126.23 |
| 14 | G | 1112 | CLA | CMB-C2B-C3B | 3.40 | 131.05 | 124.68 |
| 14 | q | 513 | CLA | CMB-C2B-C3B | 3.40 | 131.05 | 124.68 |
| 14 | 1 | 518 | CLA | CMB-C2B-C1B | -3.40 | 123.23 | 128.46 |
| 17 | L | 4019 | BCR | C16-C17-C18 | -3.40 | 122.45 | 127.31 |
| 14 | b | 507 | CLA | O2D-CGD-O1D | -3.40 | 117.18 | 123.84 |
| 14 | f | 1205 | CLA | CMB-C2B-C1B | -3.40 | 123.23 | 128.46 |
| 17 | 3 | 523 | BCR | C16-C17-C18 | -3.40 | 122.45 | 127.31 |
| 17 | n | 4019 | BCR | C16-C17-C18 | -3.40 | 122.45 | 127.31 |
| 14 | G | 1139 | CLA | CMB-C2B-C3B | 3.40 | 131.04 | 124.68 |
| 14 | e | 1103 | CLA | CHB-C4A-NA | 3.40 | 129.22 | 124.51 |
| 14 | 4 | 507 | CLA | O2D-CGD-O1D | -3.40 | 117.19 | 123.84 |
| 14 | f | 1216 | CLA | CMB-C2B-C1B | -3.40 | 123.24 | 128.46 |
| 17 | q | 523 | BCR | C28-C27-C26 | -3.40 | 108.01 | 114.08 |
| 17 | c | 523 | BCR | C16-C17-C18 | -3.40 | 122.46 | 127.31 |
| 14 | f | 1204 | CLA | O2D-CGD-O1D | -3.40 | 117.19 | 123.84 |
| 17 | s | 524 | BCR | C33-C5-C6 | -3.40 | 120.71 | 124.53 |
| 17 | a | 523 | BCR | C16-C17-C18 | -3.40 | 122.46 | 127.31 |
| 14 | A | 1103 | CLA | CHB-C4A-NA | 3.40 | 129.21 | 124.51 |
| 17 | t | 522 | BCR | C7-C8-C9 | -3.40 | 121.10 | 126.23 |
| 14 | 1 | 513 | CLA | CMB-C2B-C3B | 3.40 | 131.03 | 124.68 |
| 14 | A | 1139 | CLA | CMB-C2B-C3B | 3.40 | 131.03 | 124.68 |
| 17 | a | 524 | BCR | C24-C23-C22 | -3.40 | 121.10 | 126.23 |
| 14 | 2 | 516 | CLA | CMB-C2B-C1B | -3.40 | 123.25 | 128.46 |
| 17 | 1 | 523 | BCR | C28-C27-C26 | -3.39 | 108.02 | 114.08 |
| 17 | Y | 523 | BCR | C28-C27-C26 | -3.39 | 108.02 | 114.08 |
| 14 | 3 | 503 | CLA | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1139 | CLA | CMB-C2B-C3B | 3.39 | 131.02 | 124.68 |
| 14 | Y | 510 | CLA | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |
| 21 | q | 822 | SQD | C4-C3-C2 | 3.39 | 116.74 | 110.82 |
| 14 | a | 503 | CLA | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |
| 14 | q | 518 | CLA | CMB-C2B-C1B | -3.39 | 123.25 | 128.46 |
| 14 | e | 1140 | CLA | CAA-C2A-C3A | -3.39 | 103.50 | 112.78 |
| 17 | f | 4005 | BCR | C16-C17-C18 | -3.39 | 122.47 | 127.31 |
| 14 | Z | 516 | CLA | CMB-C2B-C1B | -3.39 | 123.26 | 128.46 |
| 14 | Y | 518 | CLA | CMB-C2B-C1B | -3.39 | 123.26 | 128.46 |
| 14 | f | 1227 | CLA | CMB-C2B-C1B | -3.39 | 123.26 | 128.46 |
| 14 | H | 1208 | CLA | CMB-C2B-C3B | 3.39 | 131.01 | 124.68 |
| 14 | B | 1204 | CLA | O2D-CGD-O1D | -3.39 | 117.22 | 123.84 |
| 14 | G | 1124 | CLA | CAA-C2A-C1A | -3.39 | 100.88 | 111.97 |
| 14 | A | 1140 | CLA | CAA-C2A-C3A | -3.38 | 103.51 | 112.78 |
| 14 | H | 1205 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 21 | q | 822 | SQD | C3-C4-C5 | 3.38 | 116.27 | 110.24 |
| 14 | B | 1218 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 17 | u | 522 | BCR | C7-C8-C9 | -3.38 | 121.12 | 126.23 |
| 14 | G | 1140 | CLA | CAA-C2A-C3A | -3.38 | 103.52 | 112.78 |
| 14 | A | 1112 | CLA | CHB-C4A-NA | 3.38 | 129.19 | 124.51 |
| 14 | B | 1205 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 14 | q | 517 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 19 | G | 1849 | LMU | C1'-O5'-C5' | 3.38 | 120.32 | 113.69 |
| 21 | l | 822 | SQD | C3-C4-C5 | 3.38 | 116.27 | 110.24 |
| 17 | A | 4002 | BCR | C15-C14-C13 | -3.38 | 122.49 | 127.31 |
| 14 | Z | 504 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 14 | r | 504 | CLA | CMB-C2B-C1B | -3.38 | 123.27 | 128.46 |
| 19 | A | 1849 | LMU | C1'-O5'-C5' | 3.38 | 120.32 | 113.69 |
| 17 | s | 523 | BCR | C16-C17-C18 | -3.38 | 122.49 | 127.31 |
| 17 | c | 522 | BCR | C28-C27-C26 | -3.38 | 108.05 | 114.08 |
| 14 | l | 510 | CLA | CMB-C2B-C1B | -3.38 | 123.28 | 128.46 |
| 17 | 5 | 523 | BCR | C16-C17-C18 | -3.38 | 122.49 | 127.31 |
| 14 | q | 503 | CLA | CMB-C2B-C1B | -3.37 | 123.28 | 128.46 |
| 17 | G | 4002 | BCR | C15-C14-C13 | -3.37 | 122.50 | 127.31 |
| 14 | G | 1112 | CLA | CHB-C4A-NA | 3.37 | 129.18 | 124.51 |
| 14 | e | 1106 | CLA | O2A-CGA-O1A | -3.37 | 115.08 | 123.59 |
| 21 | L | 5216 | SQD | O9-S-C6 | 3.37 | 110.95 | 106.94 |
| 19 | e | 1849 | LMU | C1'-O5'-C5' | 3.37 | 120.31 | 113.69 |
| 17 | c | 524 | BCR | C16-C17-C18 | -3.37 | 122.50 | 127.31 |
| 14 | f | 1208 | CLA | CMB-C2B-C3B | 3.37 | 130.99 | 124.68 |
| 17 | 5 | 522 | BCR | C7-C8-C9 | -3.37 | 121.14 | 126.23 |
| 17 | u | 522 | BCR | C28-C27-C26 | -3.37 | 108.06 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1103 | CLA | CHB-C4A-NA | 3.37 | 129.17 | 124.51 |
| 14 | A | 1124 | CLA | CAA-C2A-C1A | -3.37 | 100.93 | 111.97 |
| 14 | f | 1218 | CLA | CMB-C2B-C1B | -3.37 | 123.28 | 128.46 |
| 14 | e | 1112 | CLA | CHB-C4A-NA | 3.37 | 129.17 | 124.51 |
| 14 | r | 503 | CLA | CMB-C2B-C3B | 3.37 | 130.98 | 124.68 |
| 17 | 5 | 524 | BCR | C16-C17-C18 | -3.37 | 122.50 | 127.31 |
| 14 | l | 517 | CLA | CMB-C2B-C1B | -3.37 | 123.29 | 128.46 |
| 14 | G | 1106 | CLA | O2A-CGA-O1A | -3.37 | 115.09 | 123.59 |
| 14 | B | 1208 | CLA | CMB-C2B-C3B | 3.37 | 130.98 | 124.68 |
| 14 | B | 1227 | CLA | CMB-C2B-C1B | -3.37 | 123.29 | 128.46 |
| 14 | B | 1221 | CLA | CHB-C4A-NA | 3.37 | 129.17 | 124.51 |
| 17 | a | 523 | BCR | C20-C21-C22 | -3.37 | 122.50 | 127.31 |
| 14 | f | 1221 | CLA | CHB-C4A-NA | 3.37 | 129.17 | 124.51 |
| 17 | e | 4002 | BCR | C15-C14-C13 | -3.37 | 122.50 | 127.31 |
| 14 | q | 510 | CLA | CMB-C2B-C1B | -3.37 | 123.29 | 128.46 |
| 21 | V | 5216 | SQD | O9-S-C6 | 3.37 | 110.94 | 106.94 |
| 17 | B | 4005 | BCR | C16-C17-C18 | -3.37 | 122.51 | 127.31 |
| 14 | H | 1221 | CLA | CHB-C4A-NA | 3.36 | 129.16 | 124.51 |
| 17 | c | 522 | BCR | C7-C8-C9 | -3.36 | 121.15 | 126.23 |
| 14 | A | 1106 | CLA | O2A-CGA-O1A | -3.36 | 115.10 | 123.59 |
| 14 | e | 1124 | CLA | CAA-C2A-C1A | -3.36 | 100.95 | 111.97 |
| 17 | n | 4022 | BCR | C16-C15-C14 | -3.36 | 116.59 | 123.47 |
| 17 | H | 4017 | BCR | C21-C20-C19 | -3.36 | 112.73 | 123.22 |
| 17 | u | 523 | BCR | C16-C17-C18 | -3.36 | 122.51 | 127.31 |
| 17 | 5 | 522 | BCR | C28-C27-C26 | -3.36 | 108.08 | 114.08 |
| 14 | 2 | 504 | CLA | CMB-C2B-C1B | -3.36 | 123.30 | 128.46 |
| 14 | Y | 503 | CLA | CMB-C2B-C1B | -3.36 | 123.30 | 128.46 |
| 14 | t | 518 | CLA | CMB-C2B-C1B | -3.36 | 123.30 | 128.46 |
| 21 | Y | 822 | SQD | C3-C4-C5 | 3.36 | 116.23 | 110.24 |
| 14 | e | 1133 | CLA | CMB-C2B-C3B | 3.36 | 130.96 | 124.68 |
| 14 | G | 1133 | CLA | CMB-C2B-C3B | 3.36 | 130.96 | 124.68 |
| 17 | B | 4017 | BCR | C21-C20-C19 | -3.36 | 112.74 | 123.22 |
| 14 | l | 503 | CLA | CMB-C2B-C1B | -3.36 | 123.31 | 128.46 |
| 17 | u | 524 | BCR | C16-C17-C18 | -3.35 | 122.52 | 127.31 |
| 14 | Z | 503 | CLA | CMB-C2B-C3B | 3.35 | 130.95 | 124.68 |
| 17 | d | 522 | BCR | C28-C27-C26 | -3.35 | 108.09 | 114.08 |
| 14 | 4 | 518 | CLA | CMB-C2B-C1B | -3.35 | 123.31 | 128.46 |
| 17 | d | 522 | BCR | C24-C23-C22 | -3.35 | 121.17 | 126.23 |
| 17 | 3 | 523 | BCR | C20-C21-C22 | -3.35 | 122.53 | 127.31 |
| 14 | b | 518 | CLA | CMB-C2B-C1B | -3.34 | 123.32 | 128.46 |
| 14 | 2 | 503 | CLA | CMB-C2B-C3B | 3.34 | 130.94 | 124.68 |
| 17 | L | 4022 | BCR | C16-C15-C14 | -3.34 | 116.62 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | n | 5216 | SQD | O9-S-C6 | 3.34 | 110.91 | 106.94 |
| 17 | f | 4017 | BCR | C21-C20-C19 | -3.34 | 112.78 | 123.22 |
| 17 | H | 4005 | BCR | C16-C17-C18 | -3.34 | 122.54 | 127.31 |
| 14 | 1 | 512 | CLA | CMB-C2B-C1B | -3.34 | 123.33 | 128.46 |
| 14 | H | 1227 | CLA | CMB-C2B-C1B | -3.34 | 123.33 | 128.46 |
| 14 | A | 1133 | CLA | CMB-C2B-C3B | 3.34 | 130.93 | 124.68 |
| 14 | f | 1214 | CLA | CMB-C2B-C1B | -3.34 | 123.33 | 128.46 |
| 17 | 6 | 522 | BCR | C28-C27-C26 | -3.34 | 108.11 | 114.08 |
| 14 | G | 1138 | CLA | O2D-CGD-O1D | -3.34 | 117.31 | 123.84 |
| 17 | G | 4011 | BCR | C16-C17-C18 | -3.34 | 122.55 | 127.31 |
| 14 | B | 1214 | CLA | CMB-C2B-C1B | -3.34 | 123.34 | 128.46 |
| 14 | 1 | 507 | CLA | CMB-C2B-C3B | 3.34 | 130.92 | 124.68 |
| 14 | Y | 517 | CLA | CMB-C2B-C1B | -3.33 | 123.34 | 128.46 |
| 17 | u | 523 | BCR | C10-C11-C12 | -3.33 | 112.81 | 123.22 |
| 17 | V | 4022 | BCR | C16-C15-C14 | -3.33 | 116.65 | 123.47 |
| 17 | v | 522 | BCR | C24-C23-C22 | -3.33 | 121.20 | 126.23 |
| 19 | l | 5105 | LMU | O5'-C1'-C2' | 3.33 | 117.40 | 110.35 |
| 17 | n | 4020 | BCR | C20-C21-C22 | -3.33 | 122.56 | 127.31 |
| 19 | T | 5105 | LMU | O5'-C1'-C2' | 3.33 | 117.40 | 110.35 |
| 17 | s | 523 | BCR | C20-C21-C22 | -3.33 | 122.56 | 127.31 |
| 17 | V | 4020 | BCR | C20-C21-C22 | -3.33 | 122.56 | 127.31 |
| 19 | J | 5105 | LMU | O5'-C1'-C2' | 3.33 | 117.39 | 110.35 |
| 14 | q | 507 | CLA | CMB-C2B-C3B | 3.33 | 130.90 | 124.68 |
| 17 | 5 | 523 | BCR | C10-C11-C12 | -3.33 | 112.83 | 123.22 |
| 14 | A | 1138 | CLA | O2D-CGD-O1D | -3.33 | 117.33 | 123.84 |
| 14 | q | 512 | CLA | CMB-C2B-C1B | -3.33 | 123.35 | 128.46 |
| 14 | Y | 512 | CLA | CMB-C2B-C1B | -3.32 | 123.35 | 128.46 |
| 14 | s | 501 | CLA | CMB-C2B-C3B | 3.32 | 130.90 | 124.68 |
| 17 | n | 4022 | BCR | C15-C14-C13 | -3.32 | 122.57 | 127.31 |
| 14 | e | 1101 | CLA | CMB-C2B-C1B | -3.32 | 123.36 | 128.46 |
| 17 | A | 4011 | BCR | C16-C17-C18 | -3.32 | 122.57 | 127.31 |
| 17 | c | 523 | BCR | C10-C11-C12 | -3.32 | 112.86 | 123.22 |
| 17 | L | 4020 | BCR | C20-C21-C22 | -3.32 | 122.57 | 127.31 |
| 17 | 6 | 522 | BCR | C24-C23-C22 | -3.32 | 121.22 | 126.23 |
| 14 | a | 501 | CLA | CMB-C2B-C3B | 3.32 | 130.88 | 124.68 |
| 14 | e | 1102 | CLA | O2D-CGD-O1D | -3.31 | 117.36 | 123.84 |
| 14 | A | 1101 | CLA | CMB-C2B-C1B | -3.31 | 123.37 | 128.46 |
| 19 | T | 5105 | LMU | C1'-O5'-C5' | 3.31 | 120.19 | 113.69 |
| 14 | e | 1138 | CLA | O2D-CGD-O1D | -3.31 | 117.36 | 123.84 |
| 17 | v | 522 | BCR | C28-C27-C26 | -3.31 | 108.16 | 114.08 |
| 14 | Y | 507 | CLA | CMB-C2B-C3B | 3.31 | 130.88 | 124.68 |
| 14 | G | 1101 | CLA | CMB-C2B-C1B | -3.31 | 123.37 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | s | 822 | SQD | O48-C23-C24 | 3.31 | 120.07 | 111.38 |
| 14 | t | 503 | CLA | CMB-C2B-C1B | -3.31 | 123.37 | 128.46 |
| 14 | G | 1102 | CLA | O2D-CGD-O1D | -3.31 | 117.36 | 123.84 |
| 14 | H | 1239 | CLA | O2D-CGD-O1D | -3.31 | 117.36 | 123.84 |
| 14 | A | 1102 | CLA | O2D-CGD-O1D | -3.31 | 117.37 | 123.84 |
| 14 | e | 1125 | CLA | C6-C5-C3 | 3.31 | 122.13 | 113.45 |
| 14 | f | 1239 | CLA | O2D-CGD-O1D | -3.31 | 117.37 | 123.84 |
| 14 | 3 | 501 | CLA | CMB-C2B-C3B | 3.31 | 130.87 | 124.68 |
| 17 | e | 4011 | BCR | C16-C17-C18 | -3.31 | 122.59 | 127.31 |
| 14 | B | 1239 | CLA | O2D-CGD-O1D | -3.31 | 117.37 | 123.84 |
| 14 | T | 1302 | CLA | CMB-C2B-C1B | -3.31 | 123.38 | 128.46 |
| 14 | G | 1125 | CLA | C6-C5-C3 | 3.31 | 122.12 | 113.45 |
| 17 | v | 522 | BCR | C15-C16-C17 | -3.31 | 116.70 | 123.47 |
| 17 | r | 523 | BCR | C20-C21-C22 | -3.31 | 122.59 | 127.31 |
| 21 | 3 | 822 | SQD | O48-C23-C24 | 3.30 | 120.05 | 111.38 |
| 21 | a | 822 | SQD | O48-C23-C24 | 3.30 | 120.04 | 111.38 |
| 17 | L | 4022 | BCR | C15-C14-C13 | -3.30 | 122.59 | 127.31 |
| 19 | J | 5105 | LMU | C1'-O5'-C5' | 3.30 | 120.17 | 113.69 |
| 14 | A | 1125 | CLA | C6-C5-C3 | 3.30 | 122.11 | 113.45 |
| 14 | Z | 513 | CLA | CMB-C2B-C1B | -3.30 | 123.39 | 128.46 |
| 14 | G | 1120 | CLA | O2D-CGD-O1D | -3.30 | 117.38 | 123.84 |
| 17 | f | 4005 | BCR | C20-C21-C22 | -3.30 | 122.60 | 127.31 |
| 21 | Y | 822 | SQD | C44-O6-C1 | 3.30 | 120.18 | 113.74 |
| 14 | 2 | 516 | CLA | O2D-CGD-O1D | -3.30 | 117.39 | 123.84 |
| 14 | H | 1214 | CLA | CMB-C2B-C1B | -3.29 | 123.40 | 128.46 |
| 14 | 2 | 513 | CLA | CMB-C2B-C1B | -3.29 | 123.40 | 128.46 |
| 14 | l | 1302 | CLA | CMB-C2B-C1B | -3.29 | 123.40 | 128.46 |
| 14 | G | 1132 | CLA | O2D-CGD-CBD | 3.29 | 117.12 | 111.27 |
| 17 | V | 4022 | BCR | C15-C14-C13 | -3.29 | 122.61 | 127.31 |
| 17 | Y | 522 | BCR | C28-C27-C26 | -3.29 | 108.20 | 114.08 |
| 14 | 4 | 503 | CLA | CMB-C2B-C1B | -3.29 | 123.40 | 128.46 |
| 14 | Z | 516 | CLA | O2D-CGD-O1D | -3.29 | 117.40 | 123.84 |
| 14 | r | 513 | CLA | CMB-C2B-C1B | -3.29 | 123.41 | 128.46 |
| 21 | q | 822 | SQD | C44-O6-C1 | 3.29 | 120.17 | 113.74 |
| 17 | B | 4005 | BCR | C20-C21-C22 | -3.29 | 122.62 | 127.31 |
| 17 | b | 522 | BCR | C11-C10-C9 | -3.29 | 122.62 | 127.31 |
| 17 | l | 522 | BCR | C28-C27-C26 | -3.29 | 108.21 | 114.08 |
| 14 | r | 516 | CLA | O2D-CGD-O1D | -3.29 | 117.41 | 123.84 |
| 14 | A | 1108 | CLA | CMB-C2B-C3B | 3.29 | 130.83 | 124.68 |
| 17 | t | 523 | BCR | C20-C21-C22 | -3.29 | 122.62 | 127.31 |
| 17 | q | 522 | BCR | C28-C27-C26 | -3.29 | 108.21 | 114.08 |
| 14 | e | 1120 | CLA | O2D-CGD-O1D | -3.29 | 117.41 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | b | 521 | BCR | C16-C17-C18 | -3.29 | 122.62 | 127.31 |
| 21 | d | 822 | SQD | C1-O5-C5 | 3.29 | 120.14 | 113.69 |
| 17 | Z | 522 | BCR | C24-C23-C22 | -3.29 | 121.27 | 126.23 |
| 14 | f | 1206 | CLA | O2D-CGD-O1D | -3.29 | 117.41 | 123.84 |
| 17 | 2 | 523 | BCR | C20-C21-C22 | -3.28 | 122.62 | 127.31 |
| 14 | J | 1302 | CLA | CMB-C2B-C1B | -3.28 | 123.42 | 128.46 |
| 14 | B | 1229 | CLA | CHD-C1D-ND | -3.28 | 121.44 | 124.45 |
| 17 | b | 523 | BCR | C33-C5-C6 | -3.28 | 120.84 | 124.53 |
| 14 | A | 1120 | CLA | O2D-CGD-O1D | -3.28 | 117.42 | 123.84 |
| 19 | l | 5105 | LMU | C1'-O5'-C5' | 3.28 | 120.13 | 113.69 |
| 14 | G | 1108 | CLA | CMB-C2B-C3B | 3.28 | 130.82 | 124.68 |
| 21 | b | 822 | SQD | C44-O6-C1 | 3.28 | 120.15 | 113.74 |
| 21 | 6 | 822 | SQD | C1-O5-C5 | 3.28 | 120.13 | 113.69 |
| 14 | e | 1108 | CLA | CMB-C2B-C3B | 3.28 | 130.82 | 124.68 |
| 21 | v | 822 | SQD | C1-O5-C5 | 3.28 | 120.13 | 113.69 |
| 14 | H | 1205 | CLA | O2A-CGA-O1A | -3.28 | 115.31 | 123.59 |
| 17 | 4 | 523 | BCR | C33-C5-C6 | -3.28 | 120.85 | 124.53 |
| 17 | J | 4013 | BCR | C15-C14-C13 | -3.28 | 122.63 | 127.31 |
| 17 | c | 523 | BCR | C28-C27-C26 | -3.28 | 108.22 | 114.08 |
| 14 | e | 1118 | CLA | CHB-C4A-NA | 3.28 | 129.04 | 124.51 |
| 14 | f | 1229 | CLA | CHD-C1D-ND | -3.28 | 121.44 | 124.45 |
| 14 | f | 1205 | CLA | O2A-CGA-O1A | -3.28 | 115.32 | 123.59 |
| 14 | A | 1132 | CLA | O2D-CGD-CBD | 3.28 | 117.09 | 111.27 |
| 17 | 6 | 522 | BCR | C15-C16-C17 | -3.28 | 116.76 | 123.47 |
| 21 | 1 | 822 | SQD | C44-O6-C1 | 3.28 | 120.14 | 113.74 |
| 17 | o | 4021 | BCR | C38-C26-C25 | -3.28 | 120.85 | 124.53 |
| 14 | B | 1205 | CLA | O2A-CGA-O1A | -3.28 | 115.33 | 123.59 |
| 21 | t | 822 | SQD | C44-O6-C1 | 3.27 | 120.14 | 113.74 |
| 17 | 4 | 522 | BCR | C11-C10-C9 | -3.27 | 122.64 | 127.31 |
| 17 | j | 4016 | BCR | C16-C17-C18 | -3.27 | 122.64 | 127.31 |
| 17 | Z | 523 | BCR | C20-C21-C22 | -3.27 | 122.64 | 127.31 |
| 17 | d | 522 | BCR | C15-C16-C17 | -3.27 | 116.77 | 123.47 |
| 14 | 6 | 513 | CLA | CMB-C2B-C1B | -3.27 | 123.43 | 128.46 |
| 17 | 5 | 524 | BCR | C11-C10-C9 | -3.27 | 122.64 | 127.31 |
| 17 | 5 | 523 | BCR | C28-C27-C26 | -3.27 | 108.24 | 114.08 |
| 17 | n | 4019 | BCR | C20-C21-C22 | -3.27 | 122.64 | 127.31 |
| 17 | t | 523 | BCR | C33-C5-C6 | -3.27 | 120.86 | 124.53 |
| 17 | F | 4016 | BCR | C16-C17-C18 | -3.27 | 122.65 | 127.31 |
| 17 | 4 | 521 | BCR | C16-C17-C18 | -3.27 | 122.65 | 127.31 |
| 17 | T | 4013 | BCR | C15-C14-C13 | -3.27 | 122.65 | 127.31 |
| 14 | A | 1134 | CLA | CMB-C2B-C1B | -3.27 | 123.44 | 128.46 |
| 14 | b | 503 | CLA | CMB-C2B-C1B | -3.27 | 123.44 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 4 | 523 | BCR | C20-C21-C22 | -3.27 | 122.65 | 127.31 |
| 14 | e | 1134 | CLA | CMB-C2B-C1B | -3.26 | 123.45 | 128.46 |
| 17 | u | 524 | BCR | C11-C10-C9 | -3.26 | 122.65 | 127.31 |
| 17 | u | 523 | BCR | C28-C27-C26 | -3.26 | 108.25 | 114.08 |
| 21 | 4 | 822 | SQD | C44-O6-C1 | 3.26 | 120.11 | 113.74 |
| 17 | R | 4016 | BCR | C16-C17-C18 | -3.26 | 122.65 | 127.31 |
| 17 | t | 521 | BCR | C16-C17-C18 | -3.26 | 122.65 | 127.31 |
| 14 | a | 507 | CLA | CMB-C2B-C3B | 3.26 | 130.78 | 124.68 |
| 14 | e | 1132 | CLA | O2D-CGD-CBD | 3.26 | 117.07 | 111.27 |
| 17 | H | 4005 | BCR | C20-C21-C22 | -3.26 | 122.65 | 127.31 |
| 17 | 4 | 521 | BCR | C3-C4-C5 | -3.26 | 108.25 | 114.08 |
| 17 | t | 521 | BCR | C3-C4-C5 | -3.26 | 108.25 | 114.08 |
| 17 | L | 4019 | BCR | C20-C21-C22 | -3.26 | 122.66 | 127.31 |
| 17 | c | 522 | BCR | C24-C23-C22 | -3.26 | 121.31 | 126.23 |
| 14 | G | 1118 | CLA | CHB-C4A-NA | 3.26 | 129.02 | 124.51 |
| 14 | d | 510 | CLA | CMB-C2B-C3B | 3.26 | 130.78 | 124.68 |
| 14 | U | 1401 | CLA | O2D-CGD-O1D | -3.26 | 117.47 | 123.84 |
| 17 | t | 522 | BCR | C11-C10-C9 | -3.26 | 122.66 | 127.31 |
| 14 | H | 1023 | CLA | CHB-C4A-NA | 3.26 | 129.02 | 124.51 |
| 17 | u | 522 | BCR | C24-C23-C22 | -3.26 | 121.31 | 126.23 |
| 14 | B | 1206 | CLA | O2D-CGD-O1D | -3.26 | 117.47 | 123.84 |
| 14 | 2 | 507 | CLA | O2D-CGD-O1D | -3.26 | 117.47 | 123.84 |
| 14 | A | 1118 | CLA | CHB-C4A-NA | 3.26 | 129.01 | 124.51 |
| 14 | e | 1119 | CLA | O2D-CGD-O1D | -3.26 | 117.47 | 123.84 |
| 14 | 1 | 519 | CLA | CMB-C2B-C1B | -3.26 | 123.46 | 128.46 |
| 14 | G | 1134 | CLA | CMB-C2B-C1B | -3.26 | 123.46 | 128.46 |
| 17 | W | 4021 | BCR | C38-C26-C25 | -3.25 | 120.87 | 124.53 |
| 17 | l | 4013 | BCR | C15-C14-C13 | -3.25 | 122.67 | 127.31 |
| 14 | A | 1119 | CLA | O2D-CGD-O1D | -3.25 | 117.48 | 123.84 |
| 14 | 3 | 507 | CLA | CMB-C2B-C3B | 3.25 | 130.77 | 124.68 |
| 14 | q | 511 | CLA | CMB-C2B-C3B | 3.25 | 130.77 | 124.68 |
| 14 | c | 513 | CLA | CMB-C2B-C1B | -3.25 | 123.46 | 128.46 |
| 14 | 5 | 513 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 17 | b | 521 | BCR | C3-C4-C5 | -3.25 | 108.27 | 114.08 |
| 17 | t | 524 | BCR | C1-C6-C5 | -3.25 | 118.03 | 122.61 |
| 14 | H | 1206 | CLA | O2D-CGD-O1D | -3.25 | 117.48 | 123.84 |
| 17 | 3 | 521 | BCR | C3-C4-C5 | -3.25 | 108.27 | 114.08 |
| 14 | Y | 511 | CLA | CMB-C2B-C3B | 3.25 | 130.76 | 124.68 |
| 17 | 4 | 524 | BCR | C1-C6-C5 | -3.25 | 118.04 | 122.61 |
| 17 | 2 | 522 | BCR | C24-C23-C22 | -3.25 | 121.33 | 126.23 |
| 14 | K | 1401 | CLA | O2D-CGD-O1D | -3.25 | 117.48 | 123.84 |
| 14 | H | 1229 | CLA | CHD-C1D-ND | -3.25 | 121.47 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | q | 519 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 17 | 5 | 522 | BCR | C24-C23-C22 | -3.25 | 121.33 | 126.23 |
| 17 | b | 523 | BCR | C20-C21-C22 | -3.25 | 122.67 | 127.31 |
| 14 | f | 1217 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 17 | c | 524 | BCR | C11-C10-C9 | -3.25 | 122.68 | 127.31 |
| 17 | M | 4021 | BCR | C38-C26-C25 | -3.25 | 120.88 | 124.53 |
| 14 | A | 1122 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 14 | c | 503 | CLA | CMB-C2B-C1B | -3.25 | 123.47 | 128.46 |
| 14 | Z | 507 | CLA | O2D-CGD-O1D | -3.25 | 117.49 | 123.84 |
| 14 | s | 507 | CLA | CMB-C2B-C3B | 3.25 | 130.75 | 124.68 |
| 14 | G | 1119 | CLA | O2D-CGD-O1D | -3.24 | 117.49 | 123.84 |
| 14 | 5 | 507 | CLA | CMB-C2B-C3B | 3.24 | 130.75 | 124.68 |
| 17 | V | 4019 | BCR | C20-C21-C22 | -3.24 | 122.68 | 127.31 |
| 17 | s | 521 | BCR | C3-C4-C5 | -3.24 | 108.29 | 114.08 |
| 14 | r | 507 | CLA | O2D-CGD-O1D | -3.24 | 117.50 | 123.84 |
| 14 | V | 1503 | CLA | CMB-C2B-C3B | 3.24 | 130.74 | 124.68 |
| 14 | u | 503 | CLA | CMB-C2B-C1B | -3.24 | 123.48 | 128.46 |
| 14 | l | 511 | CLA | CMB-C2B-C3B | 3.24 | 130.74 | 124.68 |
| 17 | f | 4005 | BCR | C11-C10-C9 | -3.24 | 122.69 | 127.31 |
| 14 | 6 | 510 | CLA | CMB-C2B-C3B | 3.24 | 130.74 | 124.68 |
| 17 | G | 4007 | BCR | C7-C8-C9 | -3.24 | 121.34 | 126.23 |
| 14 | G | 1106 | CLA | O2D-CGD-O1D | -3.24 | 117.51 | 123.84 |
| 14 | u | 507 | CLA | CMB-C2B-C3B | 3.24 | 130.73 | 124.68 |
| 17 | a | 521 | BCR | C3-C4-C5 | -3.23 | 108.30 | 114.08 |
| 14 | f | 1023 | CLA | CHB-C4A-NA | 3.23 | 128.99 | 124.51 |
| 14 | L | 1503 | CLA | CMB-C2B-C3B | 3.23 | 130.73 | 124.68 |
| 14 | B | 1023 | CLA | CHB-C4A-NA | 3.23 | 128.98 | 124.51 |
| 17 | f | 4014 | BCR | C3-C4-C5 | -3.23 | 108.30 | 114.08 |
| 14 | s | 510 | CLA | CMB-C2B-C3B | 3.23 | 130.73 | 124.68 |
| 17 | H | 4014 | BCR | C3-C4-C5 | -3.23 | 108.30 | 114.08 |
| 14 | c | 507 | CLA | CMB-C2B-C3B | 3.23 | 130.73 | 124.68 |
| 14 | A | 1106 | CLA | O2D-CGD-O1D | -3.23 | 117.52 | 123.84 |
| 14 | G | 1122 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |
| 14 | n | 1503 | CLA | CMB-C2B-C3B | 3.23 | 130.72 | 124.68 |
| 14 | f | 1202 | CLA | O2D-CGD-O1D | -3.23 | 117.52 | 123.84 |
| 21 | t | 822 | SQD | C4-C3-C2 | 3.23 | 116.47 | 110.82 |
| 14 | A | 1105 | CLA | O2D-CGD-O1D | -3.23 | 117.52 | 123.84 |
| 14 | Y | 519 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |
| 14 | 3 | 510 | CLA | CMB-C2B-C3B | 3.23 | 130.72 | 124.68 |
| 21 | b | 822 | SQD | C4-C3-C2 | 3.23 | 116.46 | 110.82 |
| 14 | m | 1401 | CLA | O2D-CGD-O1D | -3.23 | 117.52 | 123.84 |
| 14 | e | 1122 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1115 | CLA | O2D-CGD-O1D | -3.23 | 117.53 | 123.84 |
| 14 | d | 513 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |
| 17 | r | 522 | BCR | C24-C23-C22 | -3.23 | 121.36 | 126.23 |
| 14 | t | 509 | CLA | CHB-C4A-NA | 3.23 | 128.97 | 124.51 |
| 21 | 4 | 822 | SQD | C4-C3-C2 | 3.23 | 116.46 | 110.82 |
| 14 | 5 | 503 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |
| 14 | u | 513 | CLA | CMB-C2B-C1B | -3.23 | 123.50 | 128.46 |
| 14 | B | 1202 | CLA | O2D-CGD-O1D | -3.23 | 117.53 | 123.84 |
| 14 | G | 1105 | CLA | O2D-CGD-O1D | -3.23 | 117.53 | 123.84 |
| 14 | l | 1303 | CLA | O2D-CGD-O1D | -3.23 | 117.53 | 123.84 |
| 17 | b | 524 | BCR | C1-C6-C5 | -3.23 | 118.07 | 122.61 |
| 17 | 6 | 522 | BCR | C3-C4-C5 | -3.23 | 108.32 | 114.08 |
| 17 | d | 522 | BCR | C3-C4-C5 | -3.23 | 108.32 | 114.08 |
| 17 | B | 4014 | BCR | C3-C4-C5 | -3.22 | 108.32 | 114.08 |
| 14 | v | 510 | CLA | CMB-C2B-C3B | 3.22 | 130.71 | 124.68 |
| 14 | T | 1303 | CLA | O2D-CGD-O1D | -3.22 | 117.54 | 123.84 |
| 14 | G | 1138 | CLA | CHB-C4A-NA | 3.22 | 128.97 | 124.51 |
| 14 | v | 513 | CLA | CMB-C2B-C1B | -3.22 | 123.51 | 128.46 |
| 14 | H | 1202 | CLA | O2D-CGD-O1D | -3.22 | 117.54 | 123.84 |
| 17 | e | 4007 | BCR | C7-C8-C9 | -3.22 | 121.37 | 126.23 |
| 21 | Z | 822 | SQD | C1-O5-C5 | 3.22 | 120.01 | 113.69 |
| 14 | H | 1217 | CLA | CMB-C2B-C1B | -3.22 | 123.52 | 128.46 |
| 14 | 4 | 509 | CLA | CHB-C4A-NA | 3.22 | 128.96 | 124.51 |
| 17 | B | 4005 | BCR | C11-C10-C9 | -3.22 | 122.72 | 127.31 |
| 14 | e | 1106 | CLA | O2D-CGD-O1D | -3.22 | 117.55 | 123.84 |
| 14 | b | 509 | CLA | CHB-C4A-NA | 3.22 | 128.96 | 124.51 |
| 14 | e | 1105 | CLA | O2D-CGD-O1D | -3.21 | 117.55 | 123.84 |
| 17 | M | 4021 | BCR | C20-C19-C18 | -3.21 | 117.39 | 126.42 |
| 17 | Y | 522 | BCR | C24-C23-C22 | -3.21 | 121.38 | 126.23 |
| 17 | o | 4021 | BCR | C20-C19-C18 | -3.21 | 117.39 | 126.42 |
| 14 | B | 1217 | CLA | CMB-C2B-C1B | -3.21 | 123.53 | 128.46 |
| 17 | t | 523 | BCR | C28-C27-C26 | -3.21 | 108.34 | 114.08 |
| 17 | A | 4007 | BCR | C7-C8-C9 | -3.21 | 121.38 | 126.23 |
| 14 | a | 510 | CLA | CMB-C2B-C3B | 3.21 | 130.69 | 124.68 |
| 14 | J | 1303 | CLA | O2D-CGD-O1D | -3.21 | 117.56 | 123.84 |
| 17 | t | 521 | BCR | C28-C27-C26 | -3.21 | 108.34 | 114.08 |
| 14 | A | 1115 | CLA | O2D-CGD-O1D | -3.21 | 117.56 | 123.84 |
| 17 | H | 4004 | BCR | C33-C5-C6 | -3.21 | 120.92 | 124.53 |
| 14 | d | 507 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 14 | 6 | 507 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 17 | 1 | 522 | BCR | C24-C23-C22 | -3.21 | 121.39 | 126.23 |
| 17 | 4 | 521 | BCR | C28-C27-C26 | -3.21 | 108.35 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 5 | 506 | CLA | CMB-C2B-C3B | 3.21 | 130.68 | 124.68 |
| 14 | A | 1138 | CLA | CHB-C4A-NA | 3.21 | 128.94 | 124.51 |
| 17 | L | 4019 | BCR | C28-C27-C26 | -3.21 | 108.35 | 114.08 |
| 17 | n | 4019 | BCR | C28-C27-C26 | -3.21 | 108.35 | 114.08 |
| 14 | G | 1115 | CLA | O2D-CGD-O1D | -3.20 | 117.57 | 123.84 |
| 14 | c | 506 | CLA | CMB-C2B-C3B | 3.20 | 130.67 | 124.68 |
| 14 | q | 509 | CLA | CMB-C2B-C3B | 3.20 | 130.67 | 124.68 |
| 17 | V | 4019 | BCR | C28-C27-C26 | -3.20 | 108.36 | 114.08 |
| 14 | v | 507 | CLA | CMB-C2B-C3B | 3.20 | 130.67 | 124.68 |
| 17 | H | 4005 | BCR | C11-C10-C9 | -3.20 | 122.74 | 127.31 |
| 17 | v | 522 | BCR | C3-C4-C5 | -3.20 | 108.36 | 114.08 |
| 17 | q | 522 | BCR | C24-C23-C22 | -3.20 | 121.40 | 126.23 |
| 21 | 2 | 822 | SQD | C1-O5-C5 | 3.20 | 119.97 | 113.69 |
| 14 | t | 510 | CLA | CMB-C2B-C3B | 3.20 | 130.67 | 124.68 |
| 21 | d | 822 | SQD | C44-O6-C1 | 3.20 | 119.99 | 113.74 |
| 17 | Y | 521 | BCR | C7-C8-C9 | -3.20 | 121.40 | 126.23 |
| 14 | 4 | 510 | CLA | CMB-C2B-C3B | 3.20 | 130.66 | 124.68 |
| 14 | b | 510 | CLA | CMB-C2B-C3B | 3.20 | 130.66 | 124.68 |
| 17 | W | 4021 | BCR | C20-C19-C18 | -3.20 | 117.43 | 126.42 |
| 14 | v | 511 | CLA | CMB-C2B-C3B | 3.20 | 130.66 | 124.68 |
| 21 | b | 822 | SQD | O7-S-C6 | 3.20 | 110.74 | 106.94 |
| 21 | r | 822 | SQD | C1-O5-C5 | 3.20 | 119.96 | 113.69 |
| 17 | c | 521 | BCR | C11-C10-C9 | -3.20 | 122.75 | 127.31 |
| 17 | b | 521 | BCR | C28-C27-C26 | -3.20 | 108.37 | 114.08 |
| 17 | B | 4004 | BCR | C33-C5-C6 | -3.20 | 120.94 | 124.53 |
| 17 | 4 | 523 | BCR | C28-C27-C26 | -3.20 | 108.37 | 114.08 |
| 14 | u | 506 | CLA | CMB-C2B-C3B | 3.19 | 130.65 | 124.68 |
| 17 | 2 | 522 | BCR | C28-C27-C26 | -3.19 | 108.38 | 114.08 |
| 14 | H | 1209 | CLA | CMB-C2B-C3B | 3.19 | 130.65 | 124.68 |
| 14 | 1 | 509 | CLA | CMB-C2B-C3B | 3.19 | 130.65 | 124.68 |
| 17 | G | 4001 | BCR | C24-C23-C22 | -3.19 | 121.41 | 126.23 |
| 17 | s | 521 | BCR | C11-C10-C9 | -3.19 | 122.76 | 127.31 |
| 17 | 3 | 521 | BCR | C11-C10-C9 | -3.19 | 122.76 | 127.31 |
| 17 | G | 4007 | BCR | C20-C21-C22 | -3.19 | 122.76 | 127.31 |
| 17 | 1 | 524 | BCR | C8-C7-C6 | -3.19 | 118.25 | 127.20 |
| 14 | H | 1205 | CLA | CBA-CAA-C2A | 3.19 | 123.27 | 113.86 |
| 14 | G | 1103 | CLA | O2D-CGD-O1D | -3.19 | 117.61 | 123.84 |
| 14 | f | 1205 | CLA | CBA-CAA-C2A | 3.19 | 123.27 | 113.86 |
| 21 | 4 | 822 | SQD | O7-S-C6 | 3.19 | 110.72 | 106.94 |
| 17 | 5 | 521 | BCR | C11-C10-C9 | -3.19 | 122.76 | 127.31 |
| 14 | A | 1103 | CLA | O2D-CGD-O1D | -3.18 | 117.61 | 123.84 |
| 17 | r | 522 | BCR | C28-C27-C26 | -3.18 | 108.39 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | Z | 518 | CLA | CMB-C2B-C3B | 3.18 | 130.63 | 124.68 |
| 14 | s | 505 | CLA | CMB-C2B-C3B | 3.18 | 130.63 | 124.68 |
| 17 | Z | 522 | BCR | C28-C27-C26 | -3.18 | 108.39 | 114.08 |
| 17 | Y | 524 | BCR | C11-C10-C9 | -3.18 | 122.77 | 127.31 |
| 17 | u | 521 | BCR | C11-C10-C9 | -3.18 | 122.77 | 127.31 |
| 14 | e | 1106 | CLA | C1-C2-C3 | -3.18 | 120.54 | 126.04 |
| 17 | Y | 524 | BCR | C8-C7-C6 | -3.18 | 118.27 | 127.20 |
| 21 | 6 | 822 | SQD | C44-O6-C1 | 3.18 | 119.95 | 113.74 |
| 14 | B | 1205 | CLA | CBA-CAA-C2A | 3.18 | 123.25 | 113.86 |
| 17 | Y | 523 | BCR | C21-C20-C19 | -3.18 | 113.29 | 123.22 |
| 17 | s | 522 | BCR | C11-C12-C13 | -3.18 | 117.48 | 126.42 |
| 17 | q | 524 | BCR | C8-C7-C6 | -3.18 | 118.27 | 127.20 |
| 17 | S | 4018 | BCR | C11-C10-C9 | -3.18 | 122.77 | 127.31 |
| 14 | d | 511 | CLA | CMB-C2B-C3B | 3.18 | 130.62 | 124.68 |
| 17 | A | 4001 | BCR | C24-C23-C22 | -3.18 | 121.43 | 126.23 |
| 17 | l | 523 | BCR | C21-C20-C19 | -3.18 | 113.30 | 123.22 |
| 17 | b | 523 | BCR | C28-C27-C26 | -3.18 | 108.40 | 114.08 |
| 14 | u | 519 | CLA | CMB-C2B-C1B | -3.18 | 123.58 | 128.46 |
| 14 | B | 1209 | CLA | CMB-C2B-C3B | 3.18 | 130.62 | 124.68 |
| 17 | l | 521 | BCR | C7-C8-C9 | -3.18 | 121.44 | 126.23 |
| 14 | G | 1137 | CLA | CMB-C2B-C3B | 3.18 | 130.62 | 124.68 |
| 14 | 6 | 511 | CLA | CMB-C2B-C3B | 3.18 | 130.62 | 124.68 |
| 14 | u | 508 | CLA | CHB-C4A-NA | 3.18 | 128.90 | 124.51 |
| 14 | G | 1132 | CLA | CMB-C2B-C1B | -3.18 | 123.58 | 128.46 |
| 14 | s | 513 | CLA | CMB-C2B-C1B | -3.17 | 123.58 | 128.46 |
| 17 | q | 523 | BCR | C21-C20-C19 | -3.17 | 113.31 | 123.22 |
| 14 | 3 | 505 | CLA | CMB-C2B-C3B | 3.17 | 130.62 | 124.68 |
| 17 | q | 524 | BCR | C11-C10-C9 | -3.17 | 122.78 | 127.31 |
| 14 | G | 1106 | CLA | C1-C2-C3 | -3.17 | 120.56 | 126.04 |
| 14 | H | 1207 | CLA | CMB-C2B-C1B | -3.17 | 123.59 | 128.46 |
| 17 | A | 4007 | BCR | C20-C21-C22 | -3.17 | 122.78 | 127.31 |
| 14 | d | 517 | CLA | CMB-C2B-C3B | 3.17 | 130.61 | 124.68 |
| 17 | l | 524 | BCR | C11-C10-C9 | -3.17 | 122.78 | 127.31 |
| 14 | e | 1137 | CLA | CMB-C2B-C3B | 3.17 | 130.61 | 124.68 |
| 14 | f | 1209 | CLA | CMB-C2B-C3B | 3.17 | 130.61 | 124.68 |
| 17 | f | 4004 | BCR | C33-C5-C6 | -3.17 | 120.97 | 124.53 |
| 17 | H | 4009 | BCR | C3-C4-C5 | -3.17 | 108.42 | 114.08 |
| 21 | v | 822 | SQD | C44-O6-C1 | 3.17 | 119.93 | 113.74 |
| 17 | 5 | 521 | BCR | C24-C23-C22 | -3.17 | 121.45 | 126.23 |
| 14 | 6 | 517 | CLA | CMB-C2B-C3B | 3.17 | 130.60 | 124.68 |
| 14 | Y | 509 | CLA | CMB-C2B-C3B | 3.17 | 130.60 | 124.68 |
| 14 | c | 519 | CLA | CMB-C2B-C1B | -3.17 | 123.60 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 505 | CLA | CMB-C2B-C3B | 3.17 | 130.60 | 124.68 |
| 14 | 5 | 519 | CLA | CMB-C2B-C1B | -3.16 | 123.60 | 128.46 |
| 14 | e | 1132 | CLA | CMB-C2B-C1B | -3.16 | 123.60 | 128.46 |
| 14 | r | 518 | CLA | CMB-C2B-C3B | 3.16 | 130.60 | 124.68 |
| 14 | f | 1221 | CLA | O2D-CGD-O1D | -3.16 | 117.65 | 123.84 |
| 17 | c | 521 | BCR | C24-C23-C22 | -3.16 | 121.45 | 126.23 |
| 14 | e | 1103 | CLA | O2D-CGD-O1D | -3.16 | 117.65 | 123.84 |
| 17 | e | 4001 | BCR | C24-C23-C22 | -3.16 | 121.46 | 126.23 |
| 17 | s | 523 | BCR | C24-C23-C22 | -3.16 | 121.46 | 126.23 |
| 14 | A | 1106 | CLA | C1-C2-C3 | -3.16 | 120.58 | 126.04 |
| 21 | t | 822 | SQD | O7-S-C6 | 3.16 | 110.69 | 106.94 |
| 14 | q | 508 | CLA | CHB-C4A-NA | 3.16 | 128.88 | 124.51 |
| 17 | k | 4018 | BCR | C11-C10-C9 | -3.16 | 122.80 | 127.31 |
| 14 | b | 506 | CLA | CMB-C2B-C3B | 3.16 | 130.59 | 124.68 |
| 14 | q | 505 | CLA | CMB-C2B-C3B | 3.16 | 130.59 | 124.68 |
| 14 | B | 1207 | CLA | CMB-C2B-C1B | -3.16 | 123.61 | 128.46 |
| 17 | e | 4007 | BCR | C20-C21-C22 | -3.16 | 122.80 | 127.31 |
| 17 | 3 | 522 | BCR | C11-C12-C13 | -3.16 | 117.55 | 126.42 |
| 14 | B | 1202 | CLA | CHB-C4A-NA | 3.16 | 128.88 | 124.51 |
| 17 | a | 522 | BCR | C11-C12-C13 | -3.16 | 117.55 | 126.42 |
| 14 | 4 | 505 | CLA | CMB-C2B-C1B | -3.16 | 123.61 | 128.46 |
| 14 | 1 | 505 | CLA | CMB-C2B-C3B | 3.16 | 130.58 | 124.68 |
| 14 | 2 | 518 | CLA | CMB-C2B-C3B | 3.16 | 130.58 | 124.68 |
| 17 | f | 4009 | BCR | C3-C4-C5 | -3.16 | 108.44 | 114.08 |
| 14 | Y | 505 | CLA | CMB-C2B-C3B | 3.16 | 130.58 | 124.68 |
| 14 | A | 1137 | CLA | CMB-C2B-C3B | 3.16 | 130.58 | 124.68 |
| 14 | s | 516 | CLA | CMB-C2B-C3B | 3.16 | 130.58 | 124.68 |
| 17 | B | 4009 | BCR | C3-C4-C5 | -3.15 | 108.44 | 114.08 |
| 14 | e | 1138 | CLA | CHB-C4A-NA | 3.15 | 128.87 | 124.51 |
| 14 | 3 | 513 | CLA | CMB-C2B-C1B | -3.15 | 123.62 | 128.46 |
| 14 | B | 1023 | CLA | O2D-CGD-O1D | -3.15 | 117.67 | 123.84 |
| 14 | B | 1221 | CLA | O2D-CGD-O1D | -3.15 | 117.67 | 123.84 |
| 14 | H | 1023 | CLA | O2D-CGD-O1D | -3.15 | 117.67 | 123.84 |
| 14 | f | 1202 | CLA | CHB-C4A-NA | 3.15 | 128.87 | 124.51 |
| 14 | b | 516 | CLA | CMB-C2B-C3B | 3.15 | 130.57 | 124.68 |
| 17 | a | 521 | BCR | C11-C10-C9 | -3.15 | 122.81 | 127.31 |
| 17 | q | 521 | BCR | C7-C8-C9 | -3.15 | 121.47 | 126.23 |
| 14 | v | 517 | CLA | CMB-C2B-C3B | 3.15 | 130.57 | 124.68 |
| 14 | v | 516 | CLA | CMB-C2B-C3B | 3.15 | 130.57 | 124.68 |
| 14 | H | 1221 | CLA | O2D-CGD-O1D | -3.15 | 117.68 | 123.84 |
| 14 | 4 | 506 | CLA | CMB-C2B-C3B | 3.15 | 130.57 | 124.68 |
| 14 | A | 1132 | CLA | CMB-C2B-C1B | -3.15 | 123.62 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 5 | 508 | CLA | CHB-C4A-NA | 3.15 | 128.87 | 124.51 |
| 14 | n | 1502 | CLA | CHB-C4A-NA | 3.15 | 128.87 | 124.51 |
| 17 | 3 | 523 | BCR | C24-C23-C22 | -3.15 | 121.48 | 126.23 |
| 14 | a | 516 | CLA | CBC-CAC-C3C | 3.15 | 121.11 | 112.43 |
| 14 | t | 516 | CLA | CMB-C2B-C3B | 3.15 | 130.57 | 124.68 |
| 14 | Z | 501 | CLA | CHB-C4A-NA | 3.15 | 128.86 | 124.51 |
| 17 | I | 4018 | BCR | C11-C10-C9 | -3.15 | 122.82 | 127.31 |
| 14 | H | 1012 | CLA | C1B-CHB-C4A | -3.15 | 123.89 | 130.12 |
| 14 | G | 1108 | CLA | O2D-CGD-O1D | -3.14 | 117.69 | 123.84 |
| 14 | 3 | 516 | CLA | CBC-CAC-C3C | 3.14 | 121.10 | 112.43 |
| 14 | A | 1013 | CLA | CAA-CBA-CGA | -3.14 | 104.07 | 113.25 |
| 14 | e | 1013 | CLA | CAA-CBA-CGA | -3.14 | 104.07 | 113.25 |
| 14 | b | 505 | CLA | CMB-C2B-C1B | -3.14 | 123.63 | 128.46 |
| 14 | f | 1023 | CLA | O2D-CGD-O1D | -3.14 | 117.69 | 123.84 |
| 14 | K | 1105 | CLA | CMC-C2C-C1C | -3.14 | 120.25 | 125.04 |
| 14 | U | 1105 | CLA | CMC-C2C-C1C | -3.14 | 120.25 | 125.04 |
| 14 | V | 1502 | CLA | CHD-C1D-ND | -3.14 | 121.57 | 124.45 |
| 14 | c | 501 | CLA | CMB-C2B-C3B | 3.14 | 130.55 | 124.68 |
| 14 | G | 1101 | CLA | CHB-C4A-NA | 3.14 | 128.85 | 124.51 |
| 20 | H | 5002 | LMG | O6-C1-O1 | -3.14 | 102.54 | 109.97 |
| 14 | 5 | 518 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 14 | 3 | 516 | CLA | CMB-C2B-C3B | 3.14 | 130.55 | 124.68 |
| 14 | e | 1101 | CLA | CHB-C4A-NA | 3.14 | 128.85 | 124.51 |
| 14 | t | 504 | CLA | CMB-C2B-C3B | 3.14 | 130.55 | 124.68 |
| 14 | a | 513 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 14 | f | 1207 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 14 | t | 505 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 14 | 4 | 516 | CLA | CMB-C2B-C3B | 3.14 | 130.55 | 124.68 |
| 17 | I | 4018 | BCR | C1-C6-C5 | -3.14 | 118.20 | 122.61 |
| 14 | u | 518 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 21 | Z | 822 | SQD | O5-C5-C4 | 3.14 | 115.39 | 109.69 |
| 14 | c | 518 | CLA | CMB-C2B-C1B | -3.14 | 123.64 | 128.46 |
| 14 | f | 1213 | CLA | CHB-C4A-NA | 3.13 | 128.85 | 124.51 |
| 17 | f | 4006 | BCR | C16-C17-C18 | -3.13 | 122.84 | 127.31 |
| 14 | 5 | 501 | CLA | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |
| 14 | f | 1012 | CLA | C1B-CHB-C4A | -3.13 | 123.91 | 130.12 |
| 17 | Z | 521 | BCR | C7-C8-C9 | -3.13 | 121.50 | 126.23 |
| 14 | G | 1013 | CLA | CAA-CBA-CGA | -3.13 | 104.10 | 113.25 |
| 14 | b | 504 | CLA | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |
| 14 | B | 1205 | CLA | O2D-CGD-O1D | -3.13 | 117.72 | 123.84 |
| 17 | a | 523 | BCR | C24-C23-C22 | -3.13 | 121.50 | 126.23 |
| 14 | 6 | 516 | CLA | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | t | 506 | CLA | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |
| 21 | 2 | 822 | SQD | O5-C5-C4 | 3.13 | 115.38 | 109.69 |
| 14 | d | 516 | CLA | CMB-C2B-C3B | 3.13 | 130.54 | 124.68 |
| 14 | B | 1213 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 14 | 2 | 501 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 14 | B | 1012 | CLA | C1B-CHB-C4A | -3.13 | 123.92 | 130.12 |
| 14 | f | 1205 | CLA | O2D-CGD-O1D | -3.13 | 117.72 | 123.84 |
| 17 | u | 521 | BCR | C24-C23-C22 | -3.13 | 121.51 | 126.23 |
| 14 | m | 1105 | CLA | CMC-C2C-C1C | -3.13 | 120.27 | 125.04 |
| 20 | B | 5002 | LMG | O6-C1-O1 | -3.13 | 102.56 | 109.97 |
| 14 | 4 | 504 | CLA | CMB-C2B-C3B | 3.13 | 130.53 | 124.68 |
| 14 | s | 516 | CLA | CBC-CAC-C3C | 3.13 | 121.05 | 112.43 |
| 14 | f | 1220 | CLA | CMB-C2B-C1B | -3.13 | 123.66 | 128.46 |
| 17 | k | 4018 | BCR | C1-C6-C5 | -3.13 | 118.21 | 122.61 |
| 21 | r | 822 | SQD | O5-C5-C4 | 3.13 | 115.37 | 109.69 |
| 14 | n | 1502 | CLA | CHD-C1D-ND | -3.13 | 121.58 | 124.45 |
| 17 | S | 4018 | BCR | C20-C21-C22 | -3.13 | 122.85 | 127.31 |
| 14 | a | 502 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 14 | A | 1108 | CLA | O2D-CGD-O1D | -3.12 | 117.73 | 123.84 |
| 14 | L | 1502 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 14 | l | 508 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 17 | Y | 524 | BCR | C7-C8-C9 | -3.12 | 121.52 | 126.23 |
| 17 | T | 4013 | BCR | C2-C1-C6 | 3.12 | 115.29 | 110.48 |
| 14 | e | 1137 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 14 | H | 1205 | CLA | O2D-CGD-O1D | -3.12 | 117.73 | 123.84 |
| 17 | 2 | 521 | BCR | C7-C8-C9 | -3.12 | 121.52 | 126.23 |
| 14 | L | 1502 | CLA | CHD-C1D-ND | -3.12 | 121.58 | 124.45 |
| 14 | B | 1201 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 14 | Y | 508 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 14 | c | 508 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 14 | r | 501 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 20 | f | 5002 | LMG | O6-C1-O1 | -3.12 | 102.58 | 109.97 |
| 14 | a | 516 | CLA | CMB-C2B-C3B | 3.12 | 130.52 | 124.68 |
| 14 | u | 501 | CLA | CMB-C2B-C3B | 3.12 | 130.52 | 124.68 |
| 17 | m | 4104 | BCR | C11-C10-C9 | -3.12 | 122.86 | 127.31 |
| 17 | l | 524 | BCR | C7-C8-C9 | -3.12 | 121.52 | 126.23 |
| 14 | e | 1108 | CLA | O2D-CGD-O1D | -3.12 | 117.74 | 123.84 |
| 14 | B | 1220 | CLA | CMB-C2B-C1B | -3.12 | 123.67 | 128.46 |
| 14 | A | 1101 | CLA | CHB-C4A-NA | 3.12 | 128.82 | 124.51 |
| 17 | q | 524 | BCR | C7-C8-C9 | -3.12 | 121.53 | 126.23 |
| 14 | l | 504 | CLA | O2D-CGD-CBD | 3.11 | 116.80 | 111.27 |
| 14 | H | 1220 | CLA | CMB-C2B-C1B | -3.11 | 123.68 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1213 | CLA | CHB-C4A-NA | 3.11 | 128.82 | 124.51 |
| 17 | I | 4018 | BCR | C20-C21-C22 | -3.11 | 122.87 | 127.31 |
| 14 | V | 1502 | CLA | CHB-C4A-NA | 3.11 | 128.81 | 124.51 |
| 14 | q | 504 | CLA | O2D-CGD-CBD | 3.11 | 116.80 | 111.27 |
| 14 | f | 1201 | CLA | CHB-C4A-NA | 3.11 | 128.81 | 124.51 |
| 14 | G | 1237 | CLA | C4-C3-C5 | 3.11 | 120.50 | 115.27 |
| 17 | T | 4015 | BCR | C20-C21-C22 | -3.11 | 122.87 | 127.31 |
| 14 | H | 1202 | CLA | CHB-C4A-NA | 3.11 | 128.81 | 124.51 |
| 17 | r | 521 | BCR | C7-C8-C9 | -3.11 | 121.54 | 126.23 |
| 17 | H | 4009 | BCR | C16-C17-C18 | -3.11 | 122.87 | 127.31 |
| 14 | H | 1201 | CLA | O2D-CGD-O1D | -3.11 | 117.76 | 123.84 |
| 17 | d | 524 | BCR | C15-C16-C17 | -3.11 | 117.11 | 123.47 |
| 14 | 3 | 502 | CLA | CHB-C4A-NA | 3.11 | 128.81 | 124.51 |
| 14 | A | 1132 | CLA | CAC-C3C-C4C | 3.11 | 128.84 | 124.81 |
| 17 | k | 4018 | BCR | C20-C21-C22 | -3.11 | 122.88 | 127.31 |
| 21 | 3 | 822 | SQD | O47-C7-C8 | 3.11 | 119.46 | 110.80 |
| 17 | l | 4013 | BCR | C2-C1-C6 | 3.11 | 115.26 | 110.48 |
| 14 | L | 1503 | CLA | O2D-CGD-O1D | -3.11 | 117.77 | 123.84 |
| 17 | B | 4006 | BCR | C16-C17-C18 | -3.10 | 122.88 | 127.31 |
| 14 | Y | 504 | CLA | O2D-CGD-CBD | 3.10 | 116.78 | 111.27 |
| 17 | B | 4006 | BCR | C31-C1-C6 | -3.10 | 105.26 | 110.30 |
| 14 | B | 1201 | CLA | O2D-CGD-O1D | -3.10 | 117.77 | 123.84 |
| 14 | n | 1503 | CLA | O2D-CGD-O1D | -3.10 | 117.77 | 123.84 |
| 14 | s | 502 | CLA | CHB-C4A-NA | 3.10 | 128.80 | 124.51 |
| 17 | 6 | 524 | BCR | C15-C16-C17 | -3.10 | 117.12 | 123.47 |
| 17 | J | 4013 | BCR | C2-C1-C6 | 3.10 | 115.26 | 110.48 |
| 14 | e | 1132 | CLA | CAC-C3C-C4C | 3.10 | 128.84 | 124.81 |
| 21 | a | 822 | SQD | O47-C7-C8 | 3.10 | 119.45 | 110.80 |
| 14 | G | 1137 | CLA | CHB-C4A-NA | 3.10 | 128.80 | 124.51 |
| 17 | G | 4001 | BCR | C11-C10-C9 | -3.10 | 122.88 | 127.31 |
| 17 | f | 4006 | BCR | C31-C1-C6 | -3.10 | 105.27 | 110.30 |
| 14 | A | 1137 | CLA | CHB-C4A-NA | 3.10 | 128.80 | 124.51 |
| 14 | H | 1023 | CLA | C1B-CHB-C4A | -3.10 | 123.98 | 130.12 |
| 14 | V | 1503 | CLA | O2D-CGD-O1D | -3.10 | 117.78 | 123.84 |
| 17 | e | 4001 | BCR | C11-C10-C9 | -3.10 | 122.89 | 127.31 |
| 21 | V | 5216 | SQD | O47-C7-C8 | 3.10 | 118.17 | 111.50 |
| 14 | e | 1237 | CLA | O2D-CGD-O1D | -3.10 | 117.78 | 123.84 |
| 14 | f | 1201 | CLA | O2D-CGD-O1D | -3.10 | 117.78 | 123.84 |
| 17 | V | 4219 | BCR | C11-C10-C9 | -3.10 | 122.89 | 127.31 |
| 14 | H | 1201 | CLA | CHB-C4A-NA | 3.10 | 128.79 | 124.51 |
| 17 | J | 4015 | BCR | C20-C21-C22 | -3.10 | 122.89 | 127.31 |
| 21 | s | 822 | SQD | O47-C7-C8 | 3.10 | 119.43 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | t | 523 | BCR | C10-C11-C12 | -3.10 | 113.56 | 123.22 |
| 14 | B | 1023 | CLA | C1B-CHB-C4A | -3.09 | 123.99 | 130.12 |
| 17 | S | 4018 | BCR | C1-C6-C5 | -3.09 | 118.25 | 122.61 |
| 21 | L | 5216 | SQD | O47-C7-C8 | 3.09 | 118.17 | 111.50 |
| 17 | L | 4219 | BCR | C11-C10-C9 | -3.09 | 122.90 | 127.31 |
| 14 | G | 1132 | CLA | CAC-C3C-C4C | 3.09 | 128.82 | 124.81 |
| 17 | 4 | 523 | BCR | C10-C11-C12 | -3.09 | 113.57 | 123.22 |
| 14 | f | 1236 | CLA | O2D-CGD-O1D | -3.09 | 117.80 | 123.84 |
| 14 | f | 1023 | CLA | C1B-CHB-C4A | -3.09 | 124.00 | 130.12 |
| 17 | H | 4006 | BCR | C31-C1-C6 | -3.09 | 105.29 | 110.30 |
| 17 | A | 4001 | BCR | C11-C10-C9 | -3.09 | 122.90 | 127.31 |
| 17 | b | 523 | BCR | C10-C11-C12 | -3.09 | 113.58 | 123.22 |
| 14 | A | 1237 | CLA | C4-C3-C5 | 3.09 | 120.46 | 115.27 |
| 14 | f | 1215 | CLA | O2D-CGD-O1D | -3.09 | 117.80 | 123.84 |
| 17 | H | 4006 | BCR | C16-C17-C18 | -3.09 | 122.91 | 127.31 |
| 17 | Z | 523 | BCR | C28-C27-C26 | -3.09 | 108.57 | 114.08 |
| 17 | U | 4104 | BCR | C15-C14-C13 | -3.08 | 122.91 | 127.31 |
| 21 | u | 822 | SQD | O6-C1-C2 | 3.08 | 113.12 | 108.30 |
| 21 | 5 | 822 | SQD | O6-C1-C2 | 3.08 | 113.11 | 108.30 |
| 21 | n | 5216 | SQD | O47-C7-C8 | 3.08 | 118.14 | 111.50 |
| 17 | v | 524 | BCR | C15-C16-C17 | -3.08 | 117.16 | 123.47 |
| 17 | m | 4104 | BCR | C15-C14-C13 | -3.08 | 122.91 | 127.31 |
| 17 | B | 4009 | BCR | C16-C17-C18 | -3.08 | 122.92 | 127.31 |
| 17 | K | 4104 | BCR | C11-C10-C9 | -3.08 | 122.92 | 127.31 |
| 17 | A | 4011 | BCR | C20-C19-C18 | -3.08 | 117.77 | 126.42 |
| 18 | G | 5003 | LHG | O8-C23-C24 | 3.08 | 121.57 | 111.91 |
| 17 | 2 | 523 | BCR | C28-C27-C26 | -3.08 | 108.58 | 114.08 |
| 14 | A | 1237 | CLA | O2D-CGD-O1D | -3.08 | 117.82 | 123.84 |
| 14 | G | 1140 | CLA | CMB-C2B-C3B | 3.07 | 130.43 | 124.68 |
| 14 | L | 1501 | CLA | CMB-C2B-C3B | 3.07 | 130.43 | 124.68 |
| 18 | A | 5003 | LHG | O8-C23-C24 | 3.07 | 121.55 | 111.91 |
| 17 | e | 4011 | BCR | C20-C19-C18 | -3.07 | 117.78 | 126.42 |
| 17 | r | 523 | BCR | C28-C27-C26 | -3.07 | 108.59 | 114.08 |
| 14 | A | 1131 | CLA | O2D-CGD-O1D | -3.07 | 117.83 | 123.84 |
| 14 | 4 | 513 | CLA | CMB-C2B-C3B | 3.07 | 130.43 | 124.68 |
| 17 | G | 4008 | BCR | C10-C11-C12 | -3.07 | 113.63 | 123.22 |
| 14 | V | 1501 | CLA | CMB-C2B-C3B | 3.07 | 130.42 | 124.68 |
| 18 | e | 5003 | LHG | O8-C23-C24 | 3.07 | 121.54 | 111.91 |
| 21 | c | 822 | SQD | O6-C1-C2 | 3.07 | 113.09 | 108.30 |
| 17 | f | 4009 | BCR | C16-C17-C18 | -3.07 | 122.93 | 127.31 |
| 17 | n | 4219 | BCR | C11-C10-C9 | -3.07 | 122.93 | 127.31 |
| 14 | e | 1131 | CLA | CMB-C2B-C1B | -3.07 | 123.75 | 128.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1131 | CLA | O2D-CGD-O1D | -3.07 | 117.84 | 123.84 |
| 17 | K | 4104 | BCR | C15-C14-C13 | -3.07 | 122.93 | 127.31 |
| 14 | e | 1237 | CLA | C4-C3-C5 | 3.07 | 120.43 | 115.27 |
| 14 | e | 1118 | CLA | CMB-C2B-C3B | 3.07 | 130.42 | 124.68 |
| 14 | 6 | 519 | CLA | CMB-C2B-C1B | -3.07 | 123.75 | 128.46 |
| 17 | G | 4011 | BCR | C20-C19-C18 | -3.07 | 117.80 | 126.42 |
| 14 | B | 1236 | CLA | O2D-CGD-O1D | -3.07 | 117.84 | 123.84 |
| 17 | U | 4104 | BCR | C11-C10-C9 | -3.06 | 122.94 | 127.31 |
| 17 | l | 4015 | BCR | C20-C21-C22 | -3.06 | 122.94 | 127.31 |
| 14 | n | 1501 | CLA | CMB-C2B-C3B | 3.06 | 130.41 | 124.68 |
| 17 | 2 | 521 | BCR | C3-C4-C5 | -3.06 | 108.61 | 114.08 |
| 14 | t | 513 | CLA | CMB-C2B-C3B | 3.06 | 130.41 | 124.68 |
| 14 | A | 1118 | CLA | CMB-C2B-C3B | 3.06 | 130.41 | 124.68 |
| 14 | 5 | 510 | CLA | CMB-C2B-C3B | 3.06 | 130.41 | 124.68 |
| 14 | d | 519 | CLA | CMB-C2B-C1B | -3.06 | 123.76 | 128.46 |
| 14 | v | 519 | CLA | CMB-C2B-C1B | -3.06 | 123.76 | 128.46 |
| 14 | G | 1237 | CLA | O2D-CGD-O1D | -3.06 | 117.85 | 123.84 |
| 17 | r | 521 | BCR | C3-C4-C5 | -3.06 | 108.61 | 114.08 |
| 14 | H | 1230 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 17 | W | 4021 | BCR | C11-C10-C9 | -3.06 | 122.94 | 127.31 |
| 14 | G | 1101 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 14 | e | 1131 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 17 | Z | 521 | BCR | C3-C4-C5 | -3.06 | 108.62 | 114.08 |
| 14 | 2 | 509 | CLA | CHB-C4A-NA | 3.06 | 128.74 | 124.51 |
| 14 | u | 504 | CLA | CMB-C2B-C3B | 3.06 | 130.40 | 124.68 |
| 17 | e | 4008 | BCR | C10-C11-C12 | -3.06 | 113.68 | 123.22 |
| 17 | t | 521 | BCR | C15-C14-C13 | -3.06 | 122.95 | 127.31 |
| 14 | e | 1140 | CLA | CMB-C2B-C3B | 3.06 | 130.40 | 124.68 |
| 14 | H | 1228 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 14 | 4 | 507 | CLA | CMB-C2B-C3B | 3.06 | 130.39 | 124.68 |
| 17 | A | 4008 | BCR | C10-C11-C12 | -3.06 | 113.68 | 123.22 |
| 14 | c | 510 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |
| 21 | 1 | 822 | SQD | O8-S-C6 | 3.05 | 110.61 | 105.74 |
| 14 | 5 | 504 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |
| 14 | f | 1225 | CLA | C1B-CHB-C4A | -3.05 | 124.07 | 130.12 |
| 14 | e | 1101 | CLA | O2D-CGD-O1D | -3.05 | 117.87 | 123.84 |
| 14 | A | 1140 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |
| 14 | B | 1225 | CLA | C1B-CHB-C4A | -3.05 | 124.07 | 130.12 |
| 17 | R | 4016 | BCR | C28-C27-C26 | -3.05 | 108.63 | 114.08 |
| 14 | B | 1215 | CLA | O2D-CGD-O1D | -3.05 | 117.87 | 123.84 |
| 14 | B | 1230 | CLA | O2D-CGD-O1D | -3.05 | 117.87 | 123.84 |
| 14 | r | 501 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | M | 4021 | BCR | C11-C10-C9 | -3.05 | 122.95 | 127.31 |
| 14 | b | 507 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |
| 14 | u | 510 | CLA | CMB-C2B-C3B | 3.05 | 130.39 | 124.68 |
| 17 | G | 4008 | BCR | C11-C10-C9 | -3.05 | 122.96 | 127.31 |
| 14 | b | 513 | CLA | CMB-C2B-C3B | 3.05 | 130.38 | 124.68 |
| 14 | Z | 509 | CLA | CHB-C4A-NA | 3.05 | 128.73 | 124.51 |
| 14 | a | 519 | CLA | CMB-C2B-C1B | -3.05 | 123.78 | 128.46 |
| 14 | b | 519 | CLA | O2D-CGD-O1D | -3.05 | 117.88 | 123.84 |
| 14 | B | 1228 | CLA | O2D-CGD-O1D | -3.05 | 117.88 | 123.84 |
| 14 | G | 1118 | CLA | CMB-C2B-C3B | 3.05 | 130.38 | 124.68 |
| 14 | 2 | 502 | CLA | CMB-C2B-C1B | -3.05 | 123.78 | 128.46 |
| 14 | A | 1101 | CLA | O2D-CGD-O1D | -3.05 | 117.88 | 123.84 |
| 14 | Z | 501 | CLA | CMB-C2B-C3B | 3.05 | 130.38 | 124.68 |
| 17 | L | 4219 | BCR | C37-C22-C23 | 3.05 | 122.88 | 118.08 |
| 14 | f | 1227 | CLA | CHB-C4A-NA | 3.05 | 128.72 | 124.51 |
| 17 | T | 4012 | BCR | C16-C17-C18 | -3.05 | 122.96 | 127.31 |
| 14 | f | 1228 | CLA | O2D-CGD-O1D | -3.05 | 117.88 | 123.84 |
| 17 | n | 4219 | BCR | C37-C22-C23 | 3.05 | 122.88 | 118.08 |
| 21 | q | 822 | SQD | O8-S-C6 | 3.04 | 110.59 | 105.74 |
| 17 | B | 4010 | BCR | C33-C5-C4 | 3.04 | 119.47 | 113.62 |
| 14 | H | 1228 | CLA | CHB-C4A-NA | 3.04 | 128.72 | 124.51 |
| 14 | r | 509 | CLA | CHB-C4A-NA | 3.04 | 128.72 | 124.51 |
| 14 | u | 512 | CLA | CMB-C2B-C3B | 3.04 | 130.37 | 124.68 |
| 17 | j | 4016 | BCR | C28-C27-C26 | -3.04 | 108.64 | 114.08 |
| 14 | 2 | 501 | CLA | O2D-CGD-O1D | -3.04 | 117.89 | 123.84 |
| 14 | t | 519 | CLA | O2D-CGD-O1D | -3.04 | 117.89 | 123.84 |
| 17 | r | 522 | BCR | C15-C16-C17 | -3.04 | 117.24 | 123.47 |
| 17 | H | 4010 | BCR | C33-C5-C4 | 3.04 | 119.46 | 113.62 |
| 17 | F | 4016 | BCR | C28-C27-C26 | -3.04 | 108.64 | 114.08 |
| 14 | f | 1230 | CLA | O2D-CGD-O1D | -3.04 | 117.89 | 123.84 |
| 14 | K | 1103 | CLA | CMB-C2B-C1B | -3.04 | 123.79 | 128.46 |
| 21 | Y | 822 | SQD | O8-S-C6 | 3.04 | 110.59 | 105.74 |
| 17 | f | 4010 | BCR | C33-C5-C4 | 3.04 | 119.46 | 113.62 |
| 14 | G | 1115 | CLA | CHB-C4A-NA | 3.04 | 128.72 | 124.51 |
| 14 | 2 | 501 | CLA | CMB-C2B-C3B | 3.04 | 130.37 | 124.68 |
| 14 | H | 1225 | CLA | C1B-CHB-C4A | -3.04 | 124.09 | 130.12 |
| 14 | A | 1131 | CLA | CMB-C2B-C1B | -3.04 | 123.79 | 128.46 |
| 14 | H | 1236 | CLA | O2D-CGD-O1D | -3.04 | 117.89 | 123.84 |
| 17 | b | 521 | BCR | C15-C14-C13 | -3.04 | 122.97 | 127.31 |
| 17 | f | 4014 | BCR | C28-C27-C26 | -3.04 | 108.65 | 114.08 |
| 14 | r | 501 | CLA | O2D-CGD-O1D | -3.04 | 117.89 | 123.84 |
| 14 | t | 507 | CLA | CMB-C2B-C3B | 3.04 | 130.37 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1227 | CLA | CHB-C4A-NA | 3.04 | 128.72 | 124.51 |
| 14 | a | 509 | CLA | CHB-C4A-NA | 3.04 | 128.72 | 124.51 |
| 14 | q | 502 | CLA | CMB-C2B-C1B | -3.04 | 123.79 | 128.46 |
| 17 | c | 523 | BCR | C24-C23-C22 | -3.04 | 121.64 | 126.23 |
| 14 | H | 1203 | CLA | O2D-CGD-O1D | -3.04 | 117.90 | 123.84 |
| 14 | l | 502 | CLA | CMB-C2B-C1B | -3.04 | 123.80 | 128.46 |
| 14 | G | 1131 | CLA | CMB-C2B-C1B | -3.04 | 123.80 | 128.46 |
| 14 | U | 1103 | CLA | CMB-C2B-C1B | -3.04 | 123.80 | 128.46 |
| 17 | 4 | 521 | BCR | C15-C14-C13 | -3.04 | 122.98 | 127.31 |
| 21 | b | 822 | SQD | O8-S-C6 | 3.04 | 110.58 | 105.74 |
| 14 | 4 | 519 | CLA | O2D-CGD-O1D | -3.04 | 117.90 | 123.84 |
| 17 | v | 523 | BCR | C24-C23-C22 | -3.03 | 121.65 | 126.23 |
| 21 | t | 822 | SQD | O8-S-C6 | 3.03 | 110.58 | 105.74 |
| 14 | f | 1236 | CLA | CMB-C2B-C1B | -3.03 | 123.80 | 128.46 |
| 14 | B | 1227 | CLA | CHB-C4A-NA | 3.03 | 128.71 | 124.51 |
| 17 | B | 4005 | BCR | C33-C5-C6 | -3.03 | 121.12 | 124.53 |
| 14 | Z | 502 | CLA | CMB-C2B-C1B | -3.03 | 123.80 | 128.46 |
| 14 | f | 1229 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 17 | B | 4014 | BCR | C28-C27-C26 | -3.03 | 108.66 | 114.08 |
| 17 | V | 4219 | BCR | C37-C22-C23 | 3.03 | 122.86 | 118.08 |
| 14 | H | 1215 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 14 | c | 504 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 14 | d | 501 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 14 | 5 | 512 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 14 | c | 505 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 14 | H | 1235 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 14 | r | 502 | CLA | CMB-C2B-C1B | -3.03 | 123.80 | 128.46 |
| 14 | 6 | 501 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 14 | G | 1119 | CLA | C1B-CHB-C4A | -3.03 | 124.11 | 130.12 |
| 14 | e | 1119 | CLA | C1B-CHB-C4A | -3.03 | 124.11 | 130.12 |
| 14 | e | 1130 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 14 | Y | 503 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 14 | Z | 501 | CLA | O2D-CGD-O1D | -3.03 | 117.91 | 123.84 |
| 14 | r | 517 | CLA | CMB-C2B-C3B | 3.03 | 130.35 | 124.68 |
| 14 | e | 1112 | CLA | O2D-CGD-O1D | -3.03 | 117.92 | 123.84 |
| 17 | H | 4014 | BCR | C28-C27-C26 | -3.03 | 108.67 | 114.08 |
| 21 | u | 822 | SQD | O8-S-C6 | 3.03 | 110.56 | 105.74 |
| 17 | e | 4008 | BCR | C11-C10-C9 | -3.03 | 122.99 | 127.31 |
| 14 | J | 1302 | CLA | CHB-C4A-NA | 3.03 | 128.70 | 124.51 |
| 21 | 4 | 822 | SQD | O8-S-C6 | 3.03 | 110.56 | 105.74 |
| 19 | l | 5105 | LMU | O5'-C5'-C4' | 3.03 | 115.19 | 109.69 |
| 17 | J | 4012 | BCR | C33-C5-C6 | -3.03 | 121.13 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 2 | 522 | BCR | C15-C16-C17 | -3.02 | 117.28 | 123.47 |
| 14 | u | 505 | CLA | CMB-C2B-C3B | 3.02 | 130.33 | 124.68 |
| 17 | H | 4005 | BCR | C33-C5-C6 | -3.02 | 121.13 | 124.53 |
| 14 | G | 1130 | CLA | O2D-CGD-O1D | -3.02 | 117.93 | 123.84 |
| 17 | J | 4012 | BCR | C16-C17-C18 | -3.02 | 123.00 | 127.31 |
| 17 | o | 4021 | BCR | C11-C10-C9 | -3.02 | 123.00 | 127.31 |
| 14 | A | 1115 | CLA | CHB-C4A-NA | 3.02 | 128.69 | 124.51 |
| 14 | 1 | 503 | CLA | O2D-CGD-O1D | -3.02 | 117.93 | 123.84 |
| 17 | u | 523 | BCR | C24-C23-C22 | -3.02 | 121.67 | 126.23 |
| 14 | A | 1119 | CLA | C1B-CHB-C4A | -3.02 | 124.13 | 130.12 |
| 17 | Z | 522 | BCR | C15-C16-C17 | -3.02 | 117.29 | 123.47 |
| 14 | H | 1216 | CLA | O2D-CGD-O1D | -3.02 | 117.93 | 123.84 |
| 14 | B | 1228 | CLA | CHB-C4A-NA | 3.02 | 128.69 | 124.51 |
| 14 | s | 519 | CLA | CMB-C2B-C1B | -3.02 | 123.82 | 128.46 |
| 17 | v | 521 | BCR | C11-C10-C9 | -3.02 | 123.00 | 127.31 |
| 18 | e | 5004 | LHG | O8-C23-C24 | 3.02 | 121.38 | 111.91 |
| 14 | f | 1235 | CLA | CMB-C2B-C3B | 3.02 | 130.32 | 124.68 |
| 14 | B | 1234 | CLA | O2D-CGD-O1D | -3.02 | 117.94 | 123.84 |
| 17 | T | 4012 | BCR | C33-C5-C6 | -3.02 | 121.14 | 124.53 |
| 17 | l | 4012 | BCR | C16-C17-C18 | -3.02 | 123.00 | 127.31 |
| 14 | B | 1235 | CLA | O2D-CGD-O1D | -3.02 | 117.94 | 123.84 |
| 17 | n | 4020 | BCR | C10-C11-C12 | -3.02 | 113.80 | 123.22 |
| 14 | 5 | 505 | CLA | CMB-C2B-C3B | 3.02 | 130.32 | 124.68 |
| 17 | 6 | 523 | BCR | C24-C23-C22 | -3.02 | 121.68 | 126.23 |
| 17 | T | 4015 | BCR | C24-C23-C22 | -3.02 | 121.68 | 126.23 |
| 14 | B | 1216 | CLA | O2D-CGD-O1D | -3.02 | 117.94 | 123.84 |
| 14 | f | 1203 | CLA | O2D-CGD-O1D | -3.02 | 117.94 | 123.84 |
| 14 | m | 1103 | CLA | CMB-C2B-C1B | -3.02 | 123.83 | 128.46 |
| 21 | q | 822 | SQD | O9-S-C6 | 3.02 | 110.52 | 106.94 |
| 14 | 2 | 517 | CLA | CMB-C2B-C3B | 3.02 | 130.32 | 124.68 |
| 17 | S | 4018 | BCR | C21-C20-C19 | -3.01 | 113.81 | 123.22 |
| 17 | A | 4008 | BCR | C11-C10-C9 | -3.01 | 123.01 | 127.31 |
| 14 | e | 1115 | CLA | CHB-C4A-NA | 3.01 | 128.68 | 124.51 |
| 14 | B | 1203 | CLA | O2D-CGD-O1D | -3.01 | 117.94 | 123.84 |
| 17 | I | 4018 | BCR | C21-C20-C19 | -3.01 | 113.81 | 123.22 |
| 14 | A | 1130 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 14 | q | 503 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 14 | 3 | 519 | CLA | CMB-C2B-C1B | -3.01 | 123.83 | 128.46 |
| 14 | 3 | 509 | CLA | CHB-C4A-NA | 3.01 | 128.68 | 124.51 |
| 14 | s | 504 | CLA | CHB-C4A-NA | 3.01 | 128.68 | 124.51 |
| 14 | e | 1110 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 14 | A | 1140 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | v | 501 | CLA | CMB-C2B-C3B | 3.01 | 130.31 | 124.68 |
| 17 | J | 4015 | BCR | C24-C23-C22 | -3.01 | 121.69 | 126.23 |
| 14 | f | 1234 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 21 | f | 1852 | SQD | O9-S-C6 | 3.01 | 110.52 | 106.94 |
| 20 | H | 5002 | LMG | O1-C7-C8 | -3.01 | 103.64 | 110.90 |
| 19 | J | 5105 | LMU | O5'-C5'-C4' | 3.01 | 115.16 | 109.69 |
| 18 | G | 5004 | LHG | O8-C23-C24 | 3.01 | 121.35 | 111.91 |
| 14 | H | 1215 | CLA | CHB-C4A-NA | 3.01 | 128.67 | 124.51 |
| 21 | 5 | 822 | SQD | O8-S-C6 | 3.01 | 110.53 | 105.74 |
| 14 | G | 1140 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 14 | f | 1235 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 14 | B | 1235 | CLA | CMB-C2B-C3B | 3.01 | 130.31 | 124.68 |
| 20 | B | 5002 | LMG | O1-C7-C8 | -3.01 | 103.64 | 110.90 |
| 14 | l | 1302 | CLA | CHB-C4A-NA | 3.01 | 128.67 | 124.51 |
| 17 | L | 4020 | BCR | C10-C11-C12 | -3.01 | 113.83 | 123.22 |
| 20 | f | 5002 | LMG | O1-C7-C8 | -3.01 | 103.64 | 110.90 |
| 17 | a | 524 | BCR | C7-C8-C9 | -3.01 | 121.69 | 126.23 |
| 14 | c | 512 | CLA | CMB-C2B-C3B | 3.01 | 130.31 | 124.68 |
| 17 | l | 4012 | BCR | C33-C5-C6 | -3.01 | 121.15 | 124.53 |
| 18 | A | 5004 | LHG | O8-C23-C24 | 3.01 | 121.34 | 111.91 |
| 14 | e | 1126 | CLA | C1B-CHB-C4A | -3.01 | 124.16 | 130.12 |
| 14 | Y | 502 | CLA | CMB-C2B-C1B | -3.01 | 123.84 | 128.46 |
| 14 | f | 1216 | CLA | O2D-CGD-O1D | -3.01 | 117.96 | 123.84 |
| 17 | f | 4005 | BCR | C33-C5-C6 | -3.01 | 121.15 | 124.53 |
| 14 | Z | 517 | CLA | CMB-C2B-C3B | 3.01 | 130.30 | 124.68 |
| 14 | f | 1228 | CLA | CHB-C4A-NA | 3.01 | 128.67 | 124.51 |
| 14 | B | 1229 | CLA | O2D-CGD-O1D | -3.01 | 117.96 | 123.84 |
| 17 | k | 4018 | BCR | C21-C20-C19 | -3.00 | 113.84 | 123.22 |
| 17 | V | 4020 | BCR | C10-C11-C12 | -3.00 | 113.84 | 123.22 |
| 14 | A | 1126 | CLA | C1B-CHB-C4A | -3.00 | 124.17 | 130.12 |
| 14 | 4 | 517 | CLA | CMB-C2B-C3B | 3.00 | 130.30 | 124.68 |
| 14 | v | 518 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 17 | 5 | 523 | BCR | C24-C23-C22 | -3.00 | 121.70 | 126.23 |
| 14 | B | 1215 | CLA | CHB-C4A-NA | 3.00 | 128.66 | 124.51 |
| 17 | d | 523 | BCR | C24-C23-C22 | -3.00 | 121.70 | 126.23 |
| 17 | v | 522 | BCR | C20-C21-C22 | -3.00 | 123.03 | 127.31 |
| 17 | 6 | 522 | BCR | C20-C21-C22 | -3.00 | 123.03 | 127.31 |
| 21 | c | 822 | SQD | O8-S-C6 | 3.00 | 110.52 | 105.74 |
| 17 | T | 4013 | BCR | C7-C8-C9 | -3.00 | 121.70 | 126.23 |
| 14 | e | 1140 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 14 | H | 1229 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 17 | 3 | 524 | BCR | C7-C8-C9 | -3.00 | 121.70 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | P | 170 | FMN | C4-N3-C2 | -3.00 | 120.10 | 125.64 |
| 17 | d | 522 | BCR | C20-C21-C22 | -3.00 | 123.03 | 127.31 |
| 14 | A | 1112 | CLA | O2D-CGD-O1D | -3.00 | 117.98 | 123.84 |
| 22 | p | 170 | FMN | C4-N3-C2 | -3.00 | 120.10 | 125.64 |
| 14 | H | 1235 | CLA | CMB-C2B-C3B | 3.00 | 130.28 | 124.68 |
| 18 | A | 5002 | LHG | O8-C23-C24 | 3.00 | 121.31 | 111.91 |
| 19 | T | 5105 | LMU | O5'-C5'-C4' | 3.00 | 115.14 | 109.69 |
| 14 | T | 1302 | CLA | CHB-C4A-NA | 3.00 | 128.66 | 124.51 |
| 14 | F | 1301 | CLA | O2D-CGD-O1D | -3.00 | 117.98 | 123.84 |
| 14 | H | 1234 | CLA | O2D-CGD-O1D | -3.00 | 117.98 | 123.84 |
| 18 | G | 5002 | LHG | O8-C23-C24 | 3.00 | 121.31 | 111.91 |
| 14 | 3 | 504 | CLA | CHB-C4A-NA | 2.99 | 128.65 | 124.51 |
| 14 | Y | 501 | CLA | CMB-C2B-C3B | 2.99 | 130.28 | 124.68 |
| 17 | s | 524 | BCR | C7-C8-C9 | -2.99 | 121.71 | 126.23 |
| 21 | H | 1852 | SQD | O9-S-C6 | 2.99 | 110.50 | 106.94 |
| 14 | G | 1112 | CLA | O2D-CGD-O1D | -2.99 | 117.99 | 123.84 |
| 14 | 1 | 501 | CLA | CMB-C2B-C3B | 2.99 | 130.28 | 124.68 |
| 17 | I | 4018 | BCR | C10-C11-C12 | -2.99 | 113.88 | 123.22 |
| 14 | e | 1104 | CLA | CHB-C4A-NA | 2.99 | 128.65 | 124.51 |
| 14 | H | 1236 | CLA | CMB-C2B-C1B | -2.99 | 123.87 | 128.46 |
| 18 | e | 5002 | LHG | O8-C23-C24 | 2.99 | 121.29 | 111.91 |
| 14 | B | 1236 | CLA | CMB-C2B-C1B | -2.99 | 123.87 | 128.46 |
| 14 | s | 509 | CLA | CHB-C4A-NA | 2.99 | 128.65 | 124.51 |
| 17 | k | 4018 | BCR | C10-C11-C12 | -2.99 | 113.89 | 123.22 |
| 17 | S | 4018 | BCR | C10-C11-C12 | -2.99 | 113.89 | 123.22 |
| 14 | 5 | 519 | CLA | O2D-CGD-O1D | -2.99 | 117.99 | 123.84 |
| 17 | H | 4006 | BCR | C8-C9-C10 | 2.99 | 123.53 | 118.94 |
| 14 | s | 507 | CLA | CHB-C4A-NA | 2.99 | 128.64 | 124.51 |
| 14 | f | 1215 | CLA | CHB-C4A-NA | 2.99 | 128.64 | 124.51 |
| 14 | b | 517 | CLA | CMB-C2B-C3B | 2.99 | 130.27 | 124.68 |
| 14 | 6 | 518 | CLA | O2D-CGD-O1D | -2.99 | 118.00 | 123.84 |
| 14 | G | 1126 | CLA | C1B-CHB-C4A | -2.99 | 124.20 | 130.12 |
| 14 | d | 518 | CLA | O2D-CGD-O1D | -2.99 | 118.00 | 123.84 |
| 14 | a | 507 | CLA | CHB-C4A-NA | 2.99 | 128.64 | 124.51 |
| 14 | q | 501 | CLA | CMB-C2B-C3B | 2.99 | 130.26 | 124.68 |
| 17 | c | 521 | BCR | C30-C25-C26 | -2.99 | 118.41 | 122.61 |
| 17 | J | 4013 | BCR | C16-C15-C14 | -2.98 | 117.36 | 123.47 |
| 14 | c | 519 | CLA | O2D-CGD-O1D | -2.98 | 118.00 | 123.84 |
| 21 | 1 | 822 | SQD | O9-S-C6 | 2.98 | 110.48 | 106.94 |
| 21 | 5 | 822 | SQD | O9-S-C6 | 2.98 | 110.48 | 106.94 |
| 17 | b | 523 | BCR | C16-C17-C18 | -2.98 | 123.05 | 127.31 |
| 14 | A | 1110 | CLA | O2D-CGD-O1D | -2.98 | 118.01 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | j | 1301 | CLA | O2D-CGD-O1D | -2.98 | 118.01 | 123.84 |
| 17 | l | 4015 | BCR | C24-C23-C22 | -2.98 | 121.73 | 126.23 |
| 14 | B | 1208 | CLA | O2D-CGD-O1D | -2.98 | 118.01 | 123.84 |
| 14 | t | 517 | CLA | CMB-C2B-C3B | 2.98 | 130.26 | 124.68 |
| 17 | 5 | 521 | BCR | C30-C25-C26 | -2.98 | 118.41 | 122.61 |
| 21 | d | 822 | SQD | O8-S-C6 | 2.98 | 110.49 | 105.74 |
| 17 | l | 4013 | BCR | C16-C15-C14 | -2.98 | 117.37 | 123.47 |
| 17 | s | 521 | BCR | C24-C23-C22 | -2.98 | 121.73 | 126.23 |
| 22 | X | 170 | FMN | C4-N3-C2 | -2.98 | 120.14 | 125.64 |
| 21 | B | 1852 | SQD | O9-S-C6 | 2.98 | 110.48 | 106.94 |
| 17 | d | 521 | BCR | C11-C10-C9 | -2.98 | 123.06 | 127.31 |
| 14 | e | 1121 | CLA | O2D-CGD-O1D | -2.98 | 118.01 | 123.84 |
| 14 | f | 1208 | CLA | O2D-CGD-O1D | -2.98 | 118.01 | 123.84 |
| 14 | c | 503 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 17 | 6 | 521 | BCR | C11-C10-C9 | -2.98 | 123.06 | 127.31 |
| 17 | A | 4011 | BCR | C34-C9-C10 | -2.98 | 118.75 | 122.92 |
| 14 | T | 1303 | CLA | CMB-C2B-C3B | 2.98 | 130.25 | 124.68 |
| 14 | a | 504 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 14 | v | 503 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 17 | l | 4015 | BCR | C2-C1-C6 | 2.98 | 115.06 | 110.48 |
| 14 | H | 1219 | CLA | CMB-C2B-C3B | 2.98 | 130.25 | 124.68 |
| 21 | v | 822 | SQD | O8-S-C6 | 2.98 | 110.48 | 105.74 |
| 14 | G | 1138 | CLA | C1B-CHB-C4A | -2.98 | 124.22 | 130.12 |
| 17 | a | 524 | BCR | C8-C7-C6 | -2.97 | 118.85 | 127.20 |
| 14 | R | 1301 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 17 | G | 4011 | BCR | C34-C9-C10 | -2.97 | 118.76 | 122.92 |
| 17 | a | 524 | BCR | C15-C16-C17 | -2.97 | 117.39 | 123.47 |
| 14 | u | 509 | CLA | CHB-C4A-NA | 2.97 | 128.62 | 124.51 |
| 14 | H | 1213 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 17 | T | 4013 | BCR | C16-C15-C14 | -2.97 | 117.39 | 123.47 |
| 14 | l | 1303 | CLA | CMB-C2B-C3B | 2.97 | 130.24 | 124.68 |
| 14 | B | 1213 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 14 | G | 1117 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 21 | Y | 822 | SQD | O9-S-C6 | 2.97 | 110.47 | 106.94 |
| 17 | J | 4013 | BCR | C7-C8-C9 | -2.97 | 121.75 | 126.23 |
| 14 | a | 518 | CLA | CMB-C2B-C1B | -2.97 | 123.90 | 128.46 |
| 14 | A | 1104 | CLA | CHB-C4A-NA | 2.97 | 128.62 | 124.51 |
| 17 | a | 521 | BCR | C24-C23-C22 | -2.97 | 121.75 | 126.23 |
| 14 | F | 1301 | CLA | CMB-C2B-C3B | 2.97 | 130.23 | 124.68 |
| 17 | 3 | 524 | BCR | C15-C16-C17 | -2.97 | 117.39 | 123.47 |
| 14 | j | 1301 | CLA | CMB-C2B-C3B | 2.97 | 130.23 | 124.68 |
| 14 | 3 | 507 | CLA | CHB-C4A-NA | 2.97 | 128.62 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1219 | CLA | CMB-C2B-C3B | 2.97 | 130.23 | 124.68 |
| 21 | u | 822 | SQD | O9-S-C6 | 2.97 | 110.47 | 106.94 |
| 17 | 3 | 521 | BCR | C24-C23-C22 | -2.97 | 121.75 | 126.23 |
| 17 | u | 523 | BCR | C20-C21-C22 | -2.97 | 123.07 | 127.31 |
| 17 | u | 521 | BCR | C30-C25-C26 | -2.97 | 118.44 | 122.61 |
| 17 | B | 4006 | BCR | C8-C9-C10 | 2.97 | 123.49 | 118.94 |
| 14 | H | 1222 | CLA | CAA-C2A-C1A | -2.97 | 102.25 | 111.97 |
| 17 | s | 524 | BCR | C15-C16-C17 | -2.97 | 117.40 | 123.47 |
| 17 | c | 521 | BCR | C38-C26-C27 | 2.97 | 119.31 | 113.62 |
| 21 | c | 822 | SQD | O9-S-C6 | 2.97 | 110.46 | 106.94 |
| 14 | R | 1301 | CLA | CMB-C2B-C3B | 2.97 | 130.23 | 124.68 |
| 17 | s | 524 | BCR | C8-C7-C6 | -2.96 | 118.88 | 127.20 |
| 14 | G | 1110 | CLA | O2D-CGD-O1D | -2.96 | 118.04 | 123.84 |
| 14 | f | 1219 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 14 | Z | 502 | CLA | CHB-C4A-NA | 2.96 | 128.61 | 124.51 |
| 14 | u | 501 | CLA | CHB-C4A-NA | 2.96 | 128.61 | 124.51 |
| 14 | A | 1121 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 14 | u | 519 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 14 | 5 | 501 | CLA | CHB-C4A-NA | 2.96 | 128.61 | 124.51 |
| 17 | 3 | 524 | BCR | C8-C7-C6 | -2.96 | 118.88 | 127.20 |
| 14 | J | 1303 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 17 | l | 4013 | BCR | C7-C8-C9 | -2.96 | 121.76 | 126.23 |
| 14 | H | 1208 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 14 | A | 1111 | CLA | CHB-C4A-NA | 2.96 | 128.61 | 124.51 |
| 14 | 3 | 518 | CLA | CMB-C2B-C1B | -2.96 | 123.91 | 128.46 |
| 17 | f | 4006 | BCR | C8-C9-C10 | 2.96 | 123.48 | 118.94 |
| 14 | H | 1207 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 14 | s | 518 | CLA | CMB-C2B-C1B | -2.96 | 123.91 | 128.46 |
| 21 | 6 | 822 | SQD | O8-S-C6 | 2.96 | 110.46 | 105.74 |
| 14 | 4 | 519 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 14 | v | 518 | CLA | CMB-C2B-C3B | 2.96 | 130.22 | 124.68 |
| 14 | G | 1126 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 17 | H | 4010 | BCR | C38-C26-C27 | 2.96 | 119.30 | 113.62 |
| 14 | H | 1223 | CLA | O2D-CGD-O1D | -2.96 | 118.05 | 123.84 |
| 14 | H | 1023 | CLA | CBC-CAC-C3C | 2.96 | 120.59 | 112.43 |
| 14 | d | 507 | CLA | CHB-C4A-NA | 2.96 | 128.60 | 124.51 |
| 14 | f | 1222 | CLA | CAA-C2A-C1A | -2.96 | 102.28 | 111.97 |
| 14 | B | 1222 | CLA | CAA-C2A-C1A | -2.96 | 102.28 | 111.97 |
| 14 | G | 1104 | CLA | CHB-C4A-NA | 2.96 | 128.60 | 124.51 |
| 19 | e | 1848 | LMU | C1B-O1B-C4' | -2.96 | 110.65 | 117.96 |
| 14 | A | 1138 | CLA | C1B-CHB-C4A | -2.96 | 124.26 | 130.12 |
| 14 | f | 1213 | CLA | O2D-CGD-O1D | -2.96 | 118.06 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1023 | CLA | CBC-CAC-C3C | 2.96 | 120.58 | 112.43 |
| 14 | B | 1216 | CLA | C1B-CHB-C4A | -2.95 | 124.27 | 130.12 |
| 14 | G | 1111 | CLA | CHB-C4A-NA | 2.95 | 128.60 | 124.51 |
| 14 | u | 503 | CLA | CHB-C4A-NA | 2.95 | 128.60 | 124.51 |
| 14 | v | 507 | CLA | CHB-C4A-NA | 2.95 | 128.60 | 124.51 |
| 14 | b | 519 | CLA | CMB-C2B-C3B | 2.95 | 130.21 | 124.68 |
| 14 | G | 1140 | CLA | CBA-CAA-C2A | 2.95 | 122.58 | 113.86 |
| 14 | A | 1109 | CLA | O2D-CGD-O1D | -2.95 | 118.06 | 123.84 |
| 14 | f | 1223 | CLA | O2D-CGD-O1D | -2.95 | 118.06 | 123.84 |
| 17 | u | 521 | BCR | C38-C26-C27 | 2.95 | 119.29 | 113.62 |
| 14 | 6 | 512 | CLA | CMB-C2B-C3B | 2.95 | 130.20 | 124.68 |
| 17 | 5 | 521 | BCR | C38-C26-C27 | 2.95 | 119.29 | 113.62 |
| 17 | J | 4015 | BCR | C2-C1-C6 | 2.95 | 115.03 | 110.48 |
| 14 | v | 513 | CLA | O2D-CGD-O1D | -2.95 | 118.07 | 123.84 |
| 14 | d | 512 | CLA | CMB-C2B-C3B | 2.95 | 130.20 | 124.68 |
| 14 | 2 | 502 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 14 | 6 | 503 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 14 | A | 1140 | CLA | CBA-CAA-C2A | 2.95 | 122.57 | 113.86 |
| 14 | Z | 518 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 14 | s | 504 | CLA | O2D-CGD-O1D | -2.95 | 118.07 | 123.84 |
| 17 | l | 4015 | BCR | C32-C1-C6 | -2.95 | 105.52 | 110.30 |
| 14 | n | 1502 | CLA | O2D-CGD-CBD | 2.95 | 116.51 | 111.27 |
| 14 | e | 1105 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 17 | t | 523 | BCR | C16-C17-C18 | -2.95 | 123.10 | 127.31 |
| 17 | b | 524 | BCR | C33-C5-C4 | 2.95 | 119.28 | 113.62 |
| 14 | c | 509 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 17 | 4 | 523 | BCR | C16-C17-C18 | -2.95 | 123.10 | 127.31 |
| 17 | B | 4010 | BCR | C38-C26-C27 | 2.95 | 119.28 | 113.62 |
| 17 | T | 4015 | BCR | C2-C1-C6 | 2.95 | 115.02 | 110.48 |
| 17 | b | 524 | BCR | C20-C21-C22 | -2.95 | 123.11 | 127.31 |
| 14 | B | 1023 | CLA | CBC-CAC-C3C | 2.95 | 120.55 | 112.43 |
| 19 | A | 1848 | LMU | C1B-O1B-C4' | -2.95 | 110.67 | 117.96 |
| 14 | U | 1103 | CLA | O2D-CGD-O1D | -2.95 | 118.08 | 123.84 |
| 14 | f | 1216 | CLA | C1B-CHB-C4A | -2.95 | 124.28 | 130.12 |
| 19 | G | 1848 | LMU | C1B-O1B-C4' | -2.94 | 110.68 | 117.96 |
| 14 | e | 1140 | CLA | CBA-CAA-C2A | 2.94 | 122.55 | 113.86 |
| 14 | A | 1117 | CLA | O2D-CGD-O1D | -2.94 | 118.08 | 123.84 |
| 14 | A | 1126 | CLA | O2D-CGD-O1D | -2.94 | 118.08 | 123.84 |
| 14 | B | 1223 | CLA | O2D-CGD-O1D | -2.94 | 118.08 | 123.84 |
| 14 | 5 | 503 | CLA | CHB-C4A-NA | 2.94 | 128.58 | 124.51 |
| 17 | F | 4016 | BCR | C20-C21-C22 | -2.94 | 123.11 | 127.31 |
| 17 | 5 | 523 | BCR | C20-C21-C22 | -2.94 | 123.11 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | c | 523 | BCR | C20-C21-C22 | -2.94 | 123.11 | 127.31 |
| 14 | L | 1502 | CLA | O2D-CGD-CBD | 2.94 | 116.50 | 111.27 |
| 17 | e | 4011 | BCR | C34-C9-C10 | -2.94 | 118.80 | 122.92 |
| 14 | B | 1207 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 14 | e | 1117 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 14 | f | 1207 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 14 | e | 1138 | CLA | C1B-CHB-C4A | -2.94 | 124.29 | 130.12 |
| 17 | 4 | 524 | BCR | C20-C21-C22 | -2.94 | 123.11 | 127.31 |
| 14 | r | 502 | CLA | CHB-C4A-NA | 2.94 | 128.58 | 124.51 |
| 17 | f | 4010 | BCR | C38-C26-C27 | 2.94 | 119.26 | 113.62 |
| 14 | 6 | 518 | CLA | CMB-C2B-C3B | 2.94 | 130.18 | 124.68 |
| 14 | e | 1109 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 14 | 6 | 507 | CLA | CHB-C4A-NA | 2.94 | 128.57 | 124.51 |
| 14 | 5 | 509 | CLA | CHB-C4A-NA | 2.94 | 128.57 | 124.51 |
| 14 | G | 1121 | CLA | O2D-CGD-O1D | -2.94 | 118.10 | 123.84 |
| 14 | 4 | 503 | CLA | CHB-C4A-NA | 2.94 | 128.57 | 124.51 |
| 14 | K | 1103 | CLA | O2D-CGD-O1D | -2.94 | 118.10 | 123.84 |
| 14 | H | 1216 | CLA | C1B-CHB-C4A | -2.94 | 124.30 | 130.12 |
| 14 | A | 1105 | CLA | CHB-C4A-NA | 2.94 | 128.57 | 124.51 |
| 14 | s | 502 | CLA | CMB-C2B-C1B | -2.93 | 123.95 | 128.46 |
| 14 | d | 513 | CLA | O2D-CGD-O1D | -2.93 | 118.10 | 123.84 |
| 14 | G | 1109 | CLA | O2D-CGD-O1D | -2.93 | 118.10 | 123.84 |
| 17 | R | 4016 | BCR | C20-C21-C22 | -2.93 | 123.12 | 127.31 |
| 14 | d | 518 | CLA | CMB-C2B-C3B | 2.93 | 130.17 | 124.68 |
| 14 | 5 | 502 | CLA | CHB-C4A-NA | 2.93 | 128.57 | 124.51 |
| 14 | G | 1132 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 14 | r | 516 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 17 | Y | 523 | BCR | C10-C11-C12 | -2.93 | 114.07 | 123.22 |
| 14 | c | 501 | CLA | CHB-C4A-NA | 2.93 | 128.57 | 124.51 |
| 14 | 2 | 516 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 14 | t | 503 | CLA | CHB-C4A-NA | 2.93 | 128.56 | 124.51 |
| 14 | G | 1139 | CLA | O2D-CGD-O1D | -2.93 | 118.11 | 123.84 |
| 14 | V | 1502 | CLA | O2D-CGD-CBD | 2.93 | 116.47 | 111.27 |
| 17 | j | 4016 | BCR | C20-C21-C22 | -2.93 | 123.13 | 127.31 |
| 17 | 4 | 524 | BCR | C33-C5-C4 | 2.93 | 119.24 | 113.62 |
| 14 | e | 1111 | CLA | CHB-C4A-NA | 2.93 | 128.56 | 124.51 |
| 14 | Y | 503 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 14 | t | 519 | CLA | CMB-C2B-C3B | 2.93 | 130.16 | 124.68 |
| 14 | v | 512 | CLA | CMB-C2B-C3B | 2.93 | 130.15 | 124.68 |
| 14 | d | 502 | CLA | CHB-C4A-NA | 2.93 | 128.56 | 124.51 |
| 17 | 1 | 523 | BCR | C10-C11-C12 | -2.92 | 114.09 | 123.22 |
| 17 | J | 4015 | BCR | C32-C1-C6 | -2.92 | 105.56 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1105 | CLA | CHB-C4A-NA | 2.92 | 128.56 | 124.51 |
| 17 | q | 523 | BCR | C10-C11-C12 | -2.92 | 114.09 | 123.22 |
| 14 | u | 516 | CLA | CMB-C2B-C3B | 2.92 | 130.15 | 124.68 |
| 14 | e | 1120 | CLA | CHB-C4A-NA | 2.92 | 128.55 | 124.51 |
| 14 | a | 512 | CLA | CMB-C2B-C3B | 2.92 | 130.15 | 124.68 |
| 14 | b | 508 | CLA | C1B-CHB-C4A | -2.92 | 124.33 | 130.12 |
| 14 | A | 1120 | CLA | CHB-C4A-NA | 2.92 | 128.55 | 124.51 |
| 17 | 5 | 524 | BCR | C33-C5-C4 | 2.92 | 119.23 | 113.62 |
| 17 | t | 524 | BCR | C33-C5-C4 | 2.92 | 119.23 | 113.62 |
| 17 | L | 4219 | BCR | C7-C8-C9 | -2.92 | 121.82 | 126.23 |
| 14 | H | 1214 | CLA | O2D-CGD-O1D | -2.92 | 118.13 | 123.84 |
| 14 | d | 503 | CLA | CHB-C4A-NA | 2.92 | 128.55 | 124.51 |
| 14 | m | 1103 | CLA | O2D-CGD-O1D | -2.92 | 118.13 | 123.84 |
| 14 | 6 | 513 | CLA | O2D-CGD-O1D | -2.92 | 118.13 | 123.84 |
| 14 | H | 1214 | CLA | CHB-C4A-NA | 2.92 | 128.55 | 124.51 |
| 14 | 3 | 502 | CLA | CMB-C2B-C1B | -2.92 | 123.98 | 128.46 |
| 14 | 1 | 503 | CLA | CMB-C2B-C3B | 2.92 | 130.14 | 124.68 |
| 14 | e | 1132 | CLA | CMB-C2B-C3B | 2.92 | 130.14 | 124.68 |
| 17 | 1 | 522 | BCR | C3-C4-C5 | -2.92 | 108.87 | 114.08 |
| 14 | s | 512 | CLA | CMB-C2B-C3B | 2.92 | 130.14 | 124.68 |
| 14 | B | 1209 | CLA | CHB-C4A-NA | 2.92 | 128.54 | 124.51 |
| 14 | e | 1126 | CLA | O2D-CGD-O1D | -2.92 | 118.14 | 123.84 |
| 14 | q | 503 | CLA | CMB-C2B-C3B | 2.92 | 130.13 | 124.68 |
| 14 | d | 503 | CLA | CMB-C2B-C3B | 2.92 | 130.13 | 124.68 |
| 14 | s | 517 | CLA | CMB-C2B-C3B | 2.92 | 130.13 | 124.68 |
| 14 | q | 507 | CLA | O2D-CGD-O1D | -2.91 | 118.14 | 123.84 |
| 17 | c | 522 | BCR | C38-C26-C25 | -2.91 | 121.25 | 124.53 |
| 14 | Z | 516 | CLA | CMB-C2B-C3B | 2.91 | 130.13 | 124.68 |
| 14 | f | 1214 | CLA | O2D-CGD-O1D | -2.91 | 118.14 | 123.84 |
| 14 | A | 1132 | CLA | CMB-C2B-C3B | 2.91 | 130.13 | 124.68 |
| 17 | f | 4010 | BCR | C7-C8-C9 | -2.91 | 121.83 | 126.23 |
| 14 | u | 502 | CLA | CHB-C4A-NA | 2.91 | 128.54 | 124.51 |
| 17 | n | 4219 | BCR | C7-C8-C9 | -2.91 | 121.83 | 126.23 |
| 14 | Y | 507 | CLA | O2D-CGD-O1D | -2.91 | 118.14 | 123.84 |
| 17 | 5 | 522 | BCR | C38-C26-C25 | -2.91 | 121.26 | 124.53 |
| 17 | c | 524 | BCR | C33-C5-C4 | 2.91 | 119.21 | 113.62 |
| 14 | H | 1207 | CLA | CMB-C2B-C3B | 2.91 | 130.13 | 124.68 |
| 14 | 2 | 518 | CLA | CHB-C4A-NA | 2.91 | 128.54 | 124.51 |
| 17 | t | 524 | BCR | C20-C21-C22 | -2.91 | 123.16 | 127.31 |
| 14 | e | 1139 | CLA | O2D-CGD-O1D | -2.91 | 118.15 | 123.84 |
| 17 | q | 522 | BCR | C3-C4-C5 | -2.91 | 108.88 | 114.08 |
| 14 | U | 1105 | CLA | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 3 | 504 | CLA | O2D-CGD-O1D | -2.91 | 118.15 | 123.84 |
| 14 | 3 | 517 | CLA | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |
| 14 | a | 517 | CLA | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |
| 17 | V | 4219 | BCR | C21-C20-C19 | -2.91 | 114.14 | 123.22 |
| 14 | c | 502 | CLA | CHB-C4A-NA | 2.91 | 128.53 | 124.51 |
| 14 | A | 1139 | CLA | O2D-CGD-O1D | -2.91 | 118.15 | 123.84 |
| 14 | q | 516 | CLA | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |
| 14 | f | 1211 | CLA | O2D-CGD-O1D | -2.91 | 118.15 | 123.84 |
| 14 | 4 | 508 | CLA | C1B-CHB-C4A | -2.91 | 124.36 | 130.12 |
| 14 | 3 | 512 | CLA | CMB-C2B-C3B | 2.91 | 130.12 | 124.68 |
| 17 | u | 524 | BCR | C33-C5-C4 | 2.91 | 119.20 | 113.62 |
| 14 | b | 503 | CLA | CHB-C4A-NA | 2.90 | 128.53 | 124.51 |
| 17 | B | 4010 | BCR | C7-C8-C9 | -2.90 | 121.85 | 126.23 |
| 17 | H | 4010 | BCR | C7-C8-C9 | -2.90 | 121.85 | 126.23 |
| 14 | 5 | 516 | CLA | CMB-C2B-C3B | 2.90 | 130.11 | 124.68 |
| 14 | c | 516 | CLA | CMB-C2B-C3B | 2.90 | 130.11 | 124.68 |
| 17 | Y | 522 | BCR | C3-C4-C5 | -2.90 | 108.89 | 114.08 |
| 14 | B | 1214 | CLA | CHB-C4A-NA | 2.90 | 128.53 | 124.51 |
| 14 | t | 502 | CLA | CHB-C4A-NA | 2.90 | 128.53 | 124.51 |
| 17 | T | 4015 | BCR | C32-C1-C6 | -2.90 | 105.59 | 110.30 |
| 14 | 5 | 504 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 14 | a | 516 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 14 | f | 1209 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 14 | a | 502 | CLA | CMB-C2B-C1B | -2.90 | 124.01 | 128.46 |
| 14 | v | 502 | CLA | CMB-C2B-C1B | -2.90 | 124.01 | 128.46 |
| 14 | t | 508 | CLA | C1B-CHB-C4A | -2.90 | 124.37 | 130.12 |
| 14 | q | 504 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 14 | a | 504 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 14 | v | 502 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 14 | e | 1118 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 17 | m | 4104 | BCR | C38-C26-C27 | 2.90 | 119.18 | 113.62 |
| 17 | a | 523 | BCR | C15-C16-C17 | -2.90 | 117.54 | 123.47 |
| 14 | B | 1214 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 14 | r | 511 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 14 | r | 518 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 14 | Y | 516 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 14 | 6 | 503 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 14 | 3 | 517 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 14 | s | 517 | CLA | O2D-CGD-O1D | -2.90 | 118.17 | 123.84 |
| 14 | 6 | 502 | CLA | CHB-C4A-NA | 2.90 | 128.52 | 124.51 |
| 14 | f | 1207 | CLA | CMB-C2B-C3B | 2.90 | 130.09 | 124.68 |
| 14 | Y | 509 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | U | 4104 | BCR | C38-C26-C27 | 2.89 | 119.18 | 113.62 |
| 14 | K | 1105 | CLA | CMB-C2B-C3B | 2.89 | 130.09 | 124.68 |
| 14 | 3 | 519 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 14 | B | 1211 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 14 | 1 | 507 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 14 | B | 1207 | CLA | CMB-C2B-C3B | 2.89 | 130.09 | 124.68 |
| 14 | 4 | 501 | CLA | CMB-C2B-C3B | 2.89 | 130.09 | 124.68 |
| 17 | B | 4009 | BCR | C33-C5-C6 | -2.89 | 121.28 | 124.53 |
| 17 | V | 4219 | BCR | C7-C8-C9 | -2.89 | 121.87 | 126.23 |
| 14 | 6 | 502 | CLA | CMB-C2B-C1B | -2.89 | 124.02 | 128.46 |
| 14 | G | 1120 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 17 | H | 4014 | BCR | C10-C11-C12 | -2.89 | 114.19 | 123.22 |
| 14 | f | 1214 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 14 | q | 509 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 14 | t | 507 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 17 | n | 4219 | BCR | C21-C20-C19 | -2.89 | 114.20 | 123.22 |
| 14 | m | 1105 | CLA | CMB-C2B-C3B | 2.89 | 130.09 | 124.68 |
| 14 | a | 517 | CLA | O2D-CGD-O1D | -2.89 | 118.19 | 123.84 |
| 14 | G | 1121 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 17 | K | 4104 | BCR | C38-C26-C27 | 2.89 | 119.17 | 113.62 |
| 14 | c | 517 | CLA | CMB-C2B-C3B | 2.89 | 130.08 | 124.68 |
| 17 | f | 4014 | BCR | C10-C11-C12 | -2.89 | 114.20 | 123.22 |
| 14 | 1 | 516 | CLA | CMB-C2B-C3B | 2.89 | 130.08 | 124.68 |
| 14 | t | 501 | CLA | CMB-C2B-C3B | 2.89 | 130.08 | 124.68 |
| 14 | b | 519 | CLA | CHB-C4A-NA | 2.89 | 128.50 | 124.51 |
| 14 | Z | 517 | CLA | O2D-CGD-O1D | -2.89 | 118.19 | 123.84 |
| 14 | f | 1222 | CLA | CAA-C2A-C3A | -2.89 | 104.87 | 112.78 |
| 14 | 2 | 511 | CLA | O2D-CGD-O1D | -2.89 | 118.19 | 123.84 |
| 14 | H | 1209 | CLA | CHB-C4A-NA | 2.89 | 128.50 | 124.51 |
| 14 | a | 519 | CLA | CHB-C4A-NA | 2.89 | 128.50 | 124.51 |
| 17 | G | 4002 | BCR | C3-C4-C5 | -2.89 | 108.92 | 114.08 |
| 14 | b | 507 | CLA | CHB-C4A-NA | 2.89 | 128.50 | 124.51 |
| 14 | d | 502 | CLA | CMB-C2B-C1B | -2.88 | 124.03 | 128.46 |
| 14 | e | 1125 | CLA | O2D-CGD-O1D | -2.88 | 118.20 | 123.84 |
| 17 | 5 | 522 | BCR | C38-C26-C27 | 2.88 | 119.16 | 113.62 |
| 14 | 4 | 507 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 14 | r | 504 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 14 | b | 518 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 14 | A | 1118 | CLA | O2D-CGD-O1D | -2.88 | 118.20 | 123.84 |
| 14 | A | 1122 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 14 | Z | 506 | CLA | CMB-C2B-C3B | 2.88 | 130.07 | 124.68 |
| 17 | L | 4219 | BCR | C21-C20-C19 | -2.88 | 114.22 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | q | 524 | BCR | C33-C5-C4 | 2.88 | 119.15 | 113.62 |
| 17 | Y | 523 | BCR | C15-C16-C17 | -2.88 | 117.57 | 123.47 |
| 14 | A | 1125 | CLA | O2D-CGD-O1D | -2.88 | 118.20 | 123.84 |
| 14 | Z | 504 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 17 | B | 4014 | BCR | C10-C11-C12 | -2.88 | 114.22 | 123.22 |
| 14 | G | 1125 | CLA | O2D-CGD-O1D | -2.88 | 118.20 | 123.84 |
| 14 | s | 519 | CLA | CHB-C4A-NA | 2.88 | 128.50 | 124.51 |
| 14 | v | 503 | CLA | CMB-C2B-C3B | 2.88 | 130.07 | 124.68 |
| 17 | H | 4004 | BCR | C28-C27-C26 | -2.88 | 108.94 | 114.08 |
| 14 | u | 502 | CLA | CMB-C2B-C1B | -2.88 | 124.04 | 128.46 |
| 14 | H | 1212 | CLA | CHB-C4A-NA | 2.88 | 128.49 | 124.51 |
| 14 | 2 | 517 | CLA | O2D-CGD-O1D | -2.88 | 118.21 | 123.84 |
| 14 | 1 | 504 | CLA | CMB-C2B-C3B | 2.88 | 130.06 | 124.68 |
| 14 | 5 | 511 | CLA | O2D-CGD-O1D | -2.88 | 118.21 | 123.84 |
| 17 | s | 523 | BCR | C15-C16-C17 | -2.88 | 117.58 | 123.47 |
| 17 | 1 | 524 | BCR | C33-C5-C4 | 2.88 | 119.14 | 113.62 |
| 17 | Y | 524 | BCR | C33-C5-C4 | 2.88 | 119.14 | 113.62 |
| 14 | B | 1222 | CLA | CAA-C2A-C3A | -2.88 | 104.90 | 112.78 |
| 17 | v | 521 | BCR | C7-C8-C9 | -2.88 | 121.89 | 126.23 |
| 17 | B | 4004 | BCR | C28-C27-C26 | -2.88 | 108.94 | 114.08 |
| 17 | c | 522 | BCR | C38-C26-C27 | 2.88 | 119.14 | 113.62 |
| 17 | H | 4009 | BCR | C33-C5-C6 | -2.88 | 121.30 | 124.53 |
| 14 | e | 1137 | CLA | C1B-CHB-C4A | -2.88 | 124.42 | 130.12 |
| 14 | 2 | 506 | CLA | CMB-C2B-C3B | 2.88 | 130.06 | 124.68 |
| 17 | t | 522 | BCR | C38-C26-C25 | -2.88 | 121.30 | 124.53 |
| 14 | c | 511 | CLA | O2D-CGD-O1D | -2.88 | 118.22 | 123.84 |
| 14 | s | 516 | CLA | CHB-C4A-NA | 2.88 | 128.49 | 124.51 |
| 14 | t | 518 | CLA | CHB-C4A-NA | 2.88 | 128.49 | 124.51 |
| 14 | f | 1227 | CLA | CMB-C2B-C3B | 2.87 | 130.06 | 124.68 |
| 14 | c | 504 | CLA | CHB-C4A-NA | 2.87 | 128.49 | 124.51 |
| 14 | q | 516 | CLA | O2D-CGD-O1D | -2.87 | 118.22 | 123.84 |
| 14 | 5 | 517 | CLA | CMB-C2B-C3B | 2.87 | 130.06 | 124.68 |
| 14 | r | 506 | CLA | CMB-C2B-C3B | 2.87 | 130.06 | 124.68 |
| 14 | u | 517 | CLA | CMB-C2B-C3B | 2.87 | 130.06 | 124.68 |
| 17 | c | 523 | BCR | C15-C16-C17 | -2.87 | 117.59 | 123.47 |
| 14 | e | 1119 | CLA | CHB-C4A-NA | 2.87 | 128.49 | 124.51 |
| 14 | t | 519 | CLA | CHB-C4A-NA | 2.87 | 128.49 | 124.51 |
| 17 | 4 | 522 | BCR | C38-C26-C25 | -2.87 | 121.30 | 124.53 |
| 14 | A | 1137 | CLA | C1B-CHB-C4A | -2.87 | 124.43 | 130.12 |
| 14 | c | 504 | CLA | O2D-CGD-O1D | -2.87 | 118.22 | 123.84 |
| 14 | b | 502 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | b | 501 | CLA | CMB-C2B-C3B | 2.87 | 130.05 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | e | 4002 | BCR | C3-C4-C5 | -2.87 | 108.95 | 114.08 |
| 14 | 4 | 501 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | Z | 511 | CLA | O2D-CGD-O1D | -2.87 | 118.22 | 123.84 |
| 17 | A | 4002 | BCR | C3-C4-C5 | -2.87 | 108.95 | 114.08 |
| 14 | Y | 504 | CLA | CMB-C2B-C3B | 2.87 | 130.05 | 124.68 |
| 14 | B | 1234 | CLA | CBC-CAC-C3C | 2.87 | 120.35 | 112.43 |
| 14 | G | 1133 | CLA | C1B-CHB-C4A | -2.87 | 124.43 | 130.12 |
| 14 | G | 1137 | CLA | C1B-CHB-C4A | -2.87 | 124.43 | 130.12 |
| 14 | 4 | 519 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | f | 1212 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 17 | 3 | 523 | BCR | C15-C16-C17 | -2.87 | 117.59 | 123.47 |
| 17 | 5 | 523 | BCR | C15-C16-C17 | -2.87 | 117.59 | 123.47 |
| 14 | e | 1135 | CLA | O2A-C1-C2 | 2.87 | 116.18 | 108.64 |
| 17 | u | 522 | BCR | C38-C26-C25 | -2.87 | 121.31 | 124.53 |
| 14 | F | 1302 | CLA | CMB-C2B-C1B | -2.87 | 124.05 | 128.46 |
| 14 | e | 1122 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | H | 1217 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 14 | A | 1135 | CLA | O2A-C1-C2 | 2.87 | 116.18 | 108.64 |
| 14 | L | 1502 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 14 | f | 1012 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 17 | s | 524 | BCR | C33-C5-C4 | 2.87 | 119.13 | 113.62 |
| 14 | l | 509 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | R | 1302 | CLA | CMB-C2B-C1B | -2.87 | 124.06 | 128.46 |
| 14 | G | 1136 | CLA | CMB-C2B-C3B | 2.87 | 130.04 | 124.68 |
| 14 | H | 1222 | CLA | CAA-C2A-C3A | -2.87 | 104.92 | 112.78 |
| 18 | G | 5003 | LHG | C11-C10-C9 | -2.87 | 99.86 | 114.42 |
| 14 | 3 | 516 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | q | 507 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | t | 501 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | q | 518 | CLA | CMB-C2B-C3B | 2.87 | 130.04 | 124.68 |
| 14 | H | 1234 | CLA | CBC-CAC-C3C | 2.87 | 120.34 | 112.43 |
| 17 | H | 4010 | BCR | C4-C5-C6 | -2.87 | 118.57 | 122.73 |
| 14 | G | 1122 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 14 | G | 1118 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 14 | H | 1211 | CLA | O2D-CGD-O1D | -2.87 | 118.23 | 123.84 |
| 14 | c | 502 | CLA | CMB-C2B-C1B | -2.87 | 124.06 | 128.46 |
| 14 | s | 511 | CLA | CHB-C4A-NA | 2.87 | 128.48 | 124.51 |
| 17 | l | 523 | BCR | C15-C16-C17 | -2.87 | 117.60 | 123.47 |
| 14 | f | 1234 | CLA | CBC-CAC-C3C | 2.87 | 120.33 | 112.43 |
| 14 | B | 1227 | CLA | CMB-C2B-C3B | 2.87 | 130.04 | 124.68 |
| 14 | A | 1119 | CLA | CHB-C4A-NA | 2.87 | 128.47 | 124.51 |
| 14 | u | 504 | CLA | CHB-C4A-NA | 2.87 | 128.47 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | A | 5003 | LHG | C11-C10-C9 | -2.87 | 99.88 | 114.42 |
| 14 | l | 518 | CLA | CMB-C2B-C3B | 2.86 | 130.04 | 124.68 |
| 14 | H | 1227 | CLA | CMB-C2B-C3B | 2.86 | 130.03 | 124.68 |
| 17 | q | 523 | BCR | C15-C16-C17 | -2.86 | 117.61 | 123.47 |
| 14 | A | 1121 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | n | 1502 | CLA | O2D-CGD-O1D | -2.86 | 118.24 | 123.84 |
| 14 | l | 507 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | Y | 507 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | e | 1013 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 18 | k | 5001 | LHG | O8-C23-C24 | 2.86 | 120.88 | 111.91 |
| 14 | G | 1119 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 18 | e | 5003 | LHG | C11-C10-C9 | -2.86 | 99.91 | 114.42 |
| 18 | n | 5220 | LHG | O8-C23-C24 | 2.86 | 120.88 | 111.91 |
| 14 | 4 | 502 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | 6 | 504 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | A | 1133 | CLA | C1B-CHB-C4A | -2.86 | 124.45 | 130.12 |
| 14 | 4 | 518 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | v | 511 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 14 | Z | 519 | CLA | CHB-C4A-NA | 2.86 | 128.46 | 124.51 |
| 17 | L | 4022 | BCR | C3-C4-C5 | -2.86 | 108.97 | 114.08 |
| 14 | V | 1502 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 14 | b | 510 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 14 | G | 1136 | CLA | CAA-C2A-C3A | -2.86 | 104.95 | 112.78 |
| 14 | Y | 518 | CLA | CMB-C2B-C3B | 2.86 | 130.02 | 124.68 |
| 17 | u | 522 | BCR | C38-C26-C27 | 2.86 | 119.10 | 113.62 |
| 17 | f | 4004 | BCR | C28-C27-C26 | -2.86 | 108.98 | 114.08 |
| 17 | V | 4022 | BCR | C16-C17-C18 | -2.86 | 123.23 | 127.31 |
| 14 | B | 1217 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 14 | l | 516 | CLA | O2D-CGD-O1D | -2.86 | 118.25 | 123.84 |
| 14 | G | 1135 | CLA | O2A-C1-C2 | 2.86 | 116.14 | 108.64 |
| 17 | 3 | 524 | BCR | C33-C5-C4 | 2.86 | 119.10 | 113.62 |
| 14 | 5 | 502 | CLA | CMB-C2B-C1B | -2.86 | 124.08 | 128.46 |
| 17 | n | 4020 | BCR | C34-C9-C8 | 2.86 | 122.58 | 118.08 |
| 17 | u | 523 | BCR | C15-C16-C17 | -2.86 | 117.62 | 123.47 |
| 14 | j | 1302 | CLA | CMB-C2B-C1B | -2.85 | 124.08 | 128.46 |
| 14 | r | 517 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 18 | L | 5220 | LHG | O8-C23-C24 | 2.85 | 120.86 | 111.91 |
| 14 | 3 | 511 | CLA | CHB-C4A-NA | 2.85 | 128.46 | 124.51 |
| 14 | u | 511 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 14 | H | 1012 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 14 | e | 1128 | CLA | C1B-CHB-C4A | -2.85 | 124.47 | 130.12 |
| 14 | 5 | 507 | CLA | CHB-C4A-NA | 2.85 | 128.46 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1226 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 14 | A | 1136 | CLA | CMB-C2B-C3B | 2.85 | 130.01 | 124.68 |
| 14 | 4 | 505 | CLA | CMB-C2B-C3B | 2.85 | 130.01 | 124.68 |
| 14 | Y | 516 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 17 | L | 4020 | BCR | C34-C9-C8 | 2.85 | 122.57 | 118.08 |
| 14 | f | 1223 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 17 | b | 522 | BCR | C38-C26-C25 | -2.85 | 121.33 | 124.53 |
| 18 | I | 5001 | LHG | O8-C23-C24 | 2.85 | 120.85 | 111.91 |
| 18 | S | 5001 | LHG | O8-C23-C24 | 2.85 | 120.85 | 111.91 |
| 14 | q | 502 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 14 | A | 1128 | CLA | C1B-CHB-C4A | -2.85 | 124.47 | 130.12 |
| 17 | a | 524 | BCR | C33-C5-C4 | 2.85 | 119.09 | 113.62 |
| 14 | B | 1212 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 14 | 4 | 510 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 14 | B | 1012 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 14 | d | 507 | CLA | O2D-CGD-O1D | -2.85 | 118.27 | 123.84 |
| 14 | b | 505 | CLA | CMB-C2B-C3B | 2.85 | 130.01 | 124.68 |
| 14 | t | 505 | CLA | CMB-C2B-C3B | 2.85 | 130.01 | 124.68 |
| 17 | B | 4010 | BCR | C4-C5-C6 | -2.85 | 118.60 | 122.73 |
| 14 | G | 1128 | CLA | C1B-CHB-C4A | -2.85 | 124.48 | 130.12 |
| 14 | 2 | 519 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 14 | v | 504 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 14 | e | 1133 | CLA | C1B-CHB-C4A | -2.85 | 124.48 | 130.12 |
| 17 | d | 521 | BCR | C7-C8-C9 | -2.85 | 121.93 | 126.23 |
| 14 | t | 510 | CLA | CHB-C4A-NA | 2.85 | 128.45 | 124.51 |
| 17 | e | 4001 | BCR | C2-C1-C6 | 2.85 | 114.86 | 110.48 |
| 14 | B | 1226 | CLA | O2D-CGD-O1D | -2.85 | 118.28 | 123.84 |
| 17 | G | 4001 | BCR | C2-C1-C6 | 2.85 | 114.86 | 110.48 |
| 14 | 2 | 504 | CLA | CHB-C4A-NA | 2.84 | 128.45 | 124.51 |
| 14 | a | 511 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 14 | d | 504 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 21 | d | 822 | SQD | O5-C5-C4 | 2.84 | 114.86 | 109.69 |
| 14 | G | 1133 | CLA | O2D-CGD-O1D | -2.84 | 118.28 | 123.84 |
| 14 | d | 511 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 18 | V | 5220 | LHG | O8-C23-C24 | 2.84 | 120.83 | 111.91 |
| 14 | 5 | 504 | CLA | O2D-CGD-O1D | -2.84 | 118.28 | 123.84 |
| 17 | n | 4022 | BCR | C3-C4-C5 | -2.84 | 109.00 | 114.08 |
| 17 | L | 4022 | BCR | C16-C17-C18 | -2.84 | 123.25 | 127.31 |
| 14 | B | 1221 | CLA | CAA-C2A-C3A | -2.84 | 105.00 | 112.78 |
| 14 | e | 1133 | CLA | O2D-CGD-O1D | -2.84 | 118.28 | 123.84 |
| 17 | 6 | 521 | BCR | C7-C8-C9 | -2.84 | 121.94 | 126.23 |
| 14 | 1 | 502 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | t | 518 | CLA | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 14 | H | 1221 | CLA | CAA-C2A-C3A | -2.84 | 105.00 | 112.78 |
| 14 | e | 1124 | CLA | CAA-C2A-C3A | -2.84 | 105.00 | 112.78 |
| 14 | e | 1136 | CLA | CAA-C2A-C3A | -2.84 | 105.00 | 112.78 |
| 14 | v | 517 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 14 | A | 1136 | CLA | CAA-C2A-C3A | -2.84 | 105.00 | 112.78 |
| 14 | f | 1226 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 14 | f | 1221 | CLA | CAA-C2A-C3A | -2.84 | 105.00 | 112.78 |
| 17 | Y | 523 | BCR | C37-C22-C23 | 2.84 | 122.55 | 118.08 |
| 17 | V | 4022 | BCR | C3-C4-C5 | -2.84 | 109.01 | 114.08 |
| 14 | f | 1021 | CLA | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 14 | A | 1133 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 14 | e | 1101 | CLA | C7-C6-C5 | -2.84 | 105.66 | 113.36 |
| 17 | u | 524 | BCR | C21-C20-C19 | -2.84 | 114.37 | 123.22 |
| 14 | b | 506 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 14 | b | 501 | CLA | CHB-C4A-NA | 2.84 | 128.43 | 124.51 |
| 17 | A | 4001 | BCR | C2-C1-C6 | 2.84 | 114.85 | 110.48 |
| 14 | u | 504 | CLA | O2D-CGD-O1D | -2.84 | 118.30 | 123.84 |
| 14 | s | 503 | CLA | CMB-C2B-C3B | 2.83 | 129.98 | 124.68 |
| 14 | 4 | 506 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 14 | l | 1303 | CLA | CHB-C4A-NA | 2.83 | 128.43 | 124.51 |
| 21 | 6 | 822 | SQD | O5-C5-C4 | 2.83 | 114.84 | 109.69 |
| 17 | f | 4010 | BCR | C4-C5-C6 | -2.83 | 118.62 | 122.73 |
| 14 | b | 502 | CLA | CMB-C2B-C1B | -2.83 | 124.11 | 128.46 |
| 17 | G | 4008 | BCR | C15-C16-C17 | -2.83 | 117.67 | 123.47 |
| 17 | l | 523 | BCR | C37-C22-C23 | 2.83 | 122.54 | 118.08 |
| 21 | v | 822 | SQD | C4-C3-C2 | 2.83 | 115.77 | 110.82 |
| 21 | 6 | 822 | SQD | C4-C3-C2 | 2.83 | 115.77 | 110.82 |
| 14 | e | 1122 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 14 | a | 503 | CLA | CMB-C2B-C3B | 2.83 | 129.98 | 124.68 |
| 14 | t | 510 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 14 | 6 | 511 | CLA | CHB-C4A-NA | 2.83 | 128.43 | 124.51 |
| 14 | u | 507 | CLA | CHB-C4A-NA | 2.83 | 128.43 | 124.51 |
| 17 | A | 4008 | BCR | C15-C16-C17 | -2.83 | 117.67 | 123.47 |
| 17 | f | 4009 | BCR | C33-C5-C6 | -2.83 | 121.35 | 124.53 |
| 14 | 3 | 503 | CLA | CMB-C2B-C3B | 2.83 | 129.98 | 124.68 |
| 14 | B | 1223 | CLA | CHB-C4A-NA | 2.83 | 128.43 | 124.51 |
| 17 | 5 | 524 | BCR | C21-C20-C19 | -2.83 | 114.38 | 123.22 |
| 14 | e | 1134 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 14 | Y | 505 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 14 | f | 1212 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 17 | t | 522 | BCR | C38-C26-C27 | 2.83 | 119.05 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | n | 4022 | BCR | C16-C17-C18 | -2.83 | 123.27 | 127.31 |
| 14 | e | 1136 | CLA | CMB-C2B-C3B | 2.83 | 129.97 | 124.68 |
| 14 | t | 506 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 17 | e | 4008 | BCR | C15-C16-C17 | -2.83 | 117.68 | 123.47 |
| 14 | G | 1122 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 17 | r | 524 | BCR | C7-C8-C9 | -2.83 | 121.96 | 126.23 |
| 14 | 6 | 507 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 14 | f | 1217 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 14 | H | 1239 | CLA | CMC-C2C-C3C | 2.83 | 133.79 | 126.12 |
| 14 | A | 1013 | CLA | CHB-C4A-NA | 2.83 | 128.42 | 124.51 |
| 14 | H | 1223 | CLA | CHB-C4A-NA | 2.83 | 128.42 | 124.51 |
| 14 | b | 518 | CLA | CMB-C2B-C3B | 2.83 | 129.97 | 124.68 |
| 14 | a | 513 | CLA | CHB-C4A-NA | 2.83 | 128.42 | 124.51 |
| 14 | 4 | 518 | CLA | CMB-C2B-C3B | 2.83 | 129.97 | 124.68 |
| 14 | q | 517 | CLA | CMB-C2B-C3B | 2.83 | 129.97 | 124.68 |
| 14 | a | 510 | CLA | CHB-C4A-NA | 2.83 | 128.42 | 124.51 |
| 14 | G | 1801 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 14 | q | 505 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 17 | 4 | 522 | BCR | C38-C26-C27 | 2.83 | 119.04 | 113.62 |
| 21 | v | 822 | SQD | O5-C5-C4 | 2.82 | 114.82 | 109.69 |
| 14 | B | 1212 | CLA | O2D-CGD-O1D | -2.82 | 118.31 | 123.84 |
| 17 | r | 521 | BCR | C33-C5-C6 | -2.82 | 121.36 | 124.53 |
| 14 | H | 1226 | CLA | C1B-CHB-C4A | -2.82 | 124.52 | 130.12 |
| 14 | Y | 518 | CLA | CHB-C4A-NA | 2.82 | 128.42 | 124.51 |
| 14 | B | 1239 | CLA | CMC-C2C-C3C | 2.82 | 133.78 | 126.12 |
| 14 | A | 1124 | CLA | CAA-C2A-C3A | -2.82 | 105.05 | 112.78 |
| 14 | A | 1117 | CLA | C1B-CHB-C4A | -2.82 | 124.53 | 130.12 |
| 17 | Y | 523 | BCR | C33-C5-C6 | -2.82 | 121.36 | 124.53 |
| 14 | 6 | 517 | CLA | O2D-CGD-O1D | -2.82 | 118.32 | 123.84 |
| 14 | v | 507 | CLA | O2D-CGD-O1D | -2.82 | 118.32 | 123.84 |
| 14 | H | 1203 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 14 | A | 1134 | CLA | O2D-CGD-O1D | -2.82 | 118.32 | 123.84 |
| 14 | H | 1239 | CLA | C16-C15-C13 | -2.82 | 106.80 | 115.92 |
| 17 | V | 4020 | BCR | C34-C9-C8 | 2.82 | 122.52 | 118.08 |
| 14 | G | 1124 | CLA | CAA-C2A-C3A | -2.82 | 105.05 | 112.78 |
| 14 | 1 | 517 | CLA | CMB-C2B-C3B | 2.82 | 129.96 | 124.68 |
| 14 | Y | 517 | CLA | CMB-C2B-C3B | 2.82 | 129.96 | 124.68 |
| 14 | G | 1117 | CLA | C1B-CHB-C4A | -2.82 | 124.53 | 130.12 |
| 14 | s | 503 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 14 | e | 1136 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 17 | u | 521 | BCR | C38-C26-C25 | -2.82 | 121.36 | 124.53 |
| 21 | d | 822 | SQD | C4-C3-C2 | 2.82 | 115.74 | 110.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1136 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 14 | 4 | 510 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 14 | t | 502 | CLA | CMB-C2B-C1B | -2.82 | 124.13 | 128.46 |
| 14 | 1 | 505 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 14 | b | 510 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 14 | r | 519 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 14 | A | 1114 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 17 | c | 524 | BCR | C21-C20-C19 | -2.82 | 114.43 | 123.22 |
| 14 | c | 507 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 14 | r | 519 | CLA | CMB-C2B-C1B | -2.82 | 124.14 | 128.46 |
| 14 | H | 1212 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 14 | A | 1101 | CLA | C7-C6-C5 | -2.82 | 105.71 | 113.36 |
| 14 | A | 1109 | CLA | O2A-CGA-O1A | -2.82 | 116.49 | 123.59 |
| 14 | e | 1137 | CLA | O2D-CGD-O1D | -2.82 | 118.33 | 123.84 |
| 17 | q | 523 | BCR | C37-C22-C23 | 2.81 | 122.51 | 118.08 |
| 14 | e | 1114 | CLA | O2D-CGD-O1D | -2.81 | 118.33 | 123.84 |
| 14 | B | 1239 | CLA | C16-C15-C13 | -2.81 | 106.82 | 115.92 |
| 17 | 2 | 521 | BCR | C33-C5-C6 | -2.81 | 121.37 | 124.53 |
| 14 | f | 1239 | CLA | CMC-C2C-C3C | 2.81 | 133.76 | 126.12 |
| 14 | G | 1013 | CLA | CHB-C4A-NA | 2.81 | 128.40 | 124.51 |
| 14 | A | 1122 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 14 | f | 1226 | CLA | C1B-CHB-C4A | -2.81 | 124.55 | 130.12 |
| 17 | 5 | 521 | BCR | C38-C26-C25 | -2.81 | 121.37 | 124.53 |
| 14 | f | 1239 | CLA | C16-C15-C13 | -2.81 | 106.83 | 115.92 |
| 14 | A | 1136 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 14 | t | 509 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 14 | e | 1117 | CLA | C1B-CHB-C4A | -2.81 | 124.55 | 130.12 |
| 14 | f | 1222 | CLA | C1B-CHB-C4A | -2.81 | 124.55 | 130.12 |
| 14 | e | 1109 | CLA | O2A-CGA-O1A | -2.81 | 116.50 | 123.59 |
| 14 | B | 1021 | CLA | CMB-C2B-C3B | 2.81 | 129.94 | 124.68 |
| 14 | R | 1302 | CLA | CHB-C4A-NA | 2.81 | 128.40 | 124.51 |
| 14 | A | 1128 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 14 | b | 504 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 17 | Z | 524 | BCR | C7-C8-C9 | -2.81 | 121.99 | 126.23 |
| 14 | Z | 519 | CLA | CMB-C2B-C1B | -2.81 | 124.15 | 128.46 |
| 14 | G | 1134 | CLA | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 14 | B | 1226 | CLA | C1B-CHB-C4A | -2.81 | 124.56 | 130.12 |
| 14 | A | 1801 | CLA | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 14 | e | 1128 | CLA | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 14 | t | 504 | CLA | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 14 | f | 1215 | CLA | C1-C2-C3 | -2.81 | 121.19 | 126.04 |
| 17 | 2 | 524 | BCR | C7-C8-C9 | -2.81 | 121.99 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1236 | CLA | C1B-CHB-C4A | -2.81 | 124.56 | 130.12 |
| 14 | 4 | 502 | CLA | CMB-C2B-C1B | -2.81 | 124.15 | 128.46 |
| 14 | n | 1503 | CLA | CHB-C4A-NA | 2.81 | 128.39 | 124.51 |
| 14 | a | 510 | CLA | O2D-CGD-O1D | -2.81 | 118.35 | 123.84 |
| 21 | L | 5216 | SQD | O8-S-C6 | 2.81 | 110.21 | 105.74 |
| 17 | Y | 522 | BCR | C33-C5-C6 | -2.81 | 121.38 | 124.53 |
| 14 | H | 1021 | CLA | CMB-C2B-C3B | 2.81 | 129.93 | 124.68 |
| 14 | G | 1101 | CLA | C7-C6-C5 | -2.81 | 105.74 | 113.36 |
| 14 | B | 1222 | CLA | C1B-CHB-C4A | -2.81 | 124.56 | 130.12 |
| 14 | f | 1236 | CLA | C1B-CHB-C4A | -2.81 | 124.56 | 130.12 |
| 14 | T | 1303 | CLA | CHB-C4A-NA | 2.81 | 128.39 | 124.51 |
| 14 | f | 1211 | CLA | C1B-CHB-C4A | -2.80 | 124.56 | 130.12 |
| 21 | u | 822 | SQD | C1-O5-C5 | 2.80 | 119.19 | 113.69 |
| 14 | 2 | 519 | CLA | CMB-C2B-C1B | -2.80 | 124.16 | 128.46 |
| 14 | 3 | 510 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 14 | 3 | 519 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 17 | c | 521 | BCR | C38-C26-C25 | -2.80 | 121.38 | 124.53 |
| 14 | 3 | 513 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 17 | R | 4016 | BCR | C16-C15-C14 | -2.80 | 117.73 | 123.47 |
| 21 | n | 5216 | SQD | O8-S-C6 | 2.80 | 110.21 | 105.74 |
| 14 | e | 1129 | CLA | O2D-CGD-CBD | 2.80 | 116.25 | 111.27 |
| 14 | G | 1134 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 14 | e | 1121 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 14 | H | 1222 | CLA | C1B-CHB-C4A | -2.80 | 124.57 | 130.12 |
| 17 | b | 522 | BCR | C38-C26-C27 | 2.80 | 119.00 | 113.62 |
| 14 | s | 519 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 14 | A | 1102 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 17 | r | 524 | BCR | C20-C21-C22 | -2.80 | 123.31 | 127.31 |
| 17 | U | 4104 | BCR | C10-C11-C12 | -2.80 | 114.48 | 123.22 |
| 14 | G | 1114 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 14 | a | 519 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 14 | F | 1302 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 14 | Y | 503 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 14 | b | 508 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 17 | K | 4104 | BCR | C3-C4-C5 | -2.80 | 109.08 | 114.08 |
| 14 | J | 1303 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 14 | 1 | 518 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 14 | Y | 502 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 14 | A | 1137 | CLA | O2D-CGD-O1D | -2.80 | 118.37 | 123.84 |
| 14 | Z | 513 | CLA | CMB-C2B-C3B | 2.80 | 129.91 | 124.68 |
| 14 | 4 | 509 | CLA | O2D-CGD-O1D | -2.80 | 118.37 | 123.84 |
| 17 | 1 | 523 | BCR | C33-C5-C6 | -2.80 | 121.39 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 1 | 507 | CLA | C2A-C1A-CHA | 2.80 | 128.75 | 123.86 |
| 14 | s | 510 | CLA | CHB-C4A-NA | 2.80 | 128.38 | 124.51 |
| 14 | 4 | 504 | CLA | O2D-CGD-O1D | -2.80 | 118.37 | 123.84 |
| 14 | e | 1109 | CLA | C1B-CHB-C4A | -2.79 | 124.58 | 130.12 |
| 17 | Z | 521 | BCR | C33-C5-C6 | -2.79 | 121.39 | 124.53 |
| 14 | 3 | 510 | CLA | CHB-C4A-NA | 2.79 | 128.38 | 124.51 |
| 14 | B | 1215 | CLA | C1B-CHB-C4A | -2.79 | 124.58 | 130.12 |
| 14 | G | 1128 | CLA | O2D-CGD-O1D | -2.79 | 118.38 | 123.84 |
| 17 | m | 4104 | BCR | C10-C11-C12 | -2.79 | 114.50 | 123.22 |
| 14 | B | 1203 | CLA | CHB-C4A-NA | 2.79 | 128.38 | 124.51 |
| 14 | e | 1102 | CLA | CHB-C4A-NA | 2.79 | 128.38 | 124.51 |
| 14 | G | 1129 | CLA | O2D-CGD-CBD | 2.79 | 116.23 | 111.27 |
| 14 | f | 1215 | CLA | O2D-CGD-CBD | 2.79 | 116.23 | 111.27 |
| 14 | s | 516 | CLA | CAC-C3C-C2C | -2.79 | 122.75 | 127.53 |
| 14 | 1 | 512 | CLA | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 14 | 3 | 503 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 14 | H | 1236 | CLA | C1B-CHB-C4A | -2.79 | 124.59 | 130.12 |
| 17 | H | 4014 | BCR | C36-C18-C19 | 2.79 | 122.48 | 118.08 |
| 17 | U | 4104 | BCR | C3-C4-C5 | -2.79 | 109.09 | 114.08 |
| 14 | s | 505 | CLA | O2D-CGD-O1D | -2.79 | 118.38 | 123.84 |
| 17 | K | 4104 | BCR | C10-C11-C12 | -2.79 | 114.50 | 123.22 |
| 17 | Y | 522 | BCR | C38-C26-C25 | -2.79 | 121.39 | 124.53 |
| 14 | T | 1302 | CLA | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 14 | d | 517 | CLA | O2D-CGD-O1D | -2.79 | 118.38 | 123.84 |
| 18 | V | 5220 | LHG | C11-C10-C9 | -2.79 | 100.26 | 114.42 |
| 14 | G | 1109 | CLA | C1B-CHB-C4A | -2.79 | 124.59 | 130.12 |
| 14 | G | 1122 | CLA | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 14 | Y | 512 | CLA | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 14 | c | 513 | CLA | CMB-C2B-C3B | 2.79 | 129.90 | 124.68 |
| 14 | 3 | 516 | CLA | CAC-C3C-C2C | -2.79 | 122.76 | 127.53 |
| 14 | j | 1302 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 14 | q | 507 | CLA | C2A-C1A-CHA | 2.79 | 128.74 | 123.86 |
| 17 | n | 4219 | BCR | C1-C6-C7 | 2.79 | 123.67 | 115.78 |
| 14 | L | 1503 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 14 | b | 517 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 14 | f | 1203 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 14 | A | 1129 | CLA | O2D-CGD-CBD | 2.79 | 116.22 | 111.27 |
| 14 | G | 1109 | CLA | O2A-CGA-O1A | -2.79 | 116.56 | 123.59 |
| 14 | B | 1211 | CLA | C1B-CHB-C4A | -2.79 | 124.59 | 130.12 |
| 14 | H | 1215 | CLA | C1B-CHB-C4A | -2.79 | 124.60 | 130.12 |
| 14 | e | 1101 | CLA | CAA-CBA-CGA | -2.79 | 105.11 | 113.25 |
| 15 | G | 2001 | PQN | C14-C13-C15 | -2.79 | 110.58 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 2 | 519 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 14 | A | 1134 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 14 | c | 519 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 17 | B | 4014 | BCR | C36-C18-C19 | 2.79 | 122.47 | 118.08 |
| 14 | A | 1109 | CLA | C1B-CHB-C4A | -2.79 | 124.60 | 130.12 |
| 14 | H | 1219 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 14 | c | 507 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 17 | 2 | 524 | BCR | C20-C21-C22 | -2.79 | 123.33 | 127.31 |
| 14 | 2 | 513 | CLA | CMB-C2B-C3B | 2.79 | 129.89 | 124.68 |
| 21 | V | 5216 | SQD | O8-S-C6 | 2.79 | 110.18 | 105.74 |
| 14 | 3 | 505 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 14 | b | 509 | CLA | O2D-CGD-O1D | -2.79 | 118.39 | 123.84 |
| 14 | q | 518 | CLA | CHB-C4A-NA | 2.78 | 128.36 | 124.51 |
| 21 | 5 | 822 | SQD | C1-O5-C5 | 2.78 | 119.15 | 113.69 |
| 17 | F | 4016 | BCR | C16-C15-C14 | -2.78 | 117.77 | 123.47 |
| 14 | f | 1219 | CLA | O2D-CGD-O1D | -2.78 | 118.39 | 123.84 |
| 14 | G | 1101 | CLA | O2D-CGD-CBD | 2.78 | 116.22 | 111.27 |
| 14 | e | 1801 | CLA | O2D-CGD-O1D | -2.78 | 118.39 | 123.84 |
| 14 | B | 1215 | CLA | C1-C2-C3 | -2.78 | 121.23 | 126.04 |
| 14 | B | 1217 | CLA | CHB-C4A-NA | 2.78 | 128.36 | 124.51 |
| 15 | A | 2001 | PQN | C14-C13-C15 | -2.78 | 110.59 | 115.27 |
| 14 | e | 1129 | CLA | C1B-CHB-C4A | -2.78 | 124.61 | 130.12 |
| 17 | L | 4219 | BCR | C1-C6-C7 | 2.78 | 123.65 | 115.78 |
| 14 | G | 1129 | CLA | C1B-CHB-C4A | -2.78 | 124.61 | 130.12 |
| 14 | c | 503 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | G | 1111 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | b | 508 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 18 | L | 5220 | LHG | C11-C10-C9 | -2.78 | 100.30 | 114.42 |
| 14 | H | 1222 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | v | 506 | CLA | CHB-C4A-NA | 2.78 | 128.36 | 124.51 |
| 14 | A | 1101 | CLA | CAA-CBA-CGA | -2.78 | 105.13 | 113.25 |
| 14 | G | 1137 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | r | 519 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | t | 508 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | Y | 507 | CLA | C2A-C1A-CHA | 2.78 | 128.72 | 123.86 |
| 14 | e | 1134 | CLA | CHB-C4A-NA | 2.78 | 128.36 | 124.51 |
| 17 | V | 4219 | BCR | C1-C6-C7 | 2.78 | 123.64 | 115.78 |
| 14 | q | 512 | CLA | CMB-C2B-C3B | 2.78 | 129.88 | 124.68 |
| 14 | c | 517 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 15 | e | 2001 | PQN | C14-C13-C15 | -2.78 | 110.59 | 115.27 |
| 14 | 4 | 508 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |
| 14 | s | 510 | CLA | O2D-CGD-O1D | -2.78 | 118.40 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | u | 513 | CLA | CMB-C2B-C3B | 2.78 | 129.88 | 124.68 |
| 14 | H | 1211 | CLA | C1B-CHB-C4A | -2.78 | 124.61 | 130.12 |
| 17 | j | 4016 | BCR | C16-C15-C14 | -2.78 | 117.78 | 123.47 |
| 14 | e | 1101 | CLA | O2D-CGD-CBD | 2.78 | 116.21 | 111.27 |
| 17 | A | 4011 | BCR | C10-C11-C12 | -2.78 | 114.55 | 123.22 |
| 14 | 5 | 513 | CLA | CMB-C2B-C3B | 2.78 | 129.88 | 124.68 |
| 14 | U | 1105 | CLA | C1B-CHB-C4A | -2.78 | 124.61 | 130.12 |
| 17 | m | 4104 | BCR | C3-C4-C5 | -2.78 | 109.12 | 114.08 |
| 14 | 5 | 507 | CLA | O2D-CGD-O1D | -2.78 | 118.41 | 123.84 |
| 14 | G | 1135 | CLA | O2D-CGD-O1D | -2.78 | 118.41 | 123.84 |
| 14 | A | 1101 | CLA | O2D-CGD-CBD | 2.78 | 116.20 | 111.27 |
| 14 | G | 1110 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 14 | s | 513 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 17 | c | 522 | BCR | C23-C24-C25 | -2.78 | 119.40 | 127.20 |
| 14 | A | 1122 | CLA | CMB-C2B-C3B | 2.78 | 129.87 | 124.68 |
| 17 | e | 4011 | BCR | C10-C11-C12 | -2.78 | 114.55 | 123.22 |
| 14 | 4 | 517 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 14 | G | 1102 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 14 | H | 1215 | CLA | C1-C2-C3 | -2.78 | 121.24 | 126.04 |
| 14 | 6 | 509 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 14 | f | 1227 | CLA | O2A-CGA-O1A | -2.78 | 116.59 | 123.59 |
| 21 | c | 822 | SQD | C1-O5-C5 | 2.78 | 119.14 | 113.69 |
| 14 | G | 1101 | CLA | CAA-CBA-CGA | -2.77 | 105.14 | 113.25 |
| 17 | 3 | 523 | BCR | C33-C5-C6 | -2.77 | 121.41 | 124.53 |
| 14 | e | 1135 | CLA | O2D-CGD-O1D | -2.77 | 118.41 | 123.84 |
| 14 | A | 1129 | CLA | C1B-CHB-C4A | -2.77 | 124.62 | 130.12 |
| 18 | n | 5220 | LHG | C11-C10-C9 | -2.77 | 100.34 | 114.42 |
| 14 | Y | 501 | CLA | CHB-C4A-NA | 2.77 | 128.35 | 124.51 |
| 17 | 1 | 522 | BCR | C33-C5-C6 | -2.77 | 121.41 | 124.53 |
| 14 | 1 | 510 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 14 | c | 503 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 14 | e | 1011 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 17 | f | 4014 | BCR | C36-C18-C19 | 2.77 | 122.45 | 118.08 |
| 14 | e | 1122 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 14 | l | 1302 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 14 | A | 1111 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | Y | 511 | CLA | CHB-C4A-NA | 2.77 | 128.35 | 124.51 |
| 14 | d | 509 | CLA | CHB-C4A-NA | 2.77 | 128.35 | 124.51 |
| 17 | Z | 524 | BCR | C33-C5-C4 | 2.77 | 118.94 | 113.62 |
| 14 | t | 503 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 14 | b | 502 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | J | 1302 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | d | 506 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | K | 1105 | CLA | C1B-CHB-C4A | -2.77 | 124.63 | 130.12 |
| 14 | A | 1135 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | B | 1215 | CLA | O2D-CGD-CBD | 2.77 | 116.19 | 111.27 |
| 14 | Z | 503 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | 5 | 503 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 14 | q | 510 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 14 | q | 519 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 17 | 5 | 522 | BCR | C23-C24-C25 | -2.77 | 119.42 | 127.20 |
| 14 | H | 1216 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | e | 1109 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | 5 | 503 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 17 | q | 523 | BCR | C33-C5-C6 | -2.77 | 121.42 | 124.53 |
| 14 | f | 1215 | CLA | C1B-CHB-C4A | -2.77 | 124.63 | 130.12 |
| 14 | r | 513 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 17 | Z | 524 | BCR | C20-C21-C22 | -2.77 | 123.36 | 127.31 |
| 17 | u | 522 | BCR | C16-C17-C18 | -2.77 | 123.36 | 127.31 |
| 14 | Y | 517 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | Z | 519 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | e | 1110 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | v | 509 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | a | 516 | CLA | CAC-C3C-C2C | -2.77 | 122.79 | 127.53 |
| 14 | G | 1110 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 14 | u | 503 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 14 | G | 1113 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | c | 510 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 14 | Y | 513 | CLA | C1B-CHB-C4A | -2.77 | 124.63 | 130.12 |
| 14 | H | 1217 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | B | 1240 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 17 | G | 4003 | BCR | C7-C8-C9 | -2.77 | 122.05 | 126.23 |
| 14 | H | 1240 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | 4 | 503 | CLA | CMB-C2B-C3B | 2.77 | 129.86 | 124.68 |
| 14 | a | 503 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | v | 519 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 18 | e | 5001 | LHG | C20-C19-C18 | -2.77 | 100.38 | 114.42 |
| 21 | 3 | 822 | SQD | C44-O6-C1 | 2.77 | 119.14 | 113.74 |
| 14 | H | 1215 | CLA | O2D-CGD-CBD | 2.77 | 116.19 | 111.27 |
| 14 | B | 1219 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | 5 | 505 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | f | 1240 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | l | 503 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | e | 1133 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | c | 513 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | u | 510 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | A | 1132 | CLA | C1B-CHB-C4A | -2.77 | 124.64 | 130.12 |
| 14 | e | 1113 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 17 | G | 4011 | BCR | C10-C11-C12 | -2.77 | 114.59 | 123.22 |
| 14 | 5 | 517 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | Y | 510 | CLA | CMB-C2B-C3B | 2.77 | 129.85 | 124.68 |
| 14 | G | 1109 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 14 | 5 | 510 | CLA | O2D-CGD-O1D | -2.77 | 118.43 | 123.84 |
| 14 | t | 502 | CLA | O2D-CGD-O1D | -2.76 | 118.43 | 123.84 |
| 14 | l | 513 | CLA | C1B-CHB-C4A | -2.76 | 124.64 | 130.12 |
| 17 | c | 522 | BCR | C16-C17-C18 | -2.76 | 123.36 | 127.31 |
| 17 | u | 522 | BCR | C23-C24-C25 | -2.76 | 119.44 | 127.20 |
| 14 | l | 508 | CLA | O2D-CGD-O1D | -2.76 | 118.43 | 123.84 |
| 14 | v | 501 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 18 | A | 5001 | LHG | C20-C19-C18 | -2.76 | 100.40 | 114.42 |
| 17 | e | 4008 | BCR | C33-C5-C6 | -2.76 | 121.42 | 124.53 |
| 14 | l | 501 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | 2 | 503 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | 4 | 508 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | B | 1222 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 18 | G | 5001 | LHG | C20-C19-C18 | -2.76 | 100.40 | 114.42 |
| 14 | d | 519 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | 5 | 519 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 17 | G | 4008 | BCR | C38-C26-C25 | -2.76 | 121.43 | 124.53 |
| 17 | s | 523 | BCR | C33-C5-C6 | -2.76 | 121.43 | 124.53 |
| 14 | l | 517 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 14 | A | 1110 | CLA | CMB-C2B-C3B | 2.76 | 129.84 | 124.68 |
| 14 | l | 519 | CLA | CMB-C2B-C3B | 2.76 | 129.84 | 124.68 |
| 14 | A | 1109 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | G | 1133 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | l | 519 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 14 | A | 1106 | CLA | O2D-CGD-CBD | 2.76 | 116.17 | 111.27 |
| 21 | r | 822 | SQD | C44-O6-C1 | 2.76 | 119.13 | 113.74 |
| 14 | Y | 508 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 14 | G | 1132 | CLA | C1B-CHB-C4A | -2.76 | 124.65 | 130.12 |
| 14 | r | 503 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 17 | r | 524 | BCR | C33-C5-C4 | 2.76 | 118.92 | 113.62 |
| 14 | u | 507 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 14 | B | 1227 | CLA | O2A-CGA-O1A | -2.76 | 116.63 | 123.59 |
| 17 | a | 523 | BCR | C33-C5-C6 | -2.76 | 121.43 | 124.53 |
| 14 | u | 519 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 505 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 14 | u | 505 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 17 | s | 524 | BCR | C21-C20-C19 | -2.76 | 114.61 | 123.22 |
| 14 | 4 | 502 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 14 | B | 1216 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | f | 1217 | CLA | CHB-C4A-NA | 2.76 | 128.33 | 124.51 |
| 14 | A | 1114 | CLA | CAA-C2A-C3A | -2.76 | 105.22 | 112.78 |
| 17 | 2 | 524 | BCR | C33-C5-C4 | 2.76 | 118.92 | 113.62 |
| 14 | e | 1113 | CLA | O2D-CGD-O1D | -2.76 | 118.45 | 123.84 |
| 14 | v | 519 | CLA | O2D-CGD-O1D | -2.76 | 118.45 | 123.84 |
| 17 | H | 4010 | BCR | C36-C18-C19 | 2.76 | 122.42 | 118.08 |
| 21 | c | 822 | SQD | O5-C5-C4 | 2.76 | 114.70 | 109.69 |
| 14 | 6 | 519 | CLA | O2D-CGD-O1D | -2.76 | 118.45 | 123.84 |
| 14 | m | 1105 | CLA | C1B-CHB-C4A | -2.76 | 124.66 | 130.12 |
| 14 | t | 508 | CLA | CHB-C4A-NA | 2.76 | 128.32 | 124.51 |
| 14 | B | 1239 | CLA | C6-C7-C8 | -2.76 | 107.01 | 115.92 |
| 14 | H | 1239 | CLA | C6-C7-C8 | -2.76 | 107.01 | 115.92 |
| 14 | e | 1111 | CLA | O2D-CGD-O1D | -2.76 | 118.45 | 123.84 |
| 17 | q | 522 | BCR | C33-C5-C6 | -2.76 | 121.43 | 124.53 |
| 17 | B | 4009 | BCR | C33-C5-C4 | 2.76 | 118.91 | 113.62 |
| 17 | q | 524 | BCR | C21-C20-C19 | -2.76 | 114.62 | 123.22 |
| 14 | e | 1114 | CLA | CAA-C2A-C3A | -2.75 | 105.23 | 112.78 |
| 14 | G | 1114 | CLA | CAA-C2A-C3A | -2.75 | 105.23 | 112.78 |
| 14 | H | 1220 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 17 | 1 | 522 | BCR | C38-C26-C25 | -2.75 | 121.44 | 124.53 |
| 17 | G | 4008 | BCR | C33-C5-C6 | -2.75 | 121.44 | 124.53 |
| 14 | q | 508 | CLA | O2D-CGD-O1D | -2.75 | 118.45 | 123.84 |
| 14 | e | 1110 | CLA | CMB-C2B-C3B | 2.75 | 129.83 | 124.68 |
| 14 | u | 511 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 14 | c | 505 | CLA | O2D-CGD-O1D | -2.75 | 118.45 | 123.84 |
| 17 | H | 4009 | BCR | C33-C5-C4 | 2.75 | 118.91 | 113.62 |
| 17 | a | 524 | BCR | C21-C20-C19 | -2.75 | 114.63 | 123.22 |
| 14 | V | 1503 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 14 | e | 1123 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 14 | Z | 513 | CLA | C1B-CHB-C4A | -2.75 | 124.67 | 130.12 |
| 17 | 3 | 524 | BCR | C21-C20-C19 | -2.75 | 114.63 | 123.22 |
| 14 | A | 1113 | CLA | O2D-CGD-O1D | -2.75 | 118.46 | 123.84 |
| 17 | Y | 524 | BCR | C21-C20-C19 | -2.75 | 114.63 | 123.22 |
| 14 | G | 1107 | CLA | C2D-C1D-ND | -2.75 | 108.08 | 110.10 |
| 14 | e | 1110 | CLA | C1-C2-C3 | -2.75 | 121.28 | 126.04 |
| 14 | H | 1238 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 14 | 6 | 506 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1131 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 14 | q | 513 | CLA | C1B-CHB-C4A | -2.75 | 124.67 | 130.12 |
| 14 | 6 | 506 | CLA | O2D-CGD-O1D | -2.75 | 118.46 | 123.84 |
| 14 | f | 1239 | CLA | C6-C7-C8 | -2.75 | 107.03 | 115.92 |
| 14 | A | 1131 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | t | 513 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | b | 503 | CLA | CMB-C2B-C3B | 2.75 | 129.82 | 124.68 |
| 17 | 1 | 523 | BCR | C23-C24-C25 | -2.75 | 119.48 | 127.20 |
| 17 | q | 523 | BCR | C23-C24-C25 | -2.75 | 119.48 | 127.20 |
| 14 | d | 506 | CLA | O2D-CGD-O1D | -2.75 | 118.46 | 123.84 |
| 17 | 1 | 524 | BCR | C21-C20-C19 | -2.75 | 114.64 | 123.22 |
| 14 | e | 1106 | CLA | O2D-CGD-CBD | 2.75 | 116.15 | 111.27 |
| 14 | A | 1011 | CLA | CMB-C2B-C3B | 2.75 | 129.82 | 124.68 |
| 14 | H | 1229 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | r | 516 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | u | 513 | CLA | O2D-CGD-O1D | -2.75 | 118.47 | 123.84 |
| 17 | r | 524 | BCR | C8-C7-C6 | -2.75 | 119.49 | 127.20 |
| 14 | 2 | 516 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 21 | Z | 822 | SQD | C44-O6-C1 | 2.75 | 119.11 | 113.74 |
| 14 | q | 508 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 14 | H | 1227 | CLA | O2A-CGA-O1A | -2.75 | 116.66 | 123.59 |
| 14 | G | 1237 | CLA | CMB-C2B-C1B | -2.75 | 124.24 | 128.46 |
| 17 | f | 4010 | BCR | C36-C18-C19 | 2.75 | 122.41 | 118.08 |
| 14 | A | 1133 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | Y | 513 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | H | 1239 | CLA | O2A-C1-C2 | -2.75 | 101.42 | 108.64 |
| 14 | e | 1131 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 14 | 1 | 511 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | q | 501 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | G | 1131 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 14 | e | 1013 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 14 | q | 517 | CLA | O2D-CGD-O1D | -2.75 | 118.47 | 123.84 |
| 14 | t | 511 | CLA | O2D-CGD-O1D | -2.75 | 118.47 | 123.84 |
| 14 | Y | 508 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 14 | d | 507 | CLA | C1B-CHB-C4A | -2.75 | 124.68 | 130.12 |
| 21 | 2 | 822 | SQD | C44-O6-C1 | 2.75 | 119.10 | 113.74 |
| 14 | 6 | 519 | CLA | CHB-C4A-NA | 2.75 | 128.31 | 124.51 |
| 14 | e | 1114 | CLA | CMB-C2B-C3B | 2.75 | 129.81 | 124.68 |
| 14 | f | 1231 | CLA | O2D-CGD-O1D | -2.75 | 118.47 | 123.84 |
| 17 | A | 4008 | BCR | C33-C5-C6 | -2.74 | 121.45 | 124.53 |
| 14 | 5 | 513 | CLA | O2D-CGD-O1D | -2.74 | 118.47 | 123.84 |
| 14 | Z | 503 | CLA | O2D-CGD-O1D | -2.74 | 118.47 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1120 | CLA | O2D-CGD-CBD | 2.74 | 116.14 | 111.27 |
| 14 | e | 1132 | CLA | C1B-CHB-C4A | -2.74 | 124.68 | 130.12 |
| 14 | r | 503 | CLA | O2D-CGD-O1D | -2.74 | 118.47 | 123.84 |
| 14 | B | 1239 | CLA | O2A-C1-C2 | -2.74 | 101.42 | 108.64 |
| 14 | Y | 519 | CLA | CMB-C2B-C3B | 2.74 | 129.81 | 124.68 |
| 17 | 5 | 522 | BCR | C16-C17-C18 | -2.74 | 123.39 | 127.31 |
| 14 | 1 | 508 | CLA | C1B-CHB-C4A | -2.74 | 124.68 | 130.12 |
| 17 | 2 | 523 | BCR | C15-C16-C17 | -2.74 | 117.86 | 123.47 |
| 14 | 4 | 511 | CLA | O2D-CGD-O1D | -2.74 | 118.47 | 123.84 |
| 14 | Y | 519 | CLA | O2D-CGD-O1D | -2.74 | 118.47 | 123.84 |
| 14 | b | 516 | CLA | O2D-CGD-O1D | -2.74 | 118.47 | 123.84 |
| 14 | q | 519 | CLA | CMB-C2B-C3B | 2.74 | 129.81 | 124.68 |
| 14 | v | 506 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 17 | f | 4017 | BCR | C20-C21-C22 | -2.74 | 123.40 | 127.31 |
| 14 | f | 1239 | CLA | O2A-C1-C2 | -2.74 | 101.43 | 108.64 |
| 14 | 4 | 506 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | H | 1231 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 14 | u | 517 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 14 | G | 1131 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 17 | e | 4003 | BCR | C7-C8-C9 | -2.74 | 122.09 | 126.23 |
| 14 | v | 507 | CLA | C1B-CHB-C4A | -2.74 | 124.69 | 130.12 |
| 17 | Z | 523 | BCR | C15-C16-C17 | -2.74 | 117.86 | 123.47 |
| 14 | A | 1113 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | 6 | 501 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | d | 519 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 17 | B | 4010 | BCR | C36-C18-C19 | 2.74 | 122.39 | 118.08 |
| 17 | l | 4013 | BCR | C10-C11-C12 | -2.74 | 114.67 | 123.22 |
| 14 | U | 1401 | CLA | O2D-CGD-CBD | 2.74 | 116.14 | 111.27 |
| 14 | A | 1123 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | d | 501 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | s | 513 | CLA | CMB-C2B-C3B | 2.74 | 129.80 | 124.68 |
| 21 | a | 822 | SQD | C44-O6-C1 | 2.74 | 119.09 | 113.74 |
| 21 | 5 | 822 | SQD | O5-C5-C4 | 2.74 | 114.67 | 109.69 |
| 14 | A | 1110 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | 4 | 513 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | f | 1239 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 21 | s | 822 | SQD | C44-O6-C1 | 2.74 | 119.09 | 113.74 |
| 17 | A | 4003 | BCR | C7-C8-C9 | -2.74 | 122.10 | 126.23 |
| 14 | d | 512 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 14 | u | 503 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 14 | Z | 516 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 17 | H | 4004 | BCR | C16-C15-C14 | -2.74 | 117.87 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1114 | CLA | CMB-C2B-C3B | 2.74 | 129.80 | 124.68 |
| 17 | s | 522 | BCR | C33-C5-C6 | -2.74 | 121.45 | 124.53 |
| 14 | l | 513 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | t | 517 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 14 | 2 | 503 | CLA | O2D-CGD-O1D | -2.74 | 118.49 | 123.84 |
| 14 | t | 516 | CLA | O2D-CGD-O1D | -2.74 | 118.49 | 123.84 |
| 14 | A | 1131 | CLA | C1B-CHB-C4A | -2.74 | 124.70 | 130.12 |
| 14 | G | 1106 | CLA | O2D-CGD-CBD | 2.74 | 116.13 | 111.27 |
| 14 | l | 506 | CLA | CHB-C4A-NA | 2.74 | 128.29 | 124.51 |
| 17 | Y | 523 | BCR | C23-C24-C25 | -2.74 | 119.52 | 127.20 |
| 14 | f | 1229 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | n | 1501 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | q | 503 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 17 | e | 4008 | BCR | C38-C26-C25 | -2.73 | 121.46 | 124.53 |
| 17 | r | 523 | BCR | C15-C16-C17 | -2.73 | 117.87 | 123.47 |
| 14 | r | 513 | CLA | C1B-CHB-C4A | -2.73 | 124.70 | 130.12 |
| 17 | 2 | 522 | BCR | C1-C6-C5 | -2.73 | 118.76 | 122.61 |
| 14 | 4 | 516 | CLA | O2D-CGD-O1D | -2.73 | 118.49 | 123.84 |
| 14 | e | 1107 | CLA | C2D-C1D-ND | -2.73 | 108.09 | 110.10 |
| 14 | b | 506 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 17 | B | 4017 | BCR | C20-C21-C22 | -2.73 | 123.41 | 127.31 |
| 14 | A | 1114 | CLA | CMB-C2B-C3B | 2.73 | 129.79 | 124.68 |
| 17 | r | 522 | BCR | C1-C6-C5 | -2.73 | 118.76 | 122.61 |
| 14 | A | 1013 | CLA | C1B-CHB-C4A | -2.73 | 124.70 | 130.12 |
| 18 | A | 5009 | LHG | O8-C23-C24 | 2.73 | 120.49 | 111.91 |
| 14 | f | 1216 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | 6 | 512 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 17 | f | 4004 | BCR | C16-C15-C14 | -2.73 | 117.88 | 123.47 |
| 17 | f | 4009 | BCR | C33-C5-C4 | 2.73 | 118.86 | 113.62 |
| 14 | l | 516 | CLA | CAC-C3C-C4C | 2.73 | 128.35 | 124.81 |
| 14 | 6 | 517 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | G | 1110 | CLA | C1-C2-C3 | -2.73 | 121.32 | 126.04 |
| 14 | B | 1220 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | 6 | 513 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 17 | J | 4013 | BCR | C20-C19-C18 | -2.73 | 118.74 | 126.42 |
| 14 | f | 1239 | CLA | CMB-C2B-C1B | -2.73 | 124.27 | 128.46 |
| 17 | Z | 522 | BCR | C1-C6-C5 | -2.73 | 118.77 | 122.61 |
| 17 | G | 4007 | BCR | C15-C16-C17 | -2.73 | 117.88 | 123.47 |
| 14 | B | 1231 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 14 | u | 508 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 14 | V | 1501 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | q | 513 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | e | 5009 | LHG | O8-C23-C24 | 2.73 | 120.48 | 111.91 |
| 14 | f | 1216 | CLA | O2A-CGA-CBA | 2.73 | 120.47 | 111.91 |
| 18 | G | 5009 | LHG | O8-C23-C24 | 2.73 | 120.47 | 111.91 |
| 14 | L | 1501 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 14 | B | 1212 | CLA | C1B-CHB-C4A | -2.73 | 124.71 | 130.12 |
| 17 | T | 4013 | BCR | C10-C11-C12 | -2.73 | 114.70 | 123.22 |
| 17 | J | 4013 | BCR | C10-C11-C12 | -2.73 | 114.70 | 123.22 |
| 17 | A | 4008 | BCR | C38-C26-C25 | -2.73 | 121.46 | 124.53 |
| 14 | b | 513 | CLA | CHB-C4A-NA | 2.73 | 128.28 | 124.51 |
| 14 | B | 1216 | CLA | O2A-CGA-CBA | 2.73 | 120.47 | 111.91 |
| 14 | c | 519 | CLA | CMB-C2B-C3B | 2.73 | 129.78 | 124.68 |
| 17 | Z | 524 | BCR | C8-C7-C6 | -2.73 | 119.54 | 127.20 |
| 17 | L | 4019 | BCR | C38-C26-C25 | -2.73 | 121.47 | 124.53 |
| 14 | H | 1217 | CLA | CMB-C2B-C3B | 2.73 | 129.78 | 124.68 |
| 17 | R | 4016 | BCR | C11-C12-C13 | -2.73 | 118.75 | 126.42 |
| 14 | Y | 504 | CLA | CHB-C4A-NA | 2.73 | 128.28 | 124.51 |
| 14 | f | 1235 | CLA | CHB-C4A-NA | 2.73 | 128.28 | 124.51 |
| 17 | q | 522 | BCR | C38-C26-C25 | -2.73 | 121.47 | 124.53 |
| 14 | H | 1213 | CLA | O2D-CGD-CBD | 2.73 | 116.11 | 111.27 |
| 14 | 2 | 513 | CLA | C1B-CHB-C4A | -2.73 | 124.72 | 130.12 |
| 17 | B | 4004 | BCR | C16-C15-C14 | -2.73 | 117.89 | 123.47 |
| 14 | Y | 510 | CLA | CHB-C4A-NA | 2.73 | 128.28 | 124.51 |
| 21 | u | 822 | SQD | O5-C5-C4 | 2.73 | 114.64 | 109.69 |
| 14 | f | 1222 | CLA | O2D-CGD-O1D | -2.73 | 118.51 | 123.84 |
| 14 | e | 1237 | CLA | CMB-C2B-C1B | -2.73 | 124.27 | 128.46 |
| 14 | f | 1238 | CLA | CHB-C4A-NA | 2.73 | 128.28 | 124.51 |
| 14 | q | 516 | CLA | CAC-C3C-C4C | 2.73 | 128.35 | 124.81 |
| 14 | A | 1110 | CLA | C1-C2-C3 | -2.73 | 121.33 | 126.04 |
| 17 | n | 4019 | BCR | C38-C26-C25 | -2.72 | 121.47 | 124.53 |
| 14 | Y | 506 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 14 | 5 | 519 | CLA | CMB-C2B-C3B | 2.72 | 129.78 | 124.68 |
| 14 | e | 1126 | CLA | O2D-CGD-CBD | 2.72 | 116.11 | 111.27 |
| 17 | 2 | 524 | BCR | C8-C7-C6 | -2.72 | 119.55 | 127.20 |
| 14 | 5 | 511 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 14 | v | 517 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 14 | G | 1013 | CLA | C1B-CHB-C4A | -2.72 | 124.72 | 130.12 |
| 17 | 3 | 522 | BCR | C15-C16-C17 | -2.72 | 117.89 | 123.47 |
| 17 | s | 522 | BCR | C15-C16-C17 | -2.72 | 117.89 | 123.47 |
| 14 | A | 1237 | CLA | CMB-C2B-C1B | -2.72 | 124.28 | 128.46 |
| 14 | r | 516 | CLA | C1B-CHB-C4A | -2.72 | 124.72 | 130.12 |
| 14 | c | 505 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 14 | 3 | 513 | CLA | CMB-C2B-C3B | 2.72 | 129.77 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1011 | CLA | CMB-C2B-C3B | 2.72 | 129.77 | 124.68 |
| 14 | B | 1213 | CLA | O2D-CGD-CBD | 2.72 | 116.11 | 111.27 |
| 14 | b | 505 | CLA | O2D-CGD-O1D | -2.72 | 118.51 | 123.84 |
| 14 | q | 504 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 14 | 5 | 508 | CLA | O2D-CGD-O1D | -2.72 | 118.52 | 123.84 |
| 14 | c | 508 | CLA | O2D-CGD-O1D | -2.72 | 118.52 | 123.84 |
| 17 | c | 524 | BCR | C15-C16-C17 | -2.72 | 117.90 | 123.47 |
| 14 | 6 | 507 | CLA | C1B-CHB-C4A | -2.72 | 124.72 | 130.12 |
| 14 | H | 1216 | CLA | O2A-CGA-CBA | 2.72 | 120.45 | 111.91 |
| 14 | t | 513 | CLA | O2D-CGD-O1D | -2.72 | 118.52 | 123.84 |
| 14 | K | 1401 | CLA | O2D-CGD-CBD | 2.72 | 116.11 | 111.27 |
| 17 | a | 522 | BCR | C15-C16-C17 | -2.72 | 117.90 | 123.47 |
| 14 | B | 1238 | CLA | CHB-C4A-NA | 2.72 | 128.28 | 124.51 |
| 17 | v | 523 | BCR | C28-C27-C26 | -2.72 | 109.22 | 114.08 |
| 14 | 4 | 505 | CLA | O2D-CGD-O1D | -2.72 | 118.52 | 123.84 |
| 14 | r | 504 | CLA | O2D-CGD-O1D | -2.72 | 118.52 | 123.84 |
| 14 | u | 510 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 14 | r | 505 | CLA | C1-C2-C3 | -2.72 | 121.34 | 126.04 |
| 17 | 5 | 524 | BCR | C15-C16-C17 | -2.72 | 117.90 | 123.47 |
| 17 | T | 4013 | BCR | C20-C19-C18 | -2.72 | 118.78 | 126.42 |
| 14 | H | 1239 | CLA | CMC-C2C-C1C | -2.72 | 120.90 | 125.04 |
| 14 | Z | 505 | CLA | C1-C2-C3 | -2.72 | 121.34 | 126.04 |
| 14 | A | 1120 | CLA | O2D-CGD-CBD | 2.72 | 116.10 | 111.27 |
| 17 | j | 4016 | BCR | C11-C12-C13 | -2.72 | 118.78 | 126.42 |
| 14 | 1 | 501 | CLA | O2D-CGD-O1D | -2.72 | 118.52 | 123.84 |
| 14 | f | 1212 | CLA | C1B-CHB-C4A | -2.72 | 124.73 | 130.12 |
| 14 | q | 506 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 17 | 6 | 523 | BCR | C28-C27-C26 | -2.72 | 109.22 | 114.08 |
| 14 | v | 513 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 17 | l | 4013 | BCR | C20-C19-C18 | -2.72 | 118.78 | 126.42 |
| 14 | 2 | 516 | CLA | C1B-CHB-C4A | -2.72 | 124.73 | 130.12 |
| 14 | f | 1213 | CLA | O2D-CGD-CBD | 2.72 | 116.10 | 111.27 |
| 14 | c | 511 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 17 | F | 4016 | BCR | C11-C12-C13 | -2.72 | 118.78 | 126.42 |
| 14 | A | 1107 | CLA | C2D-C1D-ND | -2.72 | 108.10 | 110.10 |
| 14 | H | 1212 | CLA | C1B-CHB-C4A | -2.72 | 124.74 | 130.12 |
| 14 | 5 | 510 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 21 | 4 | 822 | SQD | C1-O5-C5 | 2.72 | 119.02 | 113.69 |
| 14 | Z | 504 | CLA | O2D-CGD-O1D | -2.72 | 118.53 | 123.84 |
| 21 | 3 | 822 | SQD | O8-S-C6 | 2.72 | 110.07 | 105.74 |
| 17 | n | 4219 | BCR | C23-C22-C21 | -2.71 | 114.78 | 118.94 |
| 14 | e | 1120 | CLA | O2D-CGD-CBD | 2.71 | 116.09 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | U | 1103 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | 5 | 512 | CLA | O2D-CGD-O1D | -2.71 | 118.53 | 123.84 |
| 14 | t | 505 | CLA | O2D-CGD-O1D | -2.71 | 118.53 | 123.84 |
| 14 | m | 1401 | CLA | O2D-CGD-CBD | 2.71 | 116.09 | 111.27 |
| 17 | V | 4019 | BCR | C38-C26-C25 | -2.71 | 121.48 | 124.53 |
| 14 | 2 | 504 | CLA | O2D-CGD-O1D | -2.71 | 118.53 | 123.84 |
| 14 | Y | 501 | CLA | O2D-CGD-O1D | -2.71 | 118.53 | 123.84 |
| 14 | v | 508 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | B | 1229 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | H | 1239 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | v | 512 | CLA | O2D-CGD-O1D | -2.71 | 118.54 | 123.84 |
| 17 | H | 4017 | BCR | C20-C21-C22 | -2.71 | 123.44 | 127.31 |
| 14 | B | 1217 | CLA | CMB-C2B-C3B | 2.71 | 129.75 | 124.68 |
| 14 | c | 516 | CLA | C1B-CHB-C4A | -2.71 | 124.75 | 130.12 |
| 14 | 6 | 508 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | H | 1227 | CLA | C1B-CHB-C4A | -2.71 | 124.75 | 130.12 |
| 14 | f | 1204 | CLA | C1B-CHB-C4A | -2.71 | 124.75 | 130.12 |
| 14 | u | 519 | CLA | CMB-C2B-C3B | 2.71 | 129.75 | 124.68 |
| 14 | f | 1224 | CLA | C1B-CHB-C4A | -2.71 | 124.75 | 130.12 |
| 17 | A | 4007 | BCR | C15-C16-C17 | -2.71 | 117.92 | 123.47 |
| 14 | 2 | 504 | CLA | CMB-C2B-C3B | 2.71 | 129.75 | 124.68 |
| 17 | L | 4219 | BCR | C23-C22-C21 | -2.71 | 114.78 | 118.94 |
| 17 | v | 522 | BCR | C38-C26-C25 | -2.71 | 121.49 | 124.53 |
| 14 | l | 510 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | r | 506 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 17 | e | 4007 | BCR | C15-C16-C17 | -2.71 | 117.92 | 123.47 |
| 14 | 5 | 516 | CLA | C1B-CHB-C4A | -2.71 | 124.75 | 130.12 |
| 14 | f | 1220 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | B | 1239 | CLA | CMB-C2B-C1B | -2.71 | 124.30 | 128.46 |
| 14 | Z | 504 | CLA | CMB-C2B-C3B | 2.71 | 129.74 | 124.68 |
| 14 | G | 1123 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 14 | A | 1126 | CLA | O2D-CGD-CBD | 2.71 | 116.08 | 111.27 |
| 14 | r | 513 | CLA | CHB-C4A-NA | 2.71 | 128.25 | 124.51 |
| 17 | a | 522 | BCR | C16-C17-C18 | -2.71 | 123.45 | 127.31 |
| 14 | B | 1239 | CLA | CHB-C4A-NA | 2.71 | 128.25 | 124.51 |
| 14 | t | 516 | CLA | CHB-C4A-NA | 2.71 | 128.25 | 124.51 |
| 17 | V | 4219 | BCR | C23-C22-C21 | -2.71 | 114.79 | 118.94 |
| 17 | Y | 523 | BCR | C23-C22-C21 | -2.71 | 114.79 | 118.94 |
| 14 | t | 501 | CLA | O2D-CGD-O1D | -2.71 | 118.55 | 123.84 |
| 14 | u | 512 | CLA | O2D-CGD-O1D | -2.71 | 118.55 | 123.84 |
| 14 | 2 | 507 | CLA | CHB-C4A-NA | 2.71 | 128.25 | 124.51 |
| 14 | G | 1106 | CLA | CHB-C4A-NA | 2.71 | 128.25 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | b | 511 | CLA | O2D-CGD-O1D | -2.71 | 118.55 | 123.84 |
| 14 | G | 1126 | CLA | O2D-CGD-CBD | 2.71 | 116.08 | 111.27 |
| 17 | u | 524 | BCR | C15-C16-C17 | -2.70 | 117.93 | 123.47 |
| 14 | Z | 516 | CLA | C1B-CHB-C4A | -2.70 | 124.76 | 130.12 |
| 14 | Y | 517 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | B | 1238 | CLA | C1B-CHB-C4A | -2.70 | 124.76 | 130.12 |
| 14 | H | 1238 | CLA | C1B-CHB-C4A | -2.70 | 124.76 | 130.12 |
| 14 | Y | 516 | CLA | CAC-C3C-C4C | 2.70 | 128.32 | 124.81 |
| 14 | r | 504 | CLA | CMB-C2B-C3B | 2.70 | 129.74 | 124.68 |
| 14 | B | 1235 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | f | 1227 | CLA | C1B-CHB-C4A | -2.70 | 124.76 | 130.12 |
| 17 | d | 523 | BCR | C28-C27-C26 | -2.70 | 109.25 | 114.08 |
| 17 | d | 522 | BCR | C38-C26-C25 | -2.70 | 121.49 | 124.53 |
| 14 | a | 511 | CLA | O2D-CGD-O1D | -2.70 | 118.55 | 123.84 |
| 14 | Z | 505 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | Z | 513 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | d | 513 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | 4 | 501 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 14 | 4 | 513 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 14 | f | 1217 | CLA | CMB-C2B-C3B | 2.70 | 129.73 | 124.68 |
| 14 | G | 1112 | CLA | C1B-CHB-C4A | -2.70 | 124.77 | 130.12 |
| 14 | A | 1140 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 21 | t | 822 | SQD | C1-O5-C5 | 2.70 | 118.99 | 113.69 |
| 14 | G | 1113 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | b | 513 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 14 | 3 | 511 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 21 | b | 822 | SQD | C1-O5-C5 | 2.70 | 118.99 | 113.69 |
| 14 | a | 513 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 14 | s | 506 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 14 | t | 506 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 14 | 2 | 505 | CLA | C1-C2-C3 | -2.70 | 121.38 | 126.04 |
| 14 | G | 1140 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | b | 511 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | 6 | 507 | CLA | C2A-C1A-CHA | 2.70 | 128.58 | 123.86 |
| 14 | a | 513 | CLA | CMB-C2B-C3B | 2.70 | 129.73 | 124.68 |
| 14 | v | 511 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 14 | a | 508 | CLA | C1B-CHB-C4A | -2.70 | 124.77 | 130.12 |
| 14 | v | 507 | CLA | C2A-C1A-CHA | 2.70 | 128.58 | 123.86 |
| 14 | 6 | 511 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 17 | V | 4020 | BCR | C16-C15-C14 | -2.70 | 117.95 | 123.47 |
| 14 | d | 516 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 17 | 3 | 522 | BCR | C33-C5-C6 | -2.70 | 121.50 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 2 | 513 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | Y | 505 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | Z | 507 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | d | 517 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | f | 1238 | CLA | C1B-CHB-C4A | -2.70 | 124.78 | 130.12 |
| 14 | q | 501 | CLA | O2D-CGD-O1D | -2.70 | 118.57 | 123.84 |
| 14 | 3 | 513 | CLA | O2D-CGD-O1D | -2.70 | 118.57 | 123.84 |
| 14 | 1 | 504 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | 2 | 505 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | Z | 507 | CLA | C2A-C1A-CHA | 2.70 | 128.57 | 123.86 |
| 14 | K | 1103 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 14 | b | 501 | CLA | O2D-CGD-O1D | -2.69 | 118.57 | 123.84 |
| 14 | c | 502 | CLA | O2D-CGD-O1D | -2.69 | 118.57 | 123.84 |
| 21 | V | 5216 | SQD | O5-C5-C4 | 2.69 | 114.59 | 109.69 |
| 14 | B | 1239 | CLA | CMC-C2C-C1C | -2.69 | 120.94 | 125.04 |
| 14 | B | 1204 | CLA | C1B-CHB-C4A | -2.69 | 124.78 | 130.12 |
| 14 | c | 510 | CLA | CHB-C4A-NA | 2.69 | 128.24 | 124.51 |
| 17 | n | 4020 | BCR | C16-C15-C14 | -2.69 | 117.96 | 123.47 |
| 14 | B | 1227 | CLA | C1B-CHB-C4A | -2.69 | 124.78 | 130.12 |
| 17 | H | 4010 | BCR | C31-C1-C6 | -2.69 | 105.93 | 110.30 |
| 14 | n | 1501 | CLA | O2D-CGD-O1D | -2.69 | 118.57 | 123.84 |
| 14 | u | 506 | CLA | O2D-CGD-O1D | -2.69 | 118.57 | 123.84 |
| 17 | 6 | 522 | BCR | C38-C26-C25 | -2.69 | 121.50 | 124.53 |
| 14 | B | 1220 | CLA | O2D-CGD-O1D | -2.69 | 118.57 | 123.84 |
| 14 | u | 516 | CLA | C1B-CHB-C4A | -2.69 | 124.78 | 130.12 |
| 14 | c | 513 | CLA | CHB-C4A-NA | 2.69 | 128.24 | 124.51 |
| 17 | L | 4020 | BCR | C16-C15-C14 | -2.69 | 117.96 | 123.47 |
| 17 | 1 | 523 | BCR | C23-C22-C21 | -2.69 | 114.81 | 118.94 |
| 14 | u | 513 | CLA | C1B-CHB-C4A | -2.69 | 124.79 | 130.12 |
| 17 | 3 | 522 | BCR | C16-C17-C18 | -2.69 | 123.47 | 127.31 |
| 14 | B | 1224 | CLA | C1B-CHB-C4A | -2.69 | 124.79 | 130.12 |
| 14 | 5 | 505 | CLA | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 14 | q | 511 | CLA | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 14 | c | 512 | CLA | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 21 | n | 5216 | SQD | O48-C23-O10 | -2.69 | 116.81 | 123.59 |
| 14 | H | 1224 | CLA | C1B-CHB-C4A | -2.69 | 124.79 | 130.12 |
| 17 | f | 4017 | BCR | C15-C16-C17 | -2.69 | 117.97 | 123.47 |
| 14 | s | 513 | CLA | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 14 | V | 1502 | CLA | C1B-CHB-C4A | -2.69 | 124.79 | 130.12 |
| 21 | L | 5216 | SQD | O5-C5-C4 | 2.69 | 114.58 | 109.69 |
| 14 | f | 1220 | CLA | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 14 | H | 1204 | CLA | C1B-CHB-C4A | -2.69 | 124.79 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1128 | CLA | C7-C6-C5 | -2.69 | 106.06 | 113.36 |
| 14 | A | 1011 | CLA | C2A-C1A-CHA | 2.69 | 128.56 | 123.86 |
| 14 | L | 1501 | CLA | O2D-CGD-O1D | -2.69 | 118.58 | 123.84 |
| 14 | Z | 511 | CLA | CHB-C4A-NA | 2.69 | 128.23 | 124.51 |
| 14 | L | 1502 | CLA | C1B-CHB-C4A | -2.69 | 124.80 | 130.12 |
| 17 | c | 521 | BCR | C23-C24-C25 | -2.69 | 119.66 | 127.20 |
| 14 | n | 1502 | CLA | C1B-CHB-C4A | -2.69 | 124.80 | 130.12 |
| 21 | a | 822 | SQD | O8-S-C6 | 2.69 | 110.02 | 105.74 |
| 17 | Y | 522 | BCR | C38-C26-C27 | 2.69 | 118.78 | 113.62 |
| 14 | 3 | 506 | CLA | O2D-CGD-O1D | -2.69 | 118.59 | 123.84 |
| 14 | H | 1220 | CLA | O2D-CGD-O1D | -2.69 | 118.59 | 123.84 |
| 14 | 2 | 506 | CLA | CHB-C4A-NA | 2.69 | 128.22 | 124.51 |
| 17 | f | 4014 | BCR | C2-C1-C6 | 2.68 | 114.61 | 110.48 |
| 14 | U | 1105 | CLA | CAC-C3C-C2C | 2.68 | 132.12 | 127.53 |
| 14 | s | 511 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | c | 513 | CLA | C1B-CHB-C4A | -2.68 | 124.80 | 130.12 |
| 14 | 1 | 505 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | 4 | 516 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | H | 1227 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | V | 1501 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | m | 1105 | CLA | CAC-C3C-C2C | 2.68 | 132.12 | 127.53 |
| 14 | 2 | 507 | CLA | C2A-C1A-CHA | 2.68 | 128.55 | 123.86 |
| 17 | 5 | 521 | BCR | C23-C24-C25 | -2.68 | 119.67 | 127.20 |
| 17 | G | 4011 | BCR | C38-C26-C25 | -2.68 | 121.52 | 124.53 |
| 14 | 2 | 511 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | c | 506 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | 3 | 508 | CLA | C1B-CHB-C4A | -2.68 | 124.80 | 130.12 |
| 17 | V | 4020 | BCR | C36-C18-C19 | 2.68 | 122.30 | 118.08 |
| 14 | v | 516 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | d | 511 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | e | 1124 | CLA | O2D-CGD-O1D | -2.68 | 118.59 | 123.84 |
| 14 | A | 1106 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | q | 510 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 17 | A | 4011 | BCR | C38-C26-C25 | -2.68 | 121.52 | 124.53 |
| 21 | n | 5216 | SQD | O5-C5-C4 | 2.68 | 114.56 | 109.69 |
| 14 | e | 1124 | CLA | C1B-CHB-C4A | -2.68 | 124.81 | 130.12 |
| 17 | q | 522 | BCR | C38-C26-C27 | 2.68 | 118.77 | 113.62 |
| 17 | s | 522 | BCR | C16-C17-C18 | -2.68 | 123.48 | 127.31 |
| 14 | G | 1119 | CLA | CMC-C2C-C1C | -2.68 | 120.96 | 125.04 |
| 14 | v | 519 | CLA | CMB-C2B-C3B | 2.68 | 129.69 | 124.68 |
| 21 | s | 822 | SQD | O8-S-C6 | 2.68 | 110.01 | 105.74 |
| 17 | 6 | 523 | BCR | C20-C21-C22 | -2.68 | 123.48 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | u | 516 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 14 | B | 1230 | CLA | CAA-C2A-C3A | -2.68 | 105.44 | 112.78 |
| 14 | r | 508 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | d | 507 | CLA | C2A-C1A-CHA | 2.68 | 128.54 | 123.86 |
| 14 | q | 517 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | r | 511 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | A | 1130 | CLA | C1B-CHB-C4A | -2.68 | 124.81 | 130.12 |
| 17 | q | 522 | BCR | C11-C12-C13 | -2.68 | 118.89 | 126.42 |
| 14 | 2 | 508 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | d | 508 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 14 | f | 1239 | CLA | CMC-C2C-C1C | -2.68 | 120.96 | 125.04 |
| 14 | f | 1230 | CLA | CAA-C2A-C3A | -2.68 | 105.44 | 112.78 |
| 21 | V | 5216 | SQD | O48-C23-O10 | -2.68 | 116.83 | 123.59 |
| 14 | 3 | 506 | CLA | C1B-CHB-C4A | -2.68 | 124.81 | 130.12 |
| 17 | Y | 522 | BCR | C11-C12-C13 | -2.68 | 118.89 | 126.42 |
| 14 | 5 | 506 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 14 | A | 1124 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 14 | A | 1128 | CLA | C7-C6-C5 | -2.68 | 106.09 | 113.36 |
| 14 | H | 1239 | CLA | CMB-C2B-C1B | -2.68 | 124.35 | 128.46 |
| 14 | A | 1112 | CLA | C1B-CHB-C4A | -2.68 | 124.82 | 130.12 |
| 14 | G | 1124 | CLA | C1B-CHB-C4A | -2.68 | 124.82 | 130.12 |
| 17 | v | 523 | BCR | C20-C21-C22 | -2.68 | 123.49 | 127.31 |
| 14 | Z | 508 | CLA | CHB-C4A-NA | 2.68 | 128.21 | 124.51 |
| 17 | H | 4017 | BCR | C15-C16-C17 | -2.68 | 117.99 | 123.47 |
| 14 | 5 | 516 | CLA | O2D-CGD-O1D | -2.68 | 118.61 | 123.84 |
| 14 | G | 1130 | CLA | C1B-CHB-C4A | -2.68 | 124.82 | 130.12 |
| 14 | 5 | 513 | CLA | C1B-CHB-C4A | -2.67 | 124.82 | 130.12 |
| 14 | Z | 507 | CLA | C1B-CHB-C4A | -2.67 | 124.82 | 130.12 |
| 14 | B | 1205 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 14 | H | 1230 | CLA | CAA-C2A-C3A | -2.67 | 105.45 | 112.78 |
| 21 | L | 5216 | SQD | O48-C23-O10 | -2.67 | 116.84 | 123.59 |
| 17 | 1 | 522 | BCR | C11-C12-C13 | -2.67 | 118.90 | 126.42 |
| 17 | v | 522 | BCR | C16-C17-C18 | -2.67 | 123.49 | 127.31 |
| 17 | 4 | 524 | BCR | C24-C23-C22 | -2.67 | 122.19 | 126.23 |
| 14 | 5 | 507 | CLA | C2A-C1A-CHA | 2.67 | 128.53 | 123.86 |
| 17 | 1 | 522 | BCR | C38-C26-C27 | 2.67 | 118.75 | 113.62 |
| 14 | s | 508 | CLA | C1B-CHB-C4A | -2.67 | 124.82 | 130.12 |
| 14 | u | 508 | CLA | C1B-CHB-C4A | -2.67 | 124.82 | 130.12 |
| 14 | c | 507 | CLA | C2A-C1A-CHA | 2.67 | 128.53 | 123.86 |
| 17 | b | 524 | BCR | C24-C23-C22 | -2.67 | 122.20 | 126.23 |
| 17 | 5 | 522 | BCR | C33-C5-C6 | -2.67 | 121.53 | 124.53 |
| 17 | n | 4020 | BCR | C38-C26-C25 | 2.67 | 127.53 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 6 | 519 | CLA | CMB-C2B-C3B | 2.67 | 129.68 | 124.68 |
| 14 | m | 1103 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 14 | 2 | 507 | CLA | C1B-CHB-C4A | -2.67 | 124.83 | 130.12 |
| 14 | 5 | 502 | CLA | O2D-CGD-O1D | -2.67 | 118.61 | 123.84 |
| 14 | a | 506 | CLA | O2D-CGD-O1D | -2.67 | 118.61 | 123.84 |
| 14 | 3 | 518 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 14 | H | 1235 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 14 | a | 506 | CLA | C1B-CHB-C4A | -2.67 | 124.83 | 130.12 |
| 14 | A | 1136 | CLA | O2A-CGA-O1A | -2.67 | 116.85 | 123.59 |
| 22 | p | 170 | FMN | C4A-C4-N3 | 2.67 | 119.97 | 113.19 |
| 14 | r | 507 | CLA | C2A-C1A-CHA | 2.67 | 128.53 | 123.86 |
| 14 | e | 1140 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 17 | B | 4017 | BCR | C15-C16-C17 | -2.67 | 118.00 | 123.47 |
| 17 | f | 4010 | BCR | C31-C1-C6 | -2.67 | 105.97 | 110.30 |
| 14 | K | 1105 | CLA | CAC-C3C-C2C | 2.67 | 132.09 | 127.53 |
| 14 | e | 1136 | CLA | O2A-CGA-O1A | -2.67 | 116.86 | 123.59 |
| 17 | u | 521 | BCR | C23-C24-C25 | -2.67 | 119.71 | 127.20 |
| 14 | G | 1124 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 14 | e | 1011 | CLA | C2A-C1A-CHA | 2.67 | 128.53 | 123.86 |
| 14 | r | 507 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 14 | u | 513 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 14 | s | 506 | CLA | C1B-CHB-C4A | -2.67 | 124.83 | 130.12 |
| 14 | Z | 513 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 14 | v | 504 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 17 | 5 | 522 | BCR | C15-C16-C17 | -2.67 | 118.01 | 123.47 |
| 14 | A | 1124 | CLA | C1B-CHB-C4A | -2.67 | 124.83 | 130.12 |
| 14 | f | 1227 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 17 | a | 523 | BCR | C28-C27-C26 | -2.67 | 109.31 | 114.08 |
| 14 | B | 1227 | CLA | O2D-CGD-O1D | -2.67 | 118.62 | 123.84 |
| 17 | a | 522 | BCR | C33-C5-C6 | -2.67 | 121.53 | 124.53 |
| 14 | f | 1205 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 17 | 3 | 523 | BCR | C28-C27-C26 | -2.67 | 109.31 | 114.08 |
| 17 | u | 522 | BCR | C15-C16-C17 | -2.67 | 118.01 | 123.47 |
| 17 | L | 4020 | BCR | C36-C18-C19 | 2.67 | 122.28 | 118.08 |
| 14 | r | 517 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 22 | X | 170 | FMN | C4A-C4-N3 | 2.67 | 119.96 | 113.19 |
| 14 | 5 | 508 | CLA | C1B-CHB-C4A | -2.67 | 124.84 | 130.12 |
| 14 | e | 1237 | CLA | C11-C12-C13 | -2.67 | 107.30 | 115.92 |
| 14 | 3 | 508 | CLA | CHB-C4A-NA | 2.67 | 128.20 | 124.51 |
| 17 | c | 522 | BCR | C15-C16-C17 | -2.67 | 118.01 | 123.47 |
| 14 | G | 1136 | CLA | O2A-CGA-O1A | -2.67 | 116.87 | 123.59 |
| 14 | 5 | 506 | CLA | CHB-C4A-NA | 2.66 | 128.20 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 518 | CLA | CHB-C4A-NA | 2.66 | 128.20 | 124.51 |
| 14 | e | 1128 | CLA | C7-C6-C5 | -2.66 | 106.12 | 113.36 |
| 14 | e | 1131 | CLA | C1-C2-C3 | -2.66 | 121.44 | 126.04 |
| 14 | e | 1106 | CLA | CHB-C4A-NA | 2.66 | 128.20 | 124.51 |
| 17 | B | 4014 | BCR | C2-C1-C6 | 2.66 | 114.58 | 110.48 |
| 17 | v | 522 | BCR | C38-C26-C27 | 2.66 | 118.73 | 113.62 |
| 14 | b | 516 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 17 | B | 4010 | BCR | C31-C1-C6 | -2.66 | 105.98 | 110.30 |
| 14 | Z | 512 | CLA | CMB-C2B-C3B | 2.66 | 129.66 | 124.68 |
| 14 | r | 512 | CLA | CMB-C2B-C3B | 2.66 | 129.66 | 124.68 |
| 17 | f | 4005 | BCR | C28-C27-C26 | -2.66 | 109.32 | 114.08 |
| 14 | A | 1011 | CLA | C4D-C3D-CAD | -2.66 | 104.96 | 108.10 |
| 14 | Y | 505 | CLA | C1B-CHB-C4A | -2.66 | 124.84 | 130.12 |
| 14 | e | 1112 | CLA | C1B-CHB-C4A | -2.66 | 124.84 | 130.12 |
| 14 | H | 1238 | CLA | O2D-CGD-O1D | -2.66 | 118.63 | 123.84 |
| 14 | s | 508 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | 6 | 516 | CLA | O2D-CGD-O1D | -2.66 | 118.63 | 123.84 |
| 14 | u | 506 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | q | 510 | CLA | O2D-CGD-O1D | -2.66 | 118.64 | 123.84 |
| 22 | P | 170 | FMN | C4A-C4-N3 | 2.66 | 119.95 | 113.19 |
| 17 | 3 | 524 | BCR | C23-C24-C25 | -2.66 | 119.73 | 127.20 |
| 14 | l | 517 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | 4 | 511 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 17 | a | 524 | BCR | C23-C24-C25 | -2.66 | 119.73 | 127.20 |
| 14 | l | 505 | CLA | C1B-CHB-C4A | -2.66 | 124.85 | 130.12 |
| 14 | H | 1232 | CLA | C1B-CHB-C4A | -2.66 | 124.85 | 130.12 |
| 17 | r | 523 | BCR | C11-C10-C9 | -2.66 | 123.52 | 127.31 |
| 17 | e | 4011 | BCR | C38-C26-C25 | -2.66 | 121.54 | 124.53 |
| 14 | B | 1225 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | 5 | 513 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | u | 507 | CLA | C2A-C1A-CHA | 2.66 | 128.51 | 123.86 |
| 17 | n | 4020 | BCR | C36-C18-C19 | 2.66 | 122.27 | 118.08 |
| 14 | u | 505 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | B | 1220 | CLA | CMB-C2B-C3B | 2.66 | 129.65 | 124.68 |
| 14 | l | 510 | CLA | O2D-CGD-O1D | -2.66 | 118.64 | 123.84 |
| 14 | a | 508 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 14 | 2 | 508 | CLA | C1B-CHB-C4A | -2.66 | 124.86 | 130.12 |
| 14 | q | 505 | CLA | C1B-CHB-C4A | -2.66 | 124.86 | 130.12 |
| 14 | G | 1237 | CLA | C11-C12-C13 | -2.66 | 107.33 | 115.92 |
| 17 | u | 522 | BCR | C33-C5-C6 | -2.66 | 121.55 | 124.53 |
| 17 | s | 524 | BCR | C23-C24-C25 | -2.66 | 119.74 | 127.20 |
| 14 | d | 519 | CLA | CMB-C2B-C3B | 2.66 | 129.65 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | r | 507 | CLA | C1B-CHB-C4A | -2.66 | 124.86 | 130.12 |
| 14 | d | 518 | CLA | CHB-C4A-NA | 2.66 | 128.18 | 124.51 |
| 14 | 2 | 513 | CLA | O2D-CGD-O1D | -2.66 | 118.65 | 123.84 |
| 14 | f | 1225 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 17 | R | 4016 | BCR | C33-C5-C6 | -2.65 | 121.55 | 124.53 |
| 14 | A | 1237 | CLA | C11-C12-C13 | -2.65 | 107.34 | 115.92 |
| 17 | d | 523 | BCR | C20-C21-C22 | -2.65 | 123.52 | 127.31 |
| 17 | Y | 522 | BCR | C23-C24-C25 | -2.65 | 119.75 | 127.20 |
| 14 | 5 | 516 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 14 | c | 506 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 14 | c | 516 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 17 | 1 | 522 | BCR | C23-C24-C25 | -2.65 | 119.75 | 127.20 |
| 14 | A | 1119 | CLA | CMC-C2C-C1C | -2.65 | 121.00 | 125.04 |
| 14 | A | 1131 | CLA | C1-C2-C3 | -2.65 | 121.45 | 126.04 |
| 14 | G | 1011 | CLA | C2A-C1A-CHA | 2.65 | 128.50 | 123.86 |
| 17 | B | 4005 | BCR | C28-C27-C26 | -2.65 | 109.34 | 114.08 |
| 14 | c | 508 | CLA | C1B-CHB-C4A | -2.65 | 124.86 | 130.12 |
| 14 | f | 1220 | CLA | CMB-C2B-C3B | 2.65 | 129.64 | 124.68 |
| 14 | u | 502 | CLA | O2D-CGD-O1D | -2.65 | 118.65 | 123.84 |
| 14 | 4 | 504 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 14 | e | 1125 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 17 | H | 4005 | BCR | C28-C27-C26 | -2.65 | 109.34 | 114.08 |
| 17 | l | 4015 | BCR | C38-C26-C25 | -2.65 | 121.55 | 124.53 |
| 14 | r | 508 | CLA | C1B-CHB-C4A | -2.65 | 124.87 | 130.12 |
| 17 | q | 522 | BCR | C23-C24-C25 | -2.65 | 119.76 | 127.20 |
| 17 | q | 523 | BCR | C23-C22-C21 | -2.65 | 114.87 | 118.94 |
| 14 | e | 1130 | CLA | C1B-CHB-C4A | -2.65 | 124.87 | 130.12 |
| 17 | t | 521 | BCR | C33-C5-C6 | -2.65 | 121.55 | 124.53 |
| 14 | 2 | 512 | CLA | CMB-C2B-C3B | 2.65 | 129.64 | 124.68 |
| 17 | B | 4010 | BCR | C11-C12-C13 | -2.65 | 118.97 | 126.42 |
| 14 | Z | 508 | CLA | C1B-CHB-C4A | -2.65 | 124.87 | 130.12 |
| 17 | L | 4020 | BCR | C38-C26-C25 | 2.65 | 127.50 | 124.53 |
| 14 | f | 1232 | CLA | C1B-CHB-C4A | -2.65 | 124.87 | 130.12 |
| 17 | H | 4014 | BCR | C2-C1-C6 | 2.65 | 114.56 | 110.48 |
| 14 | q | 505 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 17 | H | 4010 | BCR | C11-C12-C13 | -2.65 | 118.98 | 126.42 |
| 14 | t | 505 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 14 | H | 1205 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 14 | 6 | 504 | CLA | O2D-CGD-O1D | -2.65 | 118.66 | 123.84 |
| 14 | f | 1232 | CLA | O2D-CGD-O1D | -2.65 | 118.66 | 123.84 |
| 17 | s | 523 | BCR | C28-C27-C26 | -2.65 | 109.35 | 114.08 |
| 14 | d | 505 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | u | 516 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 14 | 4 | 505 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 14 | r | 505 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 14 | Z | 506 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 17 | J | 4015 | BCR | C38-C26-C25 | -2.64 | 121.56 | 124.53 |
| 17 | j | 4016 | BCR | C33-C5-C6 | -2.64 | 121.56 | 124.53 |
| 14 | v | 505 | CLA | C1B-CHB-C4A | -2.64 | 124.88 | 130.12 |
| 17 | t | 524 | BCR | C24-C23-C22 | -2.64 | 122.24 | 126.23 |
| 14 | H | 1231 | CLA | CHB-C4A-NA | 2.64 | 128.17 | 124.51 |
| 14 | 6 | 503 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 17 | Z | 522 | BCR | C20-C21-C22 | -2.64 | 123.54 | 127.31 |
| 14 | c | 516 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 21 | Z | 822 | SQD | O8-S-C6 | 2.64 | 109.95 | 105.74 |
| 14 | 6 | 505 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 14 | B | 1221 | CLA | O2D-CGD-CBD | 2.64 | 115.96 | 111.27 |
| 14 | e | 1119 | CLA | CMC-C2C-C1C | -2.64 | 121.02 | 125.04 |
| 14 | 5 | 518 | CLA | CMB-C2B-C3B | 2.64 | 129.62 | 124.68 |
| 14 | A | 1125 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 14 | H | 1220 | CLA | CMB-C2B-C3B | 2.64 | 129.62 | 124.68 |
| 14 | 6 | 518 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 14 | s | 505 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 17 | V | 4020 | BCR | C38-C26-C25 | 2.64 | 127.49 | 124.53 |
| 17 | H | 4014 | BCR | C24-C23-C22 | -2.64 | 122.25 | 126.23 |
| 14 | 2 | 517 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 14 | t | 511 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 17 | 2 | 523 | BCR | C11-C10-C9 | -2.64 | 123.54 | 127.31 |
| 14 | Y | 510 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 14 | f | 1224 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 14 | v | 503 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 14 | v | 518 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 17 | f | 4010 | BCR | C11-C12-C13 | -2.64 | 119.01 | 126.42 |
| 14 | B | 1230 | CLA | CAA-C2A-C1A | -2.64 | 103.33 | 111.97 |
| 17 | f | 4014 | BCR | C24-C23-C22 | -2.64 | 122.25 | 126.23 |
| 17 | 6 | 522 | BCR | C38-C26-C27 | 2.64 | 118.68 | 113.62 |
| 14 | 2 | 510 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 14 | B | 1232 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 14 | G | 1131 | CLA | C1-C2-C3 | -2.64 | 121.48 | 126.04 |
| 14 | s | 518 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 17 | c | 522 | BCR | C33-C5-C6 | -2.64 | 121.57 | 124.53 |
| 14 | c | 518 | CLA | CMB-C2B-C3B | 2.63 | 129.61 | 124.68 |
| 14 | A | 1135 | CLA | CHB-C4A-NA | 2.63 | 128.16 | 124.51 |
| 14 | B | 1231 | CLA | CHB-C4A-NA | 2.63 | 128.16 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | b | 505 | CLA | CHB-C4A-NA | 2.63 | 128.16 | 124.51 |
| 14 | 6 | 505 | CLA | C1B-CHB-C4A | -2.63 | 124.90 | 130.12 |
| 14 | 2 | 506 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 17 | Z | 523 | BCR | C11-C10-C9 | -2.63 | 123.55 | 127.31 |
| 14 | H | 1225 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 21 | 2 | 822 | SQD | O8-S-C6 | 2.63 | 109.94 | 105.74 |
| 14 | r | 506 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 17 | H | 4014 | BCR | C34-C9-C8 | 2.63 | 122.22 | 118.08 |
| 14 | f | 1221 | CLA | O2D-CGD-CBD | 2.63 | 115.95 | 111.27 |
| 14 | f | 1229 | CLA | C6-C7-C8 | -2.63 | 107.41 | 115.92 |
| 14 | 5 | 507 | CLA | C1B-CHB-C4A | -2.63 | 124.90 | 130.12 |
| 17 | 6 | 522 | BCR | C16-C17-C18 | -2.63 | 123.55 | 127.31 |
| 14 | H | 1229 | CLA | C6-C7-C8 | -2.63 | 107.41 | 115.92 |
| 14 | B | 1224 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 14 | B | 1232 | CLA | C1B-CHB-C4A | -2.63 | 124.91 | 130.12 |
| 17 | e | 4008 | BCR | C7-C8-C9 | -2.63 | 122.26 | 126.23 |
| 14 | 4 | 517 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 14 | t | 517 | CLA | O2D-CGD-O1D | -2.63 | 118.69 | 123.84 |
| 17 | B | 4014 | BCR | C24-C23-C22 | -2.63 | 122.26 | 126.23 |
| 17 | F | 4016 | BCR | C33-C5-C6 | -2.63 | 121.58 | 124.53 |
| 14 | B | 1238 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | u | 501 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | G | 1135 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 14 | Z | 517 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 14 | f | 1205 | CLA | O2D-CGD-CBD | 2.63 | 115.94 | 111.27 |
| 14 | f | 1201 | CLA | C1B-CHB-C4A | -2.63 | 124.91 | 130.12 |
| 14 | b | 517 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 17 | b | 521 | BCR | C33-C5-C6 | -2.63 | 121.58 | 124.53 |
| 14 | u | 507 | CLA | C1B-CHB-C4A | -2.63 | 124.91 | 130.12 |
| 14 | f | 1230 | CLA | CAA-C2A-C1A | -2.63 | 103.36 | 111.97 |
| 14 | d | 505 | CLA | C1B-CHB-C4A | -2.63 | 124.91 | 130.12 |
| 14 | v | 505 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 14 | r | 513 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | 6 | 505 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | d | 504 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | G | 1125 | CLA | CHB-C4A-NA | 2.63 | 128.14 | 124.51 |
| 14 | f | 1231 | CLA | CHB-C4A-NA | 2.63 | 128.14 | 124.51 |
| 14 | e | 1117 | CLA | C1-C2-C3 | -2.63 | 121.50 | 126.04 |
| 14 | B | 1201 | CLA | C1B-CHB-C4A | -2.63 | 124.92 | 130.12 |
| 14 | G | 1011 | CLA | C4D-C3D-CAD | -2.63 | 105.00 | 108.10 |
| 14 | H | 1232 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | s | 508 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | t | 504 | CLA | CHB-C4A-NA | 2.63 | 128.14 | 124.51 |
| 14 | q | 519 | CLA | C1B-CHB-C4A | -2.63 | 124.92 | 130.12 |
| 14 | H | 1225 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 14 | H | 1221 | CLA | O2D-CGD-CBD | 2.63 | 115.93 | 111.27 |
| 17 | d | 522 | BCR | C38-C26-C27 | 2.63 | 118.66 | 113.62 |
| 17 | A | 4008 | BCR | C7-C8-C9 | -2.62 | 122.27 | 126.23 |
| 14 | B | 1229 | CLA | C6-C7-C8 | -2.62 | 107.44 | 115.92 |
| 14 | d | 505 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 14 | v | 505 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 14 | A | 1117 | CLA | C1-C2-C3 | -2.62 | 121.51 | 126.04 |
| 14 | e | 1011 | CLA | C4D-C3D-CAD | -2.62 | 105.01 | 108.10 |
| 14 | u | 518 | CLA | CMB-C2B-C3B | 2.62 | 129.58 | 124.68 |
| 14 | Z | 510 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 14 | l | 519 | CLA | C1B-CHB-C4A | -2.62 | 124.93 | 130.12 |
| 14 | A | 1111 | CLA | C1B-CHB-C4A | -2.62 | 124.93 | 130.12 |
| 14 | H | 1203 | CLA | C1-C2-C3 | -2.62 | 121.51 | 126.04 |
| 14 | d | 503 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | 3 | 505 | CLA | CHB-C4A-NA | 2.62 | 128.13 | 124.51 |
| 14 | r | 510 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | H | 1230 | CLA | CAA-C2A-C1A | -2.62 | 103.39 | 111.97 |
| 17 | 4 | 521 | BCR | C33-C5-C6 | -2.62 | 121.59 | 124.53 |
| 14 | 6 | 513 | CLA | CMB-C2B-C3B | 2.62 | 129.58 | 124.68 |
| 14 | Z | 506 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | c | 501 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | d | 513 | CLA | CMB-C2B-C3B | 2.62 | 129.58 | 124.68 |
| 14 | u | 518 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | 5 | 512 | CLA | CAA-C2A-C3A | -2.62 | 105.61 | 112.78 |
| 14 | G | 1117 | CLA | C1-C2-C3 | -2.62 | 121.52 | 126.04 |
| 14 | a | 508 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | s | 501 | CLA | CHB-C4A-NA | 2.62 | 128.13 | 124.51 |
| 14 | 3 | 508 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 14 | A | 1104 | CLA | O2A-CGA-O1A | -2.62 | 116.99 | 123.59 |
| 17 | 2 | 522 | BCR | C20-C21-C22 | -2.62 | 123.58 | 127.31 |
| 17 | e | 4007 | BCR | C38-C26-C27 | 2.62 | 118.64 | 113.62 |
| 14 | e | 1135 | CLA | CHB-C4A-NA | 2.61 | 128.13 | 124.51 |
| 14 | f | 1238 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 14 | e | 1104 | CLA | O2A-CGA-O1A | -2.61 | 116.99 | 123.59 |
| 21 | r | 822 | SQD | O8-S-C6 | 2.61 | 109.91 | 105.74 |
| 14 | Y | 511 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 14 | q | 513 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 14 | B | 1205 | CLA | O2D-CGD-CBD | 2.61 | 115.91 | 111.27 |
| 14 | l | 511 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1225 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 14 | b | 504 | CLA | CHB-C4A-NA | 2.61 | 128.13 | 124.51 |
| 14 | s | 517 | CLA | CHB-C4A-NA | 2.61 | 128.13 | 124.51 |
| 17 | Z | 523 | BCR | C24-C23-C22 | -2.61 | 122.29 | 126.23 |
| 14 | c | 507 | CLA | C1B-CHB-C4A | -2.61 | 124.94 | 130.12 |
| 14 | H | 1230 | CLA | CMB-C2B-C1B | -2.61 | 124.45 | 128.46 |
| 14 | a | 505 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 14 | Y | 519 | CLA | C1B-CHB-C4A | -2.61 | 124.94 | 130.12 |
| 17 | A | 4007 | BCR | C38-C26-C27 | 2.61 | 118.63 | 113.62 |
| 14 | 5 | 501 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 14 | a | 519 | CLA | CMB-C2B-C3B | 2.61 | 129.56 | 124.68 |
| 14 | r | 506 | CLA | C1B-CHB-C4A | -2.61 | 124.94 | 130.12 |
| 14 | a | 501 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 14 | a | 517 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 14 | G | 1104 | CLA | O2A-CGA-O1A | -2.61 | 117.00 | 123.59 |
| 14 | 3 | 518 | CLA | O2A-CGA-O1A | -2.61 | 117.00 | 123.59 |
| 14 | v | 510 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 14 | a | 518 | CLA | O2A-CGA-O1A | -2.61 | 117.00 | 123.59 |
| 14 | B | 1230 | CLA | CMB-C2B-C1B | -2.61 | 124.45 | 128.46 |
| 17 | d | 522 | BCR | C16-C17-C18 | -2.61 | 123.59 | 127.31 |
| 17 | B | 4014 | BCR | C34-C9-C8 | 2.61 | 122.19 | 118.08 |
| 17 | G | 4007 | BCR | C38-C26-C27 | 2.61 | 118.63 | 113.62 |
| 14 | H | 1201 | CLA | C1B-CHB-C4A | -2.61 | 124.95 | 130.12 |
| 14 | c | 512 | CLA | CAA-C2A-C3A | -2.61 | 105.64 | 112.78 |
| 14 | u | 512 | CLA | CAA-C2A-C3A | -2.61 | 105.64 | 112.78 |
| 17 | o | 4021 | BCR | C33-C5-C6 | -2.61 | 121.60 | 124.53 |
| 17 | r | 522 | BCR | C20-C21-C22 | -2.61 | 123.59 | 127.31 |
| 14 | B | 1225 | CLA | O2D-CGD-O1D | -2.61 | 118.74 | 123.84 |
| 14 | Z | 502 | CLA | O2D-CGD-O1D | -2.61 | 118.74 | 123.84 |
| 14 | f | 1230 | CLA | CMB-C2B-C1B | -2.61 | 124.46 | 128.46 |
| 14 | f | 1229 | CLA | C1B-CHB-C4A | -2.61 | 124.96 | 130.12 |
| 14 | l | 513 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 14 | e | 1116 | CLA | C1B-CHB-C4A | -2.60 | 124.96 | 130.12 |
| 14 | r | 502 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 17 | G | 4008 | BCR | C7-C8-C9 | -2.60 | 122.30 | 126.23 |
| 14 | a | 506 | CLA | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |
| 17 | u | 523 | BCR | C33-C5-C6 | -2.60 | 121.60 | 124.53 |
| 14 | H | 1229 | CLA | C1B-CHB-C4A | -2.60 | 124.96 | 130.12 |
| 14 | v | 519 | CLA | C1B-CHB-C4A | -2.60 | 124.96 | 130.12 |
| 17 | f | 4014 | BCR | C34-C9-C8 | 2.60 | 122.18 | 118.08 |
| 14 | G | 1111 | CLA | C1B-CHB-C4A | -2.60 | 124.96 | 130.12 |
| 14 | 3 | 506 | CLA | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1203 | CLA | C1-C2-C3 | -2.60 | 121.54 | 126.04 |
| 14 | 2 | 502 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 17 | s | 521 | BCR | C33-C5-C6 | -2.60 | 121.61 | 124.53 |
| 14 | H | 1224 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 14 | c | 518 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 14 | Y | 506 | CLA | C1B-CHB-C4A | -2.60 | 124.96 | 130.12 |
| 14 | 5 | 518 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 14 | a | 505 | CLA | C1B-CHB-C4A | -2.60 | 124.97 | 130.12 |
| 17 | T | 4015 | BCR | C38-C26-C25 | -2.60 | 121.61 | 124.53 |
| 19 | f | 1843 | LMU | C1B-O1B-C4' | -2.60 | 111.53 | 117.96 |
| 14 | 3 | 517 | CLA | CHB-C4A-NA | 2.60 | 128.11 | 124.51 |
| 14 | H | 1231 | CLA | C1B-CHB-C4A | -2.60 | 124.97 | 130.12 |
| 14 | s | 505 | CLA | C1B-CHB-C4A | -2.60 | 124.97 | 130.12 |
| 17 | 2 | 523 | BCR | C24-C23-C22 | -2.60 | 122.31 | 126.23 |
| 17 | 3 | 521 | BCR | C33-C5-C6 | -2.60 | 121.61 | 124.53 |
| 17 | a | 521 | BCR | C33-C5-C6 | -2.60 | 121.61 | 124.53 |
| 14 | s | 518 | CLA | O2A-CGA-O1A | -2.60 | 117.03 | 123.59 |
| 17 | H | 4006 | BCR | C39-C30-C25 | -2.60 | 106.08 | 110.30 |
| 17 | 5 | 523 | BCR | C33-C5-C6 | -2.60 | 121.61 | 124.53 |
| 14 | u | 518 | CLA | CHB-C4A-NA | 2.60 | 128.10 | 124.51 |
| 14 | 3 | 505 | CLA | C1B-CHB-C4A | -2.60 | 124.97 | 130.12 |
| 14 | e | 1111 | CLA | C1B-CHB-C4A | -2.60 | 124.97 | 130.12 |
| 14 | 3 | 519 | CLA | CMB-C2B-C3B | 2.60 | 129.53 | 124.68 |
| 14 | s | 519 | CLA | CMB-C2B-C3B | 2.60 | 129.53 | 124.68 |
| 14 | v | 513 | CLA | CMB-C2B-C3B | 2.60 | 129.53 | 124.68 |
| 14 | 2 | 506 | CLA | C1B-CHB-C4A | -2.60 | 124.98 | 130.12 |
| 14 | f | 1205 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 17 | 3 | 524 | BCR | C37-C22-C23 | 2.59 | 122.17 | 118.08 |
| 19 | B | 1843 | LMU | C1B-O1B-C4' | -2.59 | 111.54 | 117.96 |
| 14 | 1 | 506 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 14 | f | 1231 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 14 | H | 1203 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 14 | s | 517 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 14 | Y | 513 | CLA | O2D-CGD-O1D | -2.59 | 118.77 | 123.84 |
| 17 | a | 521 | BCR | C20-C19-C18 | -2.59 | 119.13 | 126.42 |
| 14 | H | 1240 | CLA | CHB-C4A-NA | 2.59 | 128.10 | 124.51 |
| 14 | B | 1229 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 17 | a | 522 | BCR | C20-C21-C22 | -2.59 | 123.61 | 127.31 |
| 17 | f | 4014 | BCR | C8-C7-C6 | -2.59 | 119.92 | 127.20 |
| 17 | 3 | 521 | BCR | C20-C19-C18 | -2.59 | 119.14 | 126.42 |
| 14 | e | 1122 | CLA | C1B-CHB-C4A | -2.59 | 124.98 | 130.12 |
| 14 | 3 | 501 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 507 | CLA | C1B-CHB-C4A | -2.59 | 124.99 | 130.12 |
| 14 | G | 1022 | CLA | O2D-CGD-O1D | -2.59 | 118.77 | 123.84 |
| 14 | B | 1231 | CLA | C1B-CHB-C4A | -2.59 | 124.99 | 130.12 |
| 14 | B | 1240 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 17 | 3 | 522 | BCR | C20-C21-C22 | -2.59 | 123.61 | 127.31 |
| 14 | B | 1205 | CLA | C1B-CHB-C4A | -2.59 | 124.99 | 130.12 |
| 14 | 6 | 510 | CLA | O2D-CGD-O1D | -2.59 | 118.78 | 123.84 |
| 14 | Z | 512 | CLA | O2D-CGD-O1D | -2.59 | 118.78 | 123.84 |
| 17 | 5 | 522 | BCR | C1-C6-C5 | -2.59 | 118.97 | 122.61 |
| 14 | r | 510 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 14 | A | 1116 | CLA | C1B-CHB-C4A | -2.59 | 124.99 | 130.12 |
| 14 | Y | 507 | CLA | C1B-CHB-C4A | -2.59 | 124.99 | 130.12 |
| 14 | H | 1205 | CLA | O2D-CGD-CBD | 2.59 | 115.87 | 111.27 |
| 14 | q | 511 | CLA | O2D-CGD-O1D | -2.59 | 118.78 | 123.84 |
| 14 | v | 516 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 14 | d | 519 | CLA | C1B-CHB-C4A | -2.59 | 124.99 | 130.12 |
| 17 | a | 523 | BCR | C33-C5-C4 | 2.59 | 118.58 | 113.62 |
| 14 | c | 518 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 14 | 6 | 519 | CLA | C1B-CHB-C4A | -2.59 | 125.00 | 130.12 |
| 14 | A | 1022 | CLA | O2D-CGD-O1D | -2.58 | 118.78 | 123.84 |
| 14 | e | 1237 | CLA | C6-C5-C3 | 2.58 | 120.23 | 113.45 |
| 14 | H | 1218 | CLA | CHB-C4A-NA | 2.58 | 128.09 | 124.51 |
| 14 | f | 1240 | CLA | CHB-C4A-NA | 2.58 | 128.09 | 124.51 |
| 14 | q | 516 | CLA | CHB-C4A-NA | 2.58 | 128.09 | 124.51 |
| 19 | H | 1843 | LMU | C1B-O1B-C4' | -2.58 | 111.57 | 117.96 |
| 14 | d | 510 | CLA | O2D-CGD-O1D | -2.58 | 118.78 | 123.84 |
| 17 | B | 4017 | BCR | C33-C5-C6 | -2.58 | 121.63 | 124.53 |
| 14 | A | 1134 | CLA | CMB-C2B-C3B | 2.58 | 129.51 | 124.68 |
| 14 | H | 1218 | CLA | CMB-C2B-C3B | 2.58 | 129.51 | 124.68 |
| 14 | a | 513 | CLA | C1B-CHB-C4A | -2.58 | 125.00 | 130.12 |
| 17 | U | 4104 | BCR | C30-C25-C26 | -2.58 | 118.97 | 122.61 |
| 14 | A | 1237 | CLA | C6-C5-C3 | 2.58 | 120.23 | 113.45 |
| 14 | Z | 505 | CLA | C1B-CHB-C4A | -2.58 | 125.00 | 130.12 |
| 17 | s | 522 | BCR | C20-C21-C22 | -2.58 | 123.62 | 127.31 |
| 17 | r | 522 | BCR | C38-C26-C25 | -2.58 | 121.63 | 124.53 |
| 14 | s | 506 | CLA | CHB-C4A-NA | 2.58 | 128.08 | 124.51 |
| 14 | 3 | 517 | CLA | C1B-CHB-C4A | -2.58 | 125.00 | 130.12 |
| 14 | e | 1134 | CLA | CMB-C2B-C3B | 2.58 | 129.51 | 124.68 |
| 17 | d | 523 | BCR | C10-C11-C12 | -2.58 | 115.16 | 123.22 |
| 14 | 5 | 518 | CLA | CHB-C4A-NA | 2.58 | 128.08 | 124.51 |
| 14 | G | 1134 | CLA | CMB-C2B-C3B | 2.58 | 129.51 | 124.68 |
| 17 | 3 | 523 | BCR | C33-C5-C4 | 2.58 | 118.58 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | s | 523 | BCR | C33-C5-C4 | 2.58 | 118.58 | 113.62 |
| 14 | f | 1203 | CLA | C1-C2-C3 | -2.58 | 121.58 | 126.04 |
| 17 | G | 4003 | BCR | C11-C10-C9 | -2.58 | 123.63 | 127.31 |
| 17 | s | 524 | BCR | C37-C22-C23 | 2.58 | 122.14 | 118.08 |
| 14 | s | 507 | CLA | C1B-CHB-C4A | -2.58 | 125.00 | 130.12 |
| 14 | A | 1127 | CLA | CHB-C4A-NA | 2.58 | 128.08 | 124.51 |
| 14 | Y | 516 | CLA | CHB-C4A-NA | 2.58 | 128.08 | 124.51 |
| 14 | G | 1237 | CLA | C6-C5-C3 | 2.58 | 120.22 | 113.45 |
| 14 | H | 1205 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 17 | 6 | 522 | BCR | C11-C12-C13 | -2.58 | 119.17 | 126.42 |
| 14 | e | 1022 | CLA | O2D-CGD-O1D | -2.58 | 118.79 | 123.84 |
| 19 | J | 5105 | LMU | C1'-C2'-C3' | 2.58 | 115.37 | 110.00 |
| 17 | B | 4006 | BCR | C39-C30-C25 | -2.58 | 106.11 | 110.30 |
| 18 | n | 5221 | LHG | C11-C10-C9 | -2.58 | 101.33 | 114.42 |
| 14 | A | 1103 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 14 | H | 1239 | CLA | C11-C10-C8 | -2.58 | 107.58 | 115.92 |
| 17 | d | 524 | BCR | C21-C20-C19 | -2.58 | 115.17 | 123.22 |
| 17 | u | 522 | BCR | C1-C6-C5 | -2.58 | 118.98 | 122.61 |
| 14 | l | 507 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 14 | Z | 506 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 19 | T | 5105 | LMU | C1'-C2'-C3' | 2.58 | 115.36 | 110.00 |
| 14 | e | 1103 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 18 | e | 5002 | LHG | C11-C10-C9 | -2.58 | 101.34 | 114.42 |
| 17 | 3 | 522 | BCR | C38-C26-C27 | 2.58 | 118.57 | 113.62 |
| 17 | 2 | 522 | BCR | C11-C12-C13 | -2.58 | 119.18 | 126.42 |
| 14 | e | 1119 | CLA | CHC-C1C-NC | 2.58 | 128.11 | 124.20 |
| 18 | L | 5221 | LHG | C11-C10-C9 | -2.58 | 101.34 | 114.42 |
| 17 | r | 523 | BCR | C24-C23-C22 | -2.58 | 122.34 | 126.23 |
| 14 | f | 1228 | CLA | C1B-CHB-C4A | -2.58 | 125.01 | 130.12 |
| 14 | r | 512 | CLA | O2D-CGD-O1D | -2.58 | 118.80 | 123.84 |
| 17 | s | 522 | BCR | C38-C26-C27 | 2.58 | 118.56 | 113.62 |
| 14 | B | 1239 | CLA | C11-C10-C8 | -2.58 | 107.59 | 115.92 |
| 17 | B | 4014 | BCR | C8-C7-C6 | -2.58 | 119.97 | 127.20 |
| 19 | l | 5105 | LMU | C1'-C2'-C3' | 2.58 | 115.36 | 110.00 |
| 14 | d | 516 | CLA | CHB-C4A-NA | 2.58 | 128.07 | 124.51 |
| 17 | Z | 522 | BCR | C11-C12-C13 | -2.58 | 119.18 | 126.42 |
| 18 | V | 5221 | LHG | C11-C10-C9 | -2.58 | 101.35 | 114.42 |
| 17 | s | 521 | BCR | C29-C30-C25 | 2.58 | 114.45 | 110.48 |
| 14 | q | 506 | CLA | C1B-CHB-C4A | -2.58 | 125.02 | 130.12 |
| 14 | 6 | 516 | CLA | CHB-C4A-NA | 2.58 | 128.07 | 124.51 |
| 17 | t | 524 | BCR | C8-C7-C6 | -2.57 | 119.97 | 127.20 |
| 14 | B | 1203 | CLA | C1B-CHB-C4A | -2.57 | 125.02 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1131 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 14 | f | 1239 | CLA | C11-C10-C8 | -2.57 | 107.60 | 115.92 |
| 14 | 1 | 518 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 14 | 4 | 512 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 17 | d | 522 | BCR | C11-C12-C13 | -2.57 | 119.19 | 126.42 |
| 17 | q | 524 | BCR | C1-C6-C5 | -2.57 | 118.99 | 122.61 |
| 14 | 2 | 510 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 17 | v | 523 | BCR | C33-C5-C6 | -2.57 | 121.64 | 124.53 |
| 14 | 3 | 507 | CLA | C1B-CHB-C4A | -2.57 | 125.02 | 130.12 |
| 14 | H | 1228 | CLA | C1B-CHB-C4A | -2.57 | 125.02 | 130.12 |
| 14 | t | 512 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 14 | e | 1127 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 14 | f | 1218 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 17 | 6 | 523 | BCR | C10-C11-C12 | -2.57 | 115.19 | 123.22 |
| 17 | c | 523 | BCR | C33-C5-C6 | -2.57 | 121.64 | 124.53 |
| 17 | s | 521 | BCR | C20-C19-C18 | -2.57 | 119.19 | 126.42 |
| 14 | 3 | 513 | CLA | C1B-CHB-C4A | -2.57 | 125.02 | 130.12 |
| 14 | 6 | 508 | CLA | C1B-CHB-C4A | -2.57 | 125.02 | 130.12 |
| 17 | 1 | 524 | BCR | C1-C6-C5 | -2.57 | 118.99 | 122.61 |
| 14 | 5 | 517 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 14 | e | 1131 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 17 | 6 | 524 | BCR | C21-C20-C19 | -2.57 | 115.19 | 123.22 |
| 17 | F | 4016 | BCR | C21-C20-C19 | -2.57 | 115.20 | 123.22 |
| 17 | v | 523 | BCR | C10-C11-C12 | -2.57 | 115.20 | 123.22 |
| 14 | Y | 518 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 14 | e | 1022 | CLA | C2D-C1D-ND | -2.57 | 108.21 | 110.10 |
| 14 | A | 1122 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 14 | a | 517 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 14 | H | 1207 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 14 | B | 1218 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 14 | 2 | 512 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 17 | r | 522 | BCR | C11-C12-C13 | -2.57 | 119.20 | 126.42 |
| 17 | v | 522 | BCR | C11-C12-C13 | -2.57 | 119.20 | 126.42 |
| 14 | f | 1203 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 17 | R | 4016 | BCR | C21-C20-C19 | -2.57 | 115.20 | 123.22 |
| 17 | M | 4021 | BCR | C33-C5-C6 | -2.57 | 121.64 | 124.53 |
| 17 | H | 4017 | BCR | C33-C5-C6 | -2.57 | 121.64 | 124.53 |
| 17 | e | 4003 | BCR | C11-C10-C9 | -2.57 | 123.64 | 127.31 |
| 14 | f | 1204 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 17 | j | 4016 | BCR | C21-C20-C19 | -2.57 | 115.20 | 123.22 |
| 14 | q | 518 | CLA | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 14 | u | 517 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1224 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 14 | f | 1205 | CLA | C1-C2-C3 | -2.57 | 121.60 | 126.04 |
| 14 | t | 518 | CLA | O2D-CGD-O1D | -2.57 | 118.82 | 123.84 |
| 18 | A | 5002 | LHG | C11-C10-C9 | -2.57 | 101.39 | 114.42 |
| 14 | s | 513 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 14 | v | 508 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 17 | a | 524 | BCR | C37-C22-C23 | 2.57 | 122.12 | 118.08 |
| 14 | A | 1131 | CLA | CMB-C2B-C3B | 2.57 | 129.48 | 124.68 |
| 17 | A | 4003 | BCR | C11-C10-C9 | -2.57 | 123.65 | 127.31 |
| 14 | e | 1105 | CLA | C1B-CHB-C4A | -2.57 | 125.03 | 130.12 |
| 17 | H | 4014 | BCR | C8-C7-C6 | -2.57 | 120.00 | 127.20 |
| 14 | G | 1116 | CLA | C1B-CHB-C4A | -2.56 | 125.04 | 130.12 |
| 17 | c | 522 | BCR | C1-C6-C5 | -2.56 | 119.00 | 122.61 |
| 14 | B | 1228 | CLA | C1B-CHB-C4A | -2.56 | 125.04 | 130.12 |
| 14 | c | 505 | CLA | C1B-CHB-C4A | -2.56 | 125.04 | 130.12 |
| 17 | 4 | 524 | BCR | C8-C7-C6 | -2.56 | 120.00 | 127.20 |
| 14 | G | 1137 | CLA | CAA-CBA-CGA | -2.56 | 105.76 | 113.25 |
| 14 | f | 1232 | CLA | CHB-C4A-NA | 2.56 | 128.06 | 124.51 |
| 17 | H | 4009 | BCR | C29-C30-C25 | 2.56 | 114.43 | 110.48 |
| 17 | f | 4006 | BCR | C39-C30-C25 | -2.56 | 106.14 | 110.30 |
| 14 | f | 1224 | CLA | CHB-C4A-NA | 2.56 | 128.06 | 124.51 |
| 14 | f | 1218 | CLA | CMB-C2B-C3B | 2.56 | 129.47 | 124.68 |
| 18 | G | 5002 | LHG | C11-C10-C9 | -2.56 | 101.42 | 114.42 |
| 17 | Y | 524 | BCR | C1-C6-C5 | -2.56 | 119.00 | 122.61 |
| 14 | e | 1137 | CLA | CAA-CBA-CGA | -2.56 | 105.77 | 113.25 |
| 14 | G | 1122 | CLA | C1B-CHB-C4A | -2.56 | 125.04 | 130.12 |
| 17 | 3 | 521 | BCR | C29-C30-C25 | 2.56 | 114.42 | 110.48 |
| 14 | 1 | 516 | CLA | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 14 | 2 | 505 | CLA | C1B-CHB-C4A | -2.56 | 125.04 | 130.12 |
| 14 | G | 1105 | CLA | C1B-CHB-C4A | -2.56 | 125.04 | 130.12 |
| 17 | v | 524 | BCR | C21-C20-C19 | -2.56 | 115.22 | 123.22 |
| 22 | X | 170 | FMN | C4A-C10-N10 | 2.56 | 120.22 | 116.48 |
| 14 | b | 512 | CLA | CMB-C2B-C3B | 2.56 | 129.47 | 124.68 |
| 17 | m | 4104 | BCR | C30-C25-C26 | -2.56 | 119.01 | 122.61 |
| 17 | 2 | 522 | BCR | C38-C26-C25 | -2.56 | 121.65 | 124.53 |
| 17 | f | 4017 | BCR | C33-C5-C6 | -2.56 | 121.65 | 124.53 |
| 17 | b | 524 | BCR | C8-C7-C6 | -2.56 | 120.01 | 127.20 |
| 14 | q | 507 | CLA | C1B-CHB-C4A | -2.56 | 125.05 | 130.12 |
| 14 | A | 1137 | CLA | CAA-CBA-CGA | -2.56 | 105.77 | 113.25 |
| 14 | b | 518 | CLA | O2D-CGD-O1D | -2.56 | 118.83 | 123.84 |
| 17 | v | 524 | BCR | C37-C22-C23 | 2.56 | 122.11 | 118.08 |
| 17 | H | 4014 | BCR | C24-C25-C26 | 2.56 | 127.66 | 121.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | F | 1302 | CLA | O2D-CGD-O1D | -2.56 | 118.83 | 123.84 |
| 14 | G | 1123 | CLA | C2A-C1A-CHA | 2.56 | 128.34 | 123.86 |
| 14 | G | 1132 | CLA | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 17 | f | 4009 | BCR | C29-C30-C25 | 2.56 | 114.42 | 110.48 |
| 22 | P | 170 | FMN | C4A-C10-N10 | 2.56 | 120.22 | 116.48 |
| 14 | A | 1105 | CLA | C1B-CHB-C4A | -2.56 | 125.05 | 130.12 |
| 14 | e | 1138 | CLA | O2D-CGD-CBD | 2.56 | 115.81 | 111.27 |
| 14 | G | 1103 | CLA | C1B-CHB-C4A | -2.56 | 125.05 | 130.12 |
| 14 | H | 1236 | CLA | C1-C2-C3 | -2.56 | 122.61 | 126.75 |
| 17 | K | 4104 | BCR | C30-C25-C26 | -2.56 | 119.01 | 122.61 |
| 14 | 4 | 518 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 14 | A | 1138 | CLA | O2D-CGD-CBD | 2.56 | 115.81 | 111.27 |
| 17 | f | 4014 | BCR | C24-C25-C26 | 2.56 | 127.66 | 121.46 |
| 14 | G | 1124 | CLA | C2D-C1D-ND | -2.56 | 108.22 | 110.10 |
| 14 | K | 1105 | CLA | CMC-C2C-C3C | 2.56 | 133.06 | 126.12 |
| 14 | G | 1116 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 14 | f | 1222 | CLA | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 17 | 5 | 524 | BCR | C8-C7-C6 | -2.56 | 120.03 | 127.20 |
| 14 | d | 508 | CLA | C1B-CHB-C4A | -2.56 | 125.06 | 130.12 |
| 22 | p | 170 | FMN | C4A-C10-N10 | 2.56 | 120.22 | 116.48 |
| 17 | c | 524 | BCR | C8-C7-C6 | -2.56 | 120.03 | 127.20 |
| 14 | H | 1232 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 17 | e | 4008 | BCR | C34-C9-C8 | 2.55 | 122.10 | 118.08 |
| 14 | A | 1132 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 14 | G | 1127 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 14 | A | 1123 | CLA | C2A-C1A-CHA | 2.55 | 128.32 | 123.86 |
| 17 | 6 | 523 | BCR | C33-C5-C6 | -2.55 | 121.66 | 124.53 |
| 14 | B | 1218 | CLA | O2D-CGD-O1D | -2.55 | 118.84 | 123.84 |
| 14 | b | 512 | CLA | O2D-CGD-O1D | -2.55 | 118.84 | 123.84 |
| 14 | d | 509 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 14 | e | 1237 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 14 | c | 517 | CLA | C1B-CHB-C4A | -2.55 | 125.06 | 130.12 |
| 14 | l | 506 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 17 | a | 521 | BCR | C29-C30-C25 | 2.55 | 114.41 | 110.48 |
| 14 | U | 1105 | CLA | CMC-C2C-C3C | 2.55 | 133.04 | 126.12 |
| 14 | a | 518 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 21 | V | 5216 | SQD | O48-C23-C24 | 2.55 | 119.91 | 111.91 |
| 14 | s | 501 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 14 | v | 510 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 17 | d | 523 | BCR | C33-C5-C6 | -2.55 | 121.66 | 124.53 |
| 17 | u | 523 | BCR | C21-C20-C19 | -2.55 | 115.26 | 123.22 |
| 14 | 4 | 512 | CLA | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | W | 4021 | BCR | C38-C26-C27 | 2.55 | 118.51 | 113.62 |
| 14 | m | 1105 | CLA | CMC-C2C-C3C | 2.55 | 133.04 | 126.12 |
| 14 | e | 1123 | CLA | C2A-C1A-CHA | 2.55 | 128.31 | 123.86 |
| 14 | Y | 516 | CLA | C1B-CHB-C4A | -2.55 | 125.07 | 130.12 |
| 17 | a | 522 | BCR | C38-C26-C27 | 2.55 | 118.51 | 113.62 |
| 14 | G | 1011 | CLA | C1B-CHB-C4A | -2.55 | 125.07 | 130.12 |
| 17 | B | 4009 | BCR | C29-C30-C25 | 2.55 | 114.40 | 110.48 |
| 14 | B | 1207 | CLA | CHB-C4A-NA | 2.55 | 128.03 | 124.51 |
| 14 | H | 1205 | CLA | C1-C2-C3 | -2.55 | 121.64 | 126.04 |
| 21 | a | 822 | SQD | C4-C3-C2 | 2.55 | 115.27 | 110.82 |
| 14 | B | 1218 | CLA | CHB-C4A-NA | 2.55 | 128.03 | 124.51 |
| 17 | 6 | 524 | BCR | C37-C22-C23 | 2.55 | 122.09 | 118.08 |
| 14 | q | 516 | CLA | C1B-CHB-C4A | -2.55 | 125.08 | 130.12 |
| 14 | e | 1124 | CLA | C2D-C1D-ND | -2.55 | 108.23 | 110.10 |
| 14 | s | 518 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 17 | B | 4014 | BCR | C24-C25-C26 | 2.55 | 127.63 | 121.46 |
| 17 | W | 4021 | BCR | C33-C5-C6 | -2.55 | 121.67 | 124.53 |
| 17 | 5 | 523 | BCR | C21-C20-C19 | -2.54 | 115.28 | 123.22 |
| 14 | B | 1232 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 17 | B | 4009 | BCR | C16-C15-C14 | -2.54 | 118.26 | 123.47 |
| 17 | u | 524 | BCR | C8-C7-C6 | -2.54 | 120.06 | 127.20 |
| 21 | L | 5216 | SQD | C45-O47-C7 | 2.54 | 124.05 | 117.79 |
| 14 | 3 | 518 | CLA | O2D-CGD-O1D | -2.54 | 118.86 | 123.84 |
| 17 | o | 4021 | BCR | C38-C26-C27 | 2.54 | 118.50 | 113.62 |
| 17 | H | 4009 | BCR | C16-C15-C14 | -2.54 | 118.26 | 123.47 |
| 14 | H | 1204 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 14 | A | 1119 | CLA | CHC-C1C-NC | 2.54 | 128.06 | 124.20 |
| 17 | G | 4008 | BCR | C34-C9-C8 | 2.54 | 122.08 | 118.08 |
| 14 | t | 512 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 14 | F | 1301 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 14 | Z | 510 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 14 | G | 1119 | CLA | CHC-C1C-NC | 2.54 | 128.06 | 124.20 |
| 14 | A | 1022 | CLA | C2D-C1D-ND | -2.54 | 108.23 | 110.10 |
| 14 | B | 1205 | CLA | C1-C2-C3 | -2.54 | 121.65 | 126.04 |
| 14 | R | 1301 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 14 | j | 1301 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 21 | 3 | 822 | SQD | C4-C3-C2 | 2.54 | 115.26 | 110.82 |
| 14 | f | 1218 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 17 | Z | 522 | BCR | C38-C26-C25 | -2.54 | 121.67 | 124.53 |
| 14 | f | 1207 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 21 | L | 5216 | SQD | O48-C23-C24 | 2.54 | 119.88 | 111.91 |
| 17 | b | 522 | BCR | C23-C24-C25 | -2.54 | 120.07 | 127.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1116 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 17 | L | 4022 | BCR | C33-C5-C6 | -2.54 | 121.68 | 124.53 |
| 14 | e | 1113 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 14 | Y | 506 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 21 | n | 5216 | SQD | C45-O47-C7 | 2.54 | 124.04 | 117.79 |
| 14 | 6 | 509 | CLA | O2D-CGD-O1D | -2.54 | 118.87 | 123.84 |
| 14 | c | 519 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 17 | L | 4022 | BCR | C21-C20-C19 | -2.54 | 115.30 | 123.22 |
| 14 | B | 1204 | CLA | CHB-C4A-NA | 2.54 | 128.02 | 124.51 |
| 14 | H | 1224 | CLA | CHB-C4A-NA | 2.54 | 128.02 | 124.51 |
| 21 | s | 822 | SQD | C4-C3-C2 | 2.54 | 115.25 | 110.82 |
| 14 | B | 1234 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 14 | 5 | 505 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 17 | 4 | 522 | BCR | C23-C24-C25 | -2.54 | 120.07 | 127.20 |
| 17 | L | 4020 | BCR | C8-C9-C10 | -2.54 | 115.05 | 118.94 |
| 17 | c | 523 | BCR | C21-C20-C19 | -2.54 | 115.30 | 123.22 |
| 14 | B | 1222 | CLA | CHB-C4A-NA | 2.54 | 128.02 | 124.51 |
| 14 | G | 1801 | CLA | CHB-C4A-NA | 2.54 | 128.02 | 124.51 |
| 17 | A | 4008 | BCR | C34-C9-C8 | 2.54 | 122.08 | 118.08 |
| 14 | j | 1302 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 17 | e | 4003 | BCR | C21-C20-C19 | -2.54 | 115.30 | 123.22 |
| 14 | f | 1234 | CLA | C1B-CHB-C4A | -2.54 | 125.09 | 130.12 |
| 17 | f | 4009 | BCR | C16-C15-C14 | -2.54 | 118.28 | 123.47 |
| 14 | G | 1138 | CLA | O2D-CGD-CBD | 2.54 | 115.78 | 111.27 |
| 17 | G | 4008 | BCR | C38-C26-C27 | 2.54 | 118.49 | 113.62 |
| 17 | t | 522 | BCR | C23-C24-C25 | -2.54 | 120.08 | 127.20 |
| 21 | V | 5216 | SQD | C45-O47-C7 | 2.54 | 124.03 | 117.79 |
| 14 | H | 1218 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 14 | c | 509 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 17 | e | 4002 | BCR | C23-C24-C25 | -2.54 | 120.08 | 127.20 |
| 17 | u | 522 | BCR | C21-C20-C19 | -2.54 | 115.31 | 123.22 |
| 14 | Y | 502 | CLA | O2D-CGD-O1D | -2.53 | 118.88 | 123.84 |
| 14 | B | 1210 | CLA | C1-C2-C3 | -2.53 | 121.66 | 126.04 |
| 14 | f | 1236 | CLA | C1-C2-C3 | -2.53 | 122.65 | 126.75 |
| 14 | q | 502 | CLA | O2D-CGD-O1D | -2.53 | 118.88 | 123.84 |
| 17 | c | 522 | BCR | C21-C20-C19 | -2.53 | 115.31 | 123.22 |
| 17 | Y | 522 | BCR | C20-C21-C22 | -2.53 | 123.69 | 127.31 |
| 14 | 1 | 516 | CLA | C1B-CHB-C4A | -2.53 | 125.10 | 130.12 |
| 14 | r | 505 | CLA | C1B-CHB-C4A | -2.53 | 125.10 | 130.12 |
| 17 | 2 | 524 | BCR | C37-C22-C23 | 2.53 | 122.07 | 118.08 |
| 14 | 3 | 501 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 14 | G | 1022 | CLA | C2D-C1D-ND | -2.53 | 108.24 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1236 | CLA | C1-C2-C3 | -2.53 | 122.66 | 126.75 |
| 21 | n | 5216 | SQD | O48-C23-C24 | 2.53 | 119.85 | 111.91 |
| 17 | Z | 524 | BCR | C37-C22-C23 | 2.53 | 122.07 | 118.08 |
| 17 | d | 523 | BCR | C11-C10-C9 | -2.53 | 123.70 | 127.31 |
| 17 | G | 4002 | BCR | C23-C24-C25 | -2.53 | 120.09 | 127.20 |
| 18 | A | 5006 | LHG | O8-C23-C24 | 2.53 | 119.85 | 111.91 |
| 18 | G | 5001 | LHG | O8-C23-C24 | 2.53 | 119.85 | 111.91 |
| 14 | 5 | 519 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 14 | 6 | 510 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 14 | H | 1222 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 17 | 5 | 522 | BCR | C21-C20-C19 | -2.53 | 115.32 | 123.22 |
| 14 | H | 1210 | CLA | C1-C2-C3 | -2.53 | 121.67 | 126.04 |
| 17 | A | 4002 | BCR | C23-C24-C25 | -2.53 | 120.10 | 127.20 |
| 14 | A | 1121 | CLA | O2D-CGD-CBD | 2.53 | 115.76 | 111.27 |
| 14 | A | 1102 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 14 | t | 501 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 17 | r | 522 | BCR | C33-C5-C6 | -2.53 | 121.69 | 124.53 |
| 14 | l | 502 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 14 | e | 1121 | CLA | O2D-CGD-CBD | 2.53 | 115.76 | 111.27 |
| 14 | A | 1011 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 17 | r | 522 | BCR | C38-C26-C27 | 2.53 | 118.47 | 113.62 |
| 17 | n | 4020 | BCR | C8-C9-C10 | -2.53 | 115.06 | 118.94 |
| 17 | M | 4021 | BCR | C38-C26-C27 | 2.53 | 118.47 | 113.62 |
| 14 | f | 1023 | CLA | CAA-CBA-CGA | -2.53 | 105.86 | 113.25 |
| 14 | R | 1302 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 14 | A | 1237 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 14 | K | 1401 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 14 | e | 1132 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 14 | A | 1124 | CLA | C2D-C1D-ND | -2.53 | 108.24 | 110.10 |
| 14 | H | 1234 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 14 | H | 1023 | CLA | CAA-CBA-CGA | -2.53 | 105.87 | 113.25 |
| 17 | m | 4104 | BCR | C15-C16-C17 | -2.53 | 118.30 | 123.47 |
| 14 | H | 1220 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 14 | m | 1401 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 14 | G | 1134 | CLA | O2D-CGD-CBD | 2.53 | 115.76 | 111.27 |
| 17 | A | 4003 | BCR | C21-C20-C19 | -2.53 | 115.33 | 123.22 |
| 14 | e | 1116 | CLA | O2D-CGD-O1D | -2.53 | 118.90 | 123.84 |
| 17 | d | 524 | BCR | C37-C22-C23 | 2.53 | 122.06 | 118.08 |
| 14 | A | 1140 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 14 | e | 1102 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 14 | G | 1121 | CLA | CMB-C2B-C3B | 2.53 | 129.40 | 124.68 |
| 14 | A | 1134 | CLA | O2D-CGD-CBD | 2.53 | 115.76 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1113 | CLA | C1B-CHB-C4A | -2.53 | 125.11 | 130.12 |
| 17 | n | 4022 | BCR | C21-C20-C19 | -2.53 | 115.34 | 123.22 |
| 17 | B | 4006 | BCR | C1-C6-C5 | -2.53 | 119.06 | 122.61 |
| 17 | q | 522 | BCR | C20-C21-C22 | -2.52 | 123.71 | 127.31 |
| 14 | e | 1011 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 17 | V | 4022 | BCR | C21-C20-C19 | -2.52 | 115.34 | 123.22 |
| 14 | f | 1205 | CLA | CMB-C2B-C3B | 2.52 | 129.40 | 124.68 |
| 18 | G | 5006 | LHG | O8-C23-C24 | 2.52 | 119.83 | 111.91 |
| 14 | G | 1105 | CLA | O2A-CGA-O1A | -2.52 | 117.22 | 123.59 |
| 14 | 4 | 501 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 18 | e | 5001 | LHG | O8-C23-C24 | 2.52 | 119.83 | 111.91 |
| 17 | l | 522 | BCR | C20-C21-C22 | -2.52 | 123.71 | 127.31 |
| 14 | q | 506 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 14 | G | 1113 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 14 | u | 505 | CLA | C1B-CHB-C4A | -2.52 | 125.12 | 130.12 |
| 14 | e | 1108 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 20 | B | 5002 | LMG | O1-C1-C2 | -2.52 | 104.36 | 108.30 |
| 14 | u | 509 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 14 | q | 512 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 17 | H | 4006 | BCR | C1-C6-C5 | -2.52 | 119.06 | 122.61 |
| 17 | e | 4008 | BCR | C38-C26-C27 | 2.52 | 118.46 | 113.62 |
| 14 | f | 1203 | CLA | C11-C12-C13 | -2.52 | 107.77 | 115.92 |
| 20 | f | 5002 | LMG | O1-C1-C2 | -2.52 | 104.37 | 108.30 |
| 14 | B | 1023 | CLA | CAA-CBA-CGA | -2.52 | 105.89 | 113.25 |
| 14 | f | 1234 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 17 | V | 4022 | BCR | C33-C5-C6 | -2.52 | 121.70 | 124.53 |
| 17 | T | 4015 | BCR | C21-C20-C19 | -2.52 | 115.35 | 123.22 |
| 14 | G | 1140 | CLA | C1B-CHB-C4A | -2.52 | 125.13 | 130.12 |
| 17 | n | 4022 | BCR | C33-C5-C6 | -2.52 | 121.70 | 124.53 |
| 21 | v | 822 | SQD | C45-O47-C7 | 2.52 | 122.59 | 117.90 |
| 17 | G | 4003 | BCR | C21-C20-C19 | -2.52 | 115.36 | 123.22 |
| 18 | A | 5001 | LHG | O8-C23-C24 | 2.52 | 119.81 | 111.91 |
| 14 | 5 | 509 | CLA | O2D-CGD-O1D | -2.52 | 118.92 | 123.84 |
| 17 | L | 4219 | BCR | C39-C30-C25 | -2.52 | 106.22 | 110.30 |
| 14 | Y | 512 | CLA | O2D-CGD-O1D | -2.52 | 118.92 | 123.84 |
| 21 | d | 822 | SQD | C45-O47-C7 | 2.52 | 122.59 | 117.90 |
| 14 | e | 1134 | CLA | O2D-CGD-CBD | 2.52 | 115.74 | 111.27 |
| 14 | e | 1140 | CLA | C1B-CHB-C4A | -2.52 | 125.13 | 130.12 |
| 14 | f | 1210 | CLA | C1-C2-C3 | -2.52 | 121.69 | 126.04 |
| 17 | U | 4104 | BCR | C15-C16-C17 | -2.52 | 118.32 | 123.47 |
| 17 | f | 4006 | BCR | C1-C6-C5 | -2.52 | 119.07 | 122.61 |
| 14 | t | 505 | CLA | C1B-CHB-C4A | -2.52 | 125.13 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1205 | CLA | CMB-C2B-C3B | 2.52 | 129.38 | 124.68 |
| 14 | v | 516 | CLA | C1B-CHB-C4A | -2.52 | 125.14 | 130.12 |
| 17 | A | 4008 | BCR | C38-C26-C27 | 2.51 | 118.45 | 113.62 |
| 14 | B | 1210 | CLA | CHB-C4A-NA | 2.51 | 127.99 | 124.51 |
| 18 | e | 5006 | LHG | O8-C23-C24 | 2.51 | 119.80 | 111.91 |
| 14 | q | 519 | CLA | CHB-C4A-NA | 2.51 | 127.99 | 124.51 |
| 14 | e | 1105 | CLA | O2A-CGA-O1A | -2.51 | 117.25 | 123.59 |
| 17 | V | 4020 | BCR | C8-C9-C10 | -2.51 | 115.08 | 118.94 |
| 14 | l | 512 | CLA | O2D-CGD-O1D | -2.51 | 118.92 | 123.84 |
| 14 | u | 519 | CLA | C1B-CHB-C4A | -2.51 | 125.14 | 130.12 |
| 17 | J | 4015 | BCR | C21-C20-C19 | -2.51 | 115.37 | 123.22 |
| 14 | A | 1801 | CLA | CHB-C4A-NA | 2.51 | 127.99 | 124.51 |
| 21 | 6 | 822 | SQD | C45-O47-C7 | 2.51 | 122.58 | 117.90 |
| 14 | A | 1105 | CLA | O2A-CGA-O1A | -2.51 | 117.25 | 123.59 |
| 17 | 2 | 522 | BCR | C38-C26-C27 | 2.51 | 118.44 | 113.62 |
| 14 | G | 1102 | CLA | C1B-CHB-C4A | -2.51 | 125.14 | 130.12 |
| 14 | 2 | 518 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 14 | B | 1234 | CLA | CHB-C4A-NA | 2.51 | 127.99 | 124.51 |
| 14 | G | 1237 | CLA | CHB-C4A-NA | 2.51 | 127.99 | 124.51 |
| 14 | d | 510 | CLA | CHB-C4A-NA | 2.51 | 127.99 | 124.51 |
| 14 | G | 1121 | CLA | O2D-CGD-CBD | 2.51 | 115.73 | 111.27 |
| 17 | n | 4020 | BCR | C28-C27-C26 | -2.51 | 109.59 | 114.08 |
| 17 | J | 4013 | BCR | C32-C1-C6 | -2.51 | 106.22 | 110.30 |
| 14 | b | 501 | CLA | C1B-CHB-C4A | -2.51 | 125.14 | 130.12 |
| 14 | A | 1121 | CLA | CMB-C2B-C3B | 2.51 | 129.38 | 124.68 |
| 14 | v | 509 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 17 | Y | 523 | BCR | C34-C9-C8 | 2.51 | 122.03 | 118.08 |
| 17 | v | 523 | BCR | C11-C10-C9 | -2.51 | 123.73 | 127.31 |
| 14 | A | 1126 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 18 | e | 5005 | LHG | O8-C23-C24 | 2.51 | 119.78 | 111.91 |
| 14 | e | 1126 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 14 | B | 1220 | CLA | C1B-CHB-C4A | -2.51 | 125.15 | 130.12 |
| 14 | a | 501 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 14 | G | 1108 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 14 | H | 1203 | CLA | C11-C12-C13 | -2.51 | 107.81 | 115.92 |
| 14 | A | 1134 | CLA | C2A-C1A-CHA | 2.51 | 128.24 | 123.86 |
| 17 | l | 523 | BCR | C34-C9-C8 | 2.51 | 122.03 | 118.08 |
| 17 | K | 4104 | BCR | C15-C16-C17 | -2.51 | 118.34 | 123.47 |
| 14 | H | 1234 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 17 | B | 4014 | BCR | C35-C13-C12 | 2.51 | 122.03 | 118.08 |
| 14 | r | 501 | CLA | C1B-CHB-C4A | -2.51 | 125.16 | 130.12 |
| 20 | H | 5002 | LMG | O1-C1-C2 | -2.51 | 104.39 | 108.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | T | 4013 | BCR | C32-C1-C6 | -2.50 | 106.24 | 110.30 |
| 14 | G | 1134 | CLA | C2A-C1A-CHA | 2.50 | 128.24 | 123.86 |
| 14 | 4 | 505 | CLA | C1B-CHB-C4A | -2.50 | 125.16 | 130.12 |
| 14 | f | 1220 | CLA | C1B-CHB-C4A | -2.50 | 125.16 | 130.12 |
| 18 | A | 5005 | LHG | O8-C23-C24 | 2.50 | 119.77 | 111.91 |
| 14 | B | 1203 | CLA | C11-C12-C13 | -2.50 | 107.83 | 115.92 |
| 14 | b | 505 | CLA | C1B-CHB-C4A | -2.50 | 125.16 | 130.12 |
| 17 | f | 4009 | BCR | C8-C7-C6 | -2.50 | 120.17 | 127.20 |
| 14 | A | 1108 | CLA | CHB-C4A-NA | 2.50 | 127.97 | 124.51 |
| 14 | H | 1205 | CLA | CMB-C2B-C3B | 2.50 | 129.36 | 124.68 |
| 14 | f | 1219 | CLA | O2A-CGA-O1A | -2.50 | 117.28 | 123.59 |
| 17 | q | 523 | BCR | C34-C9-C8 | 2.50 | 122.02 | 118.08 |
| 17 | Z | 522 | BCR | C38-C26-C27 | 2.50 | 118.42 | 113.62 |
| 14 | B | 1219 | CLA | O2A-CGA-O1A | -2.50 | 117.28 | 123.59 |
| 17 | l | 4013 | BCR | C32-C1-C6 | -2.50 | 106.24 | 110.30 |
| 14 | 3 | 519 | CLA | C1B-CHB-C4A | -2.50 | 125.17 | 130.12 |
| 14 | a | 503 | CLA | O2D-CGD-O1D | -2.50 | 118.95 | 123.84 |
| 14 | H | 1219 | CLA | O2A-CGA-O1A | -2.50 | 117.28 | 123.59 |
| 14 | 2 | 501 | CLA | C1B-CHB-C4A | -2.50 | 125.17 | 130.12 |
| 14 | B | 1206 | CLA | O2A-CGA-O1A | -2.50 | 117.29 | 123.59 |
| 14 | e | 1121 | CLA | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 17 | 6 | 523 | BCR | C11-C10-C9 | -2.50 | 123.75 | 127.31 |
| 14 | 1 | 519 | CLA | CHB-C4A-NA | 2.50 | 127.97 | 124.51 |
| 14 | a | 519 | CLA | C1B-CHB-C4A | -2.50 | 125.17 | 130.12 |
| 14 | d | 516 | CLA | C1B-CHB-C4A | -2.50 | 125.17 | 130.12 |
| 14 | 2 | 505 | CLA | O2D-CGD-O1D | -2.50 | 118.95 | 123.84 |
| 14 | e | 1134 | CLA | C2A-C1A-CHA | 2.50 | 128.23 | 123.86 |
| 18 | A | 5009 | LHG | C11-C10-C9 | -2.50 | 101.75 | 114.42 |
| 17 | l | 4015 | BCR | C21-C20-C19 | -2.50 | 115.42 | 123.22 |
| 17 | V | 4219 | BCR | C39-C30-C25 | -2.50 | 106.25 | 110.30 |
| 17 | B | 4009 | BCR | C8-C7-C6 | -2.50 | 120.19 | 127.20 |
| 17 | 2 | 523 | BCR | C10-C11-C12 | -2.50 | 115.43 | 123.22 |
| 14 | f | 1206 | CLA | O2A-CGA-O1A | -2.50 | 117.29 | 123.59 |
| 17 | q | 524 | BCR | C24-C23-C22 | -2.49 | 122.47 | 126.23 |
| 18 | G | 5009 | LHG | C11-C10-C9 | -2.49 | 101.76 | 114.42 |
| 18 | e | 5009 | LHG | C11-C10-C9 | -2.49 | 101.76 | 114.42 |
| 18 | G | 5005 | LHG | O8-C23-C24 | 2.49 | 119.74 | 111.91 |
| 17 | n | 4219 | BCR | C39-C30-C25 | -2.49 | 106.25 | 110.30 |
| 17 | r | 524 | BCR | C37-C22-C23 | 2.49 | 122.01 | 118.08 |
| 14 | 6 | 516 | CLA | C1B-CHB-C4A | -2.49 | 125.18 | 130.12 |
| 14 | e | 1801 | CLA | CHB-C4A-NA | 2.49 | 127.96 | 124.51 |
| 17 | 2 | 522 | BCR | C33-C5-C6 | -2.49 | 121.73 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | K | 1103 | CLA | CMB-C2B-C3B | 2.49 | 129.34 | 124.68 |
| 17 | Z | 523 | BCR | C10-C11-C12 | -2.49 | 115.44 | 123.22 |
| 14 | d | 513 | CLA | C1B-CHB-C4A | -2.49 | 125.18 | 130.12 |
| 17 | L | 4020 | BCR | C28-C27-C26 | -2.49 | 109.63 | 114.08 |
| 17 | d | 524 | BCR | C20-C21-C22 | -2.49 | 123.75 | 127.31 |
| 17 | I | 4018 | BCR | C33-C5-C4 | 2.49 | 118.40 | 113.62 |
| 17 | f | 4006 | BCR | C15-C16-C17 | -2.49 | 118.37 | 123.47 |
| 14 | G | 1126 | CLA | CHB-C4A-NA | 2.49 | 127.96 | 124.51 |
| 17 | r | 523 | BCR | C10-C11-C12 | -2.49 | 115.45 | 123.22 |
| 14 | 3 | 503 | CLA | O2D-CGD-O1D | -2.49 | 118.97 | 123.84 |
| 14 | H | 1210 | CLA | O2D-CGD-O1D | -2.49 | 118.97 | 123.84 |
| 14 | e | 1135 | CLA | C2D-C1D-ND | -2.49 | 108.27 | 110.10 |
| 14 | B | 1228 | CLA | C1-C2-C3 | -2.49 | 121.74 | 126.04 |
| 17 | s | 521 | BCR | C7-C8-C9 | -2.49 | 122.47 | 126.23 |
| 14 | s | 503 | CLA | O2D-CGD-O1D | -2.49 | 118.97 | 123.84 |
| 14 | s | 519 | CLA | C1B-CHB-C4A | -2.49 | 125.19 | 130.12 |
| 14 | v | 513 | CLA | C1B-CHB-C4A | -2.49 | 125.19 | 130.12 |
| 18 | e | 5003 | LHG | C20-C19-C18 | -2.49 | 101.80 | 114.42 |
| 14 | U | 1401 | CLA | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 17 | e | 4001 | BCR | C21-C20-C19 | -2.49 | 115.46 | 123.22 |
| 14 | Z | 518 | CLA | O2D-CGD-O1D | -2.49 | 118.98 | 123.84 |
| 14 | H | 1210 | CLA | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 14 | 6 | 513 | CLA | C1B-CHB-C4A | -2.49 | 125.19 | 130.12 |
| 17 | f | 4014 | BCR | C35-C13-C12 | 2.49 | 121.99 | 118.08 |
| 17 | H | 4009 | BCR | C8-C7-C6 | -2.49 | 120.22 | 127.20 |
| 18 | G | 5003 | LHG | C20-C19-C18 | -2.49 | 101.81 | 114.42 |
| 14 | 3 | 502 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 14 | f | 1210 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 14 | r | 518 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 17 | r | 524 | BCR | C21-C20-C19 | -2.48 | 115.46 | 123.22 |
| 14 | B | 1210 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 18 | A | 5003 | LHG | C20-C19-C18 | -2.48 | 101.81 | 114.42 |
| 14 | l | 1303 | CLA | O2D-CGD-CBD | 2.48 | 115.68 | 111.27 |
| 17 | G | 4001 | BCR | C21-C20-C19 | -2.48 | 115.47 | 123.22 |
| 17 | G | 4007 | BCR | C10-C11-C12 | -2.48 | 115.47 | 123.22 |
| 14 | A | 1237 | CLA | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 17 | k | 4018 | BCR | C33-C5-C4 | 2.48 | 118.39 | 113.62 |
| 17 | A | 4007 | BCR | C10-C11-C12 | -2.48 | 115.47 | 123.22 |
| 14 | Z | 501 | CLA | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 17 | q | 524 | BCR | C37-C22-C23 | 2.48 | 121.99 | 118.08 |
| 14 | t | 509 | CLA | O2A-CGA-O1A | -2.48 | 117.11 | 123.30 |
| 14 | Z | 505 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | r | 505 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 17 | V | 4020 | BCR | C28-C27-C26 | -2.48 | 109.64 | 114.08 |
| 14 | T | 1303 | CLA | O2D-CGD-CBD | 2.48 | 115.68 | 111.27 |
| 14 | H | 1234 | CLA | CAC-C3C-C4C | 2.48 | 128.03 | 124.81 |
| 17 | A | 4001 | BCR | C21-C20-C19 | -2.48 | 115.47 | 123.22 |
| 17 | S | 4018 | BCR | C30-C25-C26 | -2.48 | 119.12 | 122.61 |
| 17 | r | 523 | BCR | C33-C5-C6 | -2.48 | 121.74 | 124.53 |
| 14 | L | 1503 | CLA | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 14 | v | 506 | CLA | C1B-CHB-C4A | -2.48 | 125.20 | 130.12 |
| 17 | Z | 524 | BCR | C21-C20-C19 | -2.48 | 115.48 | 123.22 |
| 14 | J | 1303 | CLA | O2D-CGD-CBD | 2.48 | 115.67 | 111.27 |
| 17 | v | 524 | BCR | C20-C21-C22 | -2.48 | 123.77 | 127.31 |
| 17 | e | 4007 | BCR | C10-C11-C12 | -2.48 | 115.48 | 123.22 |
| 17 | t | 523 | BCR | C34-C9-C8 | 2.48 | 121.98 | 118.08 |
| 14 | H | 1214 | CLA | C1B-CHB-C4A | -2.48 | 125.21 | 130.12 |
| 17 | 2 | 524 | BCR | C21-C20-C19 | -2.48 | 115.48 | 123.22 |
| 14 | B | 1206 | CLA | C1B-CHB-C4A | -2.48 | 125.21 | 130.12 |
| 14 | e | 1237 | CLA | C1B-CHB-C4A | -2.48 | 125.21 | 130.12 |
| 14 | q | 517 | CLA | C1B-CHB-C4A | -2.48 | 125.21 | 130.12 |
| 14 | 4 | 509 | CLA | O2A-CGA-O1A | -2.48 | 117.13 | 123.30 |
| 17 | S | 4018 | BCR | C33-C5-C4 | 2.48 | 118.37 | 113.62 |
| 17 | f | 4006 | BCR | C33-C5-C4 | 2.47 | 118.37 | 113.62 |
| 17 | Y | 524 | BCR | C37-C22-C23 | 2.47 | 121.98 | 118.08 |
| 14 | G | 1237 | CLA | C1B-CHB-C4A | -2.47 | 125.22 | 130.12 |
| 21 | f | 1852 | SQD | O47-C7-C8 | 2.47 | 116.83 | 111.50 |
| 17 | 6 | 524 | BCR | C20-C21-C22 | -2.47 | 123.78 | 127.31 |
| 14 | f | 1228 | CLA | C1-C2-C3 | -2.47 | 121.76 | 126.04 |
| 14 | s | 502 | CLA | O2D-CGD-O1D | -2.47 | 119.00 | 123.84 |
| 14 | U | 1103 | CLA | CMB-C2B-C3B | 2.47 | 129.31 | 124.68 |
| 17 | A | 4003 | BCR | C24-C23-C22 | -2.47 | 122.50 | 126.23 |
| 18 | e | 5001 | LHG | C11-C10-C9 | -2.47 | 101.87 | 114.42 |
| 14 | B | 1214 | CLA | CMB-C2B-C3B | 2.47 | 129.31 | 124.68 |
| 17 | A | 4003 | BCR | C38-C26-C25 | -2.47 | 121.75 | 124.53 |
| 14 | f | 1210 | CLA | CHB-C4A-NA | 2.47 | 127.93 | 124.51 |
| 17 | Y | 524 | BCR | C24-C23-C22 | -2.47 | 122.50 | 126.23 |
| 17 | H | 4014 | BCR | C35-C13-C12 | 2.47 | 121.97 | 118.08 |
| 14 | Y | 517 | CLA | C1B-CHB-C4A | -2.47 | 125.22 | 130.12 |
| 14 | n | 1503 | CLA | C1B-CHB-C4A | -2.47 | 125.22 | 130.12 |
| 14 | m | 1103 | CLA | CMB-C2B-C3B | 2.47 | 129.30 | 124.68 |
| 17 | B | 4006 | BCR | C15-C16-C17 | -2.47 | 118.41 | 123.47 |
| 14 | s | 512 | CLA | O2D-CGD-O1D | -2.47 | 119.01 | 123.84 |
| 17 | G | 4002 | BCR | C10-C11-C12 | -2.47 | 115.51 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | B | 4006 | BCR | C33-C5-C4 | 2.47 | 118.36 | 113.62 |
| 17 | Y | 521 | BCR | C33-C5-C6 | -2.47 | 121.75 | 124.53 |
| 17 | A | 4002 | BCR | C10-C11-C12 | -2.47 | 115.51 | 123.22 |
| 18 | A | 5001 | LHG | C11-C10-C9 | -2.47 | 101.89 | 114.42 |
| 17 | 4 | 523 | BCR | C34-C9-C8 | 2.47 | 121.97 | 118.08 |
| 17 | 3 | 521 | BCR | C7-C8-C9 | -2.47 | 122.50 | 126.23 |
| 14 | u | 517 | CLA | CHB-C4A-NA | 2.47 | 127.92 | 124.51 |
| 14 | H | 1206 | CLA | O2A-CGA-O1A | -2.47 | 117.36 | 123.59 |
| 17 | A | 4008 | BCR | C16-C15-C14 | -2.47 | 118.42 | 123.47 |
| 17 | u | 521 | BCR | C7-C8-C9 | -2.47 | 122.51 | 126.23 |
| 14 | A | 1107 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 14 | r | 517 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 17 | G | 4008 | BCR | C16-C15-C14 | -2.47 | 118.42 | 123.47 |
| 14 | f | 1206 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 14 | f | 1235 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 14 | G | 1105 | CLA | CHD-C1D-ND | -2.47 | 122.19 | 124.45 |
| 14 | H | 1206 | CLA | C1B-CHB-C4A | -2.47 | 125.23 | 130.12 |
| 14 | f | 1214 | CLA | CMB-C2B-C3B | 2.47 | 129.29 | 124.68 |
| 14 | A | 1136 | CLA | C1B-CHB-C4A | -2.46 | 125.24 | 130.12 |
| 17 | H | 4006 | BCR | C33-C5-C4 | 2.46 | 118.35 | 113.62 |
| 17 | Z | 522 | BCR | C33-C5-C6 | -2.46 | 121.76 | 124.53 |
| 14 | b | 509 | CLA | O2A-CGA-O1A | -2.46 | 117.16 | 123.30 |
| 18 | e | 5009 | LHG | C27-C26-C25 | -2.46 | 101.92 | 114.42 |
| 17 | e | 4008 | BCR | C16-C15-C14 | -2.46 | 118.43 | 123.47 |
| 14 | Y | 519 | CLA | CHB-C4A-NA | 2.46 | 127.92 | 124.51 |
| 14 | H | 1228 | CLA | C1-C2-C3 | -2.46 | 121.78 | 126.04 |
| 17 | c | 522 | BCR | C11-C12-C13 | -2.46 | 119.50 | 126.42 |
| 14 | e | 1116 | CLA | CHB-C4A-NA | 2.46 | 127.92 | 124.51 |
| 18 | e | 5001 | LHG | O8-C23-O10 | -2.46 | 117.38 | 123.59 |
| 17 | I | 4018 | BCR | C30-C25-C26 | -2.46 | 119.14 | 122.61 |
| 18 | G | 5001 | LHG | C11-C10-C9 | -2.46 | 101.92 | 114.42 |
| 17 | 5 | 522 | BCR | C11-C12-C13 | -2.46 | 119.50 | 126.42 |
| 18 | G | 5001 | LHG | O8-C23-O10 | -2.46 | 117.38 | 123.59 |
| 14 | B | 1214 | CLA | C1B-CHB-C4A | -2.46 | 125.24 | 130.12 |
| 14 | e | 1136 | CLA | C1B-CHB-C4A | -2.46 | 125.24 | 130.12 |
| 17 | d | 522 | BCR | C33-C5-C6 | -2.46 | 121.76 | 124.53 |
| 17 | H | 4006 | BCR | C15-C16-C17 | -2.46 | 118.43 | 123.47 |
| 17 | L | 4020 | BCR | C29-C28-C27 | -2.46 | 105.88 | 111.38 |
| 17 | l | 524 | BCR | C24-C23-C22 | -2.46 | 122.52 | 126.23 |
| 17 | a | 521 | BCR | C7-C8-C9 | -2.46 | 122.52 | 126.23 |
| 14 | a | 502 | CLA | O2D-CGD-O1D | -2.46 | 119.03 | 123.84 |
| 14 | f | 1206 | CLA | CHB-C4A-NA | 2.46 | 127.92 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 3 | 512 | CLA | O2D-CGD-O1D | -2.46 | 119.03 | 123.84 |
| 18 | A | 5009 | LHG | C27-C26-C25 | -2.46 | 101.93 | 114.42 |
| 14 | A | 1127 | CLA | C1B-CHB-C4A | -2.46 | 125.24 | 130.12 |
| 18 | G | 5009 | LHG | C27-C26-C25 | -2.46 | 101.94 | 114.42 |
| 17 | Z | 523 | BCR | C33-C5-C6 | -2.46 | 121.77 | 124.53 |
| 14 | B | 1206 | CLA | CHB-C4A-NA | 2.46 | 127.91 | 124.51 |
| 14 | 4 | 506 | CLA | C1B-CHB-C4A | -2.46 | 125.25 | 130.12 |
| 14 | U | 1401 | CLA | C1B-CHB-C4A | -2.46 | 125.25 | 130.12 |
| 14 | f | 1236 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 14 | e | 1107 | CLA | C1B-CHB-C4A | -2.46 | 125.25 | 130.12 |
| 17 | l | 521 | BCR | C33-C5-C6 | -2.46 | 121.77 | 124.53 |
| 17 | e | 4003 | BCR | C38-C26-C25 | -2.46 | 121.77 | 124.53 |
| 17 | q | 521 | BCR | C33-C5-C6 | -2.46 | 121.77 | 124.53 |
| 14 | K | 1401 | CLA | C1B-CHB-C4A | -2.46 | 125.25 | 130.12 |
| 14 | B | 1236 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 17 | V | 4019 | BCR | C16-C15-C14 | -2.46 | 118.44 | 123.47 |
| 14 | l | 517 | CLA | C1B-CHB-C4A | -2.46 | 125.25 | 130.12 |
| 21 | B | 1852 | SQD | O47-C7-C8 | 2.46 | 116.79 | 111.50 |
| 17 | u | 522 | BCR | C11-C12-C13 | -2.46 | 119.52 | 126.42 |
| 14 | A | 1135 | CLA | C2D-C1D-ND | -2.45 | 108.30 | 110.10 |
| 14 | B | 1234 | CLA | CAC-C3C-C4C | 2.45 | 128.00 | 124.81 |
| 17 | e | 4002 | BCR | C10-C11-C12 | -2.45 | 115.56 | 123.22 |
| 14 | H | 1236 | CLA | CMB-C2B-C3B | 2.45 | 129.27 | 124.68 |
| 14 | A | 1115 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 14 | G | 1107 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 14 | e | 1127 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 20 | l | 5104 | LMG | O6-C1-O1 | -2.45 | 104.16 | 109.97 |
| 20 | J | 5104 | LMG | O6-C1-O1 | -2.45 | 104.17 | 109.97 |
| 17 | c | 521 | BCR | C7-C8-C9 | -2.45 | 122.53 | 126.23 |
| 17 | u | 522 | BCR | C33-C5-C4 | 2.45 | 118.33 | 113.62 |
| 14 | m | 1401 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 14 | B | 1210 | CLA | CBC-CAC-C3C | 2.45 | 119.19 | 112.43 |
| 14 | H | 1210 | CLA | CBC-CAC-C3C | 2.45 | 119.19 | 112.43 |
| 14 | f | 1210 | CLA | CBC-CAC-C3C | 2.45 | 119.19 | 112.43 |
| 17 | b | 523 | BCR | C34-C9-C8 | 2.45 | 121.94 | 118.08 |
| 14 | H | 1214 | CLA | CMB-C2B-C3B | 2.45 | 129.26 | 124.68 |
| 17 | H | 4009 | BCR | C15-C16-C17 | -2.45 | 118.45 | 123.47 |
| 17 | 5 | 522 | BCR | C33-C5-C4 | 2.45 | 118.33 | 113.62 |
| 14 | 6 | 501 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 17 | v | 522 | BCR | C33-C5-C6 | -2.45 | 121.78 | 124.53 |
| 14 | B | 1012 | CLA | C16-C15-C13 | -2.45 | 108.00 | 115.92 |
| 14 | 6 | 506 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1136 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 14 | r | 509 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 14 | t | 506 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 21 | a | 822 | SQD | C1-O5-C5 | 2.45 | 118.50 | 113.69 |
| 17 | 5 | 521 | BCR | C7-C8-C9 | -2.45 | 122.53 | 126.23 |
| 14 | V | 1503 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | f | 1214 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 17 | A | 4001 | BCR | C11-C12-C13 | -2.45 | 119.53 | 126.42 |
| 14 | B | 1235 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | G | 1101 | CLA | CMB-C2B-C3B | 2.45 | 129.26 | 124.68 |
| 14 | v | 501 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 17 | 1 | 524 | BCR | C37-C22-C23 | 2.45 | 121.94 | 118.08 |
| 14 | f | 1234 | CLA | CAC-C3C-C4C | 2.45 | 127.99 | 124.81 |
| 17 | e | 4001 | BCR | C11-C12-C13 | -2.45 | 119.54 | 126.42 |
| 14 | e | 1115 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 18 | A | 5001 | LHG | O8-C23-O10 | -2.45 | 117.42 | 123.59 |
| 21 | 3 | 822 | SQD | C1-O5-C5 | 2.45 | 118.49 | 113.69 |
| 14 | r | 516 | CLA | O2D-CGD-CBD | 2.45 | 115.62 | 111.27 |
| 14 | f | 1216 | CLA | C1-O2A-CGA | 2.45 | 122.86 | 116.44 |
| 14 | a | 510 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | H | 1206 | CLA | CHB-C4A-NA | 2.45 | 127.89 | 124.51 |
| 14 | B | 1230 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | G | 1115 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | b | 503 | CLA | O2D-CGD-O1D | -2.45 | 119.06 | 123.84 |
| 14 | r | 508 | CLA | O2D-CGD-O1D | -2.45 | 119.06 | 123.84 |
| 14 | e | 1101 | CLA | CMB-C2B-C3B | 2.45 | 129.25 | 124.68 |
| 14 | V | 1501 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | d | 506 | CLA | C1B-CHB-C4A | -2.45 | 125.27 | 130.12 |
| 14 | f | 1012 | CLA | C16-C15-C13 | -2.45 | 108.02 | 115.92 |
| 14 | a | 512 | CLA | O2D-CGD-O1D | -2.44 | 119.06 | 123.84 |
| 17 | B | 4009 | BCR | C15-C16-C17 | -2.44 | 118.47 | 123.47 |
| 17 | n | 4020 | BCR | C29-C28-C27 | -2.44 | 105.91 | 111.38 |
| 17 | G | 4003 | BCR | C24-C23-C22 | -2.44 | 122.54 | 126.23 |
| 14 | 5 | 517 | CLA | CHB-C4A-NA | 2.44 | 127.89 | 124.51 |
| 14 | f | 1230 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 17 | e | 4003 | BCR | C24-C23-C22 | -2.44 | 122.54 | 126.23 |
| 17 | u | 521 | BCR | C34-C9-C8 | 2.44 | 121.93 | 118.08 |
| 17 | 3 | 522 | BCR | C38-C26-C25 | -2.44 | 121.78 | 124.53 |
| 14 | 2 | 509 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 14 | Z | 516 | CLA | O2D-CGD-CBD | 2.44 | 115.61 | 111.27 |
| 14 | b | 506 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 14 | s | 504 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | G | 4003 | BCR | C10-C11-C12 | -2.44 | 115.60 | 123.22 |
| 14 | Y | 509 | CLA | O2D-CGD-O1D | -2.44 | 119.06 | 123.84 |
| 14 | L | 1501 | CLA | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 17 | 2 | 523 | BCR | C33-C5-C6 | -2.44 | 121.79 | 124.53 |
| 17 | 6 | 522 | BCR | C33-C5-C6 | -2.44 | 121.79 | 124.53 |
| 14 | G | 1119 | CLA | CAC-C3C-C4C | 2.44 | 127.98 | 124.81 |
| 14 | H | 1216 | CLA | C1-O2A-CGA | 2.44 | 122.85 | 116.44 |
| 17 | L | 4019 | BCR | C16-C15-C14 | -2.44 | 118.47 | 123.47 |
| 17 | G | 4007 | BCR | C21-C20-C19 | -2.44 | 115.60 | 123.22 |
| 17 | e | 4007 | BCR | C21-C20-C19 | -2.44 | 115.60 | 123.22 |
| 14 | H | 1012 | CLA | C16-C15-C13 | -2.44 | 108.03 | 115.92 |
| 17 | V | 4020 | BCR | C29-C28-C27 | -2.44 | 105.92 | 111.38 |
| 17 | U | 4104 | BCR | C28-C27-C26 | -2.44 | 109.72 | 114.08 |
| 14 | e | 1136 | CLA | C1-C2-C3 | -2.44 | 121.82 | 126.04 |
| 14 | G | 1127 | CLA | C1B-CHB-C4A | -2.44 | 125.29 | 130.12 |
| 20 | T | 5104 | LMG | O6-C1-O1 | -2.44 | 104.20 | 109.97 |
| 20 | f | 5002 | LMG | C42-C41-C40 | -2.44 | 102.05 | 114.42 |
| 14 | A | 1116 | CLA | CHB-C4A-NA | 2.44 | 127.88 | 124.51 |
| 17 | a | 522 | BCR | C38-C26-C25 | -2.44 | 121.79 | 124.53 |
| 14 | d | 501 | CLA | C1B-CHB-C4A | -2.44 | 125.29 | 130.12 |
| 14 | n | 1501 | CLA | C1B-CHB-C4A | -2.44 | 125.29 | 130.12 |
| 17 | 2 | 523 | BCR | C21-C20-C19 | -2.44 | 115.61 | 123.22 |
| 14 | 2 | 516 | CLA | O2D-CGD-CBD | 2.44 | 115.60 | 111.27 |
| 17 | B | 4014 | BCR | C37-C22-C23 | 2.44 | 121.92 | 118.08 |
| 17 | H | 4010 | BCR | C23-C22-C21 | 2.44 | 122.68 | 118.94 |
| 14 | B | 1216 | CLA | C1-O2A-CGA | 2.44 | 122.84 | 116.44 |
| 18 | L | 5221 | LHG | C20-C19-C18 | -2.44 | 102.05 | 114.42 |
| 17 | r | 523 | BCR | C21-C20-C19 | -2.44 | 115.61 | 123.22 |
| 17 | H | 4014 | BCR | C37-C22-C23 | 2.44 | 121.92 | 118.08 |
| 21 | s | 822 | SQD | C1-O5-C5 | 2.44 | 118.47 | 113.69 |
| 21 | H | 1852 | SQD | O47-C7-C8 | 2.44 | 116.75 | 111.50 |
| 17 | k | 4018 | BCR | C30-C25-C26 | -2.44 | 119.18 | 122.61 |
| 17 | f | 4009 | BCR | C15-C16-C17 | -2.44 | 118.48 | 123.47 |
| 14 | 6 | 508 | CLA | O2D-CGD-O1D | -2.44 | 119.08 | 123.84 |
| 14 | H | 1230 | CLA | C1B-CHB-C4A | -2.44 | 125.29 | 130.12 |
| 17 | H | 4006 | BCR | C3-C4-C5 | -2.44 | 109.73 | 114.08 |
| 14 | 1 | 509 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 17 | e | 4003 | BCR | C10-C11-C12 | -2.43 | 115.62 | 123.22 |
| 21 | u | 822 | SQD | C45-O47-C7 | 2.43 | 122.43 | 117.90 |
| 17 | A | 4003 | BCR | C10-C11-C12 | -2.43 | 115.62 | 123.22 |
| 14 | G | 1114 | CLA | CHB-C4A-NA | 2.43 | 127.88 | 124.51 |
| 14 | q | 509 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 509 | CLA | C1B-CHB-C4A | -2.43 | 125.30 | 130.12 |
| 17 | n | 4019 | BCR | C16-C15-C14 | -2.43 | 118.49 | 123.47 |
| 17 | m | 4104 | BCR | C28-C27-C26 | -2.43 | 109.73 | 114.08 |
| 14 | v | 503 | CLA | C1B-CHB-C4A | -2.43 | 125.30 | 130.12 |
| 14 | G | 1136 | CLA | C1-C2-C3 | -2.43 | 121.84 | 126.04 |
| 17 | G | 4003 | BCR | C38-C26-C25 | -2.43 | 121.80 | 124.53 |
| 14 | c | 517 | CLA | CHB-C4A-NA | 2.43 | 127.88 | 124.51 |
| 17 | A | 4007 | BCR | C21-C20-C19 | -2.43 | 115.63 | 123.22 |
| 17 | Z | 523 | BCR | C21-C20-C19 | -2.43 | 115.63 | 123.22 |
| 14 | Z | 509 | CLA | C1B-CHB-C4A | -2.43 | 125.30 | 130.12 |
| 14 | 2 | 508 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 14 | 2 | 517 | CLA | C1B-CHB-C4A | -2.43 | 125.30 | 130.12 |
| 14 | G | 1130 | CLA | CHB-C4A-NA | 2.43 | 127.87 | 124.51 |
| 17 | m | 4104 | BCR | C23-C24-C25 | -2.43 | 120.38 | 127.20 |
| 20 | B | 5002 | LMG | C42-C41-C40 | -2.43 | 102.09 | 114.42 |
| 14 | B | 1210 | CLA | O2A-CGA-O1A | -2.43 | 117.46 | 123.59 |
| 14 | A | 1136 | CLA | C1-C2-C3 | -2.43 | 121.84 | 126.04 |
| 17 | f | 4014 | BCR | C37-C22-C23 | 2.43 | 121.91 | 118.08 |
| 18 | V | 5221 | LHG | C20-C19-C18 | -2.43 | 102.09 | 114.42 |
| 14 | t | 503 | CLA | C2D-C1D-ND | -2.43 | 108.31 | 110.10 |
| 14 | A | 1101 | CLA | CMB-C2B-C3B | 2.43 | 129.22 | 124.68 |
| 17 | s | 524 | BCR | C27-C26-C25 | -2.43 | 119.20 | 122.73 |
| 20 | H | 5002 | LMG | C42-C41-C40 | -2.43 | 102.10 | 114.42 |
| 17 | 5 | 521 | BCR | C34-C9-C8 | 2.43 | 121.90 | 118.08 |
| 14 | s | 510 | CLA | C1B-CHB-C4A | -2.43 | 125.31 | 130.12 |
| 18 | n | 5221 | LHG | C20-C19-C18 | -2.43 | 102.11 | 114.42 |
| 17 | K | 4104 | BCR | C28-C27-C26 | -2.43 | 109.74 | 114.08 |
| 17 | U | 4104 | BCR | C23-C24-C25 | -2.43 | 120.39 | 127.20 |
| 17 | B | 4010 | BCR | C23-C22-C21 | 2.43 | 122.66 | 118.94 |
| 14 | s | 509 | CLA | C1B-CHB-C4A | -2.43 | 125.31 | 130.12 |
| 17 | G | 4001 | BCR | C11-C12-C13 | -2.43 | 119.60 | 126.42 |
| 17 | K | 4104 | BCR | C23-C24-C25 | -2.43 | 120.39 | 127.20 |
| 17 | B | 4006 | BCR | C3-C4-C5 | -2.42 | 109.75 | 114.08 |
| 21 | 5 | 822 | SQD | C45-O47-C7 | 2.42 | 122.42 | 117.90 |
| 14 | G | 1116 | CLA | CHB-C4A-NA | 2.42 | 127.86 | 124.51 |
| 14 | f | 1215 | CLA | C3C-C4C-NC | -2.42 | 107.85 | 110.57 |
| 17 | V | 4020 | BCR | C15-C14-C13 | -2.42 | 123.85 | 127.31 |
| 17 | c | 522 | BCR | C33-C5-C4 | 2.42 | 118.27 | 113.62 |
| 14 | d | 508 | CLA | O2D-CGD-O1D | -2.42 | 119.10 | 123.84 |
| 14 | b | 512 | CLA | CHB-C4A-NA | 2.42 | 127.86 | 124.51 |
| 14 | 6 | 503 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 14 | Z | 519 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1139 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 14 | A | 1114 | CLA | CHB-C4A-NA | 2.42 | 127.86 | 124.51 |
| 14 | f | 1210 | CLA | O2A-CGA-O1A | -2.42 | 117.48 | 123.59 |
| 14 | e | 1127 | CLA | C1-C2-C3 | -2.42 | 121.86 | 126.04 |
| 14 | v | 508 | CLA | O2D-CGD-O1D | -2.42 | 119.10 | 123.84 |
| 14 | 4 | 503 | CLA | O2D-CGD-O1D | -2.42 | 119.11 | 123.84 |
| 14 | 3 | 504 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 14 | 3 | 509 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 14 | H | 1215 | CLA | C3C-C4C-NC | -2.42 | 107.86 | 110.57 |
| 14 | H | 1235 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 14 | a | 518 | CLA | C1B-CHB-C4A | -2.42 | 125.32 | 130.12 |
| 14 | e | 1124 | CLA | CHD-C1D-ND | -2.42 | 122.23 | 124.45 |
| 14 | b | 519 | CLA | C1B-CHB-C4A | -2.42 | 125.33 | 130.12 |
| 14 | 3 | 510 | CLA | C1B-CHB-C4A | -2.42 | 125.33 | 130.12 |
| 14 | a | 504 | CLA | C1B-CHB-C4A | -2.42 | 125.33 | 130.12 |
| 14 | B | 1240 | CLA | C1-C2-C3 | -2.42 | 121.86 | 126.04 |
| 14 | A | 1139 | CLA | C1B-CHB-C4A | -2.42 | 125.33 | 130.12 |
| 14 | A | 1124 | CLA | CHD-C1D-ND | -2.42 | 122.23 | 124.45 |
| 14 | s | 507 | CLA | O2D-CGD-O1D | -2.42 | 119.11 | 123.84 |
| 14 | t | 503 | CLA | O2D-CGD-O1D | -2.42 | 119.11 | 123.84 |
| 17 | o | 4021 | BCR | C36-C18-C19 | 2.42 | 121.89 | 118.08 |
| 14 | A | 1127 | CLA | C1-C2-C3 | -2.42 | 121.86 | 126.04 |
| 14 | Z | 517 | CLA | C1B-CHB-C4A | -2.42 | 125.33 | 130.12 |
| 14 | H | 1210 | CLA | O2A-CGA-O1A | -2.42 | 117.49 | 123.59 |
| 14 | e | 1135 | CLA | O2A-CGA-O1A | -2.42 | 117.49 | 123.59 |
| 14 | B | 1230 | CLA | CHB-C4A-NA | 2.42 | 127.85 | 124.51 |
| 17 | t | 523 | BCR | C21-C20-C19 | -2.42 | 115.68 | 123.22 |
| 17 | I | 4018 | BCR | C38-C26-C27 | 2.42 | 118.26 | 113.62 |
| 17 | G | 4002 | BCR | C33-C5-C6 | -2.42 | 121.82 | 124.53 |
| 21 | 5 | 822 | SQD | C4-C3-C2 | 2.42 | 115.04 | 110.82 |
| 17 | c | 521 | BCR | C34-C9-C8 | 2.41 | 121.88 | 118.08 |
| 14 | e | 1119 | CLA | CAC-C3C-C4C | 2.41 | 127.94 | 124.81 |
| 14 | b | 511 | CLA | C1B-CHB-C4A | -2.41 | 125.33 | 130.12 |
| 14 | 4 | 503 | CLA | C2D-C1D-ND | -2.41 | 108.33 | 110.10 |
| 14 | d | 503 | CLA | C1B-CHB-C4A | -2.41 | 125.34 | 130.12 |
| 14 | e | 1105 | CLA | CHD-C1D-ND | -2.41 | 122.24 | 124.45 |
| 14 | U | 1105 | CLA | CHB-C4A-NA | 2.41 | 127.85 | 124.51 |
| 21 | c | 822 | SQD | C45-O47-C7 | 2.41 | 122.39 | 117.90 |
| 14 | 3 | 507 | CLA | O2D-CGD-O1D | -2.41 | 119.12 | 123.84 |
| 14 | e | 1114 | CLA | CHB-C4A-NA | 2.41 | 127.85 | 124.51 |
| 14 | G | 1139 | CLA | C1B-CHB-C4A | -2.41 | 125.34 | 130.12 |
| 18 | L | 5218 | LHG | C27-C26-C25 | -2.41 | 102.18 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 518 | CLA | CMB-C2B-C3B | 2.41 | 129.19 | 124.68 |
| 17 | f | 4006 | BCR | C3-C4-C5 | -2.41 | 109.77 | 114.08 |
| 17 | u | 522 | BCR | C1-C6-C7 | 2.41 | 122.60 | 115.78 |
| 14 | f | 1235 | CLA | CHD-C1D-ND | -2.41 | 122.24 | 124.45 |
| 14 | G | 1135 | CLA | C2D-C1D-ND | -2.41 | 108.33 | 110.10 |
| 18 | I | 5001 | LHG | C20-C19-C18 | -2.41 | 102.18 | 114.42 |
| 17 | f | 4014 | BCR | C15-C14-C13 | -2.41 | 123.87 | 127.31 |
| 14 | A | 1136 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 14 | A | 1130 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 18 | n | 5218 | LHG | C27-C26-C25 | -2.41 | 102.19 | 114.42 |
| 14 | t | 509 | CLA | C1B-CHB-C4A | -2.41 | 125.34 | 130.12 |
| 14 | A | 1119 | CLA | CAC-C3C-C4C | 2.41 | 127.94 | 124.81 |
| 17 | a | 522 | BCR | C23-C24-C25 | -2.41 | 120.44 | 127.20 |
| 17 | 5 | 522 | BCR | C1-C6-C7 | 2.41 | 122.59 | 115.78 |
| 18 | S | 5001 | LHG | C20-C19-C18 | -2.41 | 102.20 | 114.42 |
| 18 | k | 5001 | LHG | C20-C19-C18 | -2.41 | 102.20 | 114.42 |
| 14 | e | 1136 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 17 | A | 4002 | BCR | C20-C19-C18 | -2.41 | 119.65 | 126.42 |
| 17 | e | 4002 | BCR | C20-C19-C18 | -2.41 | 119.65 | 126.42 |
| 14 | a | 507 | CLA | O2D-CGD-O1D | -2.41 | 119.13 | 123.84 |
| 14 | G | 1135 | CLA | O2A-CGA-O1A | -2.41 | 117.52 | 123.59 |
| 17 | M | 4021 | BCR | C36-C18-C19 | 2.41 | 121.87 | 118.08 |
| 17 | s | 522 | BCR | C38-C26-C25 | -2.41 | 121.83 | 124.53 |
| 14 | A | 1105 | CLA | CHD-C1D-ND | -2.41 | 122.24 | 124.45 |
| 14 | v | 502 | CLA | O2D-CGD-O1D | -2.41 | 119.13 | 123.84 |
| 18 | V | 5218 | LHG | C27-C26-C25 | -2.41 | 102.21 | 114.42 |
| 17 | H | 4014 | BCR | C15-C14-C13 | -2.41 | 123.88 | 127.31 |
| 14 | 3 | 518 | CLA | C1B-CHB-C4A | -2.41 | 125.35 | 130.12 |
| 14 | f | 1230 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 17 | q | 522 | BCR | C30-C25-C26 | -2.41 | 119.22 | 122.61 |
| 17 | e | 4002 | BCR | C33-C5-C6 | -2.41 | 121.83 | 124.53 |
| 14 | G | 1136 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 14 | 3 | 518 | CLA | CMB-C2B-C3B | 2.41 | 129.18 | 124.68 |
| 17 | 4 | 524 | BCR | C3-C4-C5 | -2.40 | 109.78 | 114.08 |
| 14 | s | 518 | CLA | CMB-C2B-C3B | 2.40 | 129.18 | 124.68 |
| 17 | k | 4018 | BCR | C38-C26-C27 | 2.40 | 118.23 | 113.62 |
| 14 | G | 1124 | CLA | CHD-C1D-ND | -2.40 | 122.25 | 124.45 |
| 14 | G | 1127 | CLA | C1-C2-C3 | -2.40 | 121.89 | 126.04 |
| 21 | u | 822 | SQD | C4-C3-C2 | 2.40 | 115.02 | 110.82 |
| 14 | G | 1117 | CLA | C7-C6-C5 | -2.40 | 106.83 | 113.36 |
| 17 | b | 524 | BCR | C3-C4-C5 | -2.40 | 109.79 | 114.08 |
| 14 | Z | 508 | CLA | O2D-CGD-O1D | -2.40 | 119.14 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | e | 4001 | BCR | C35-C13-C12 | 2.40 | 121.86 | 118.08 |
| 14 | t | 511 | CLA | C1B-CHB-C4A | -2.40 | 125.36 | 130.12 |
| 17 | c | 522 | BCR | C1-C6-C7 | 2.40 | 122.57 | 115.78 |
| 17 | 6 | 524 | BCR | C23-C24-C25 | -2.40 | 120.46 | 127.20 |
| 17 | H | 4010 | BCR | C20-C19-C18 | -2.40 | 119.67 | 126.42 |
| 14 | e | 1102 | CLA | O2D-CGD-CBD | 2.40 | 115.53 | 111.27 |
| 14 | A | 1135 | CLA | O2A-CGA-O1A | -2.40 | 117.53 | 123.59 |
| 17 | Y | 522 | BCR | C30-C25-C26 | -2.40 | 119.23 | 122.61 |
| 14 | A | 1134 | CLA | C1B-CHB-C4A | -2.40 | 125.36 | 130.12 |
| 17 | G | 4003 | BCR | C16-C15-C14 | -2.40 | 118.56 | 123.47 |
| 17 | S | 4018 | BCR | C38-C26-C27 | 2.40 | 118.23 | 113.62 |
| 14 | 4 | 512 | CLA | CHB-C4A-NA | 2.40 | 127.83 | 124.51 |
| 17 | 4 | 523 | BCR | C21-C20-C19 | -2.40 | 115.73 | 123.22 |
| 14 | t | 512 | CLA | CHB-C4A-NA | 2.40 | 127.83 | 124.51 |
| 22 | X | 170 | FMN | O4-C4-C4A | -2.40 | 120.23 | 126.60 |
| 20 | B | 5002 | LMG | C38-C37-C36 | -2.40 | 102.25 | 114.42 |
| 14 | t | 519 | CLA | C1B-CHB-C4A | -2.40 | 125.36 | 130.12 |
| 14 | e | 1127 | CLA | CAA-CBA-CGA | -2.40 | 106.24 | 113.25 |
| 15 | G | 2001 | PQN | C2M-C2-C3 | -2.40 | 120.49 | 124.40 |
| 14 | H | 1213 | CLA | C11-C10-C8 | -2.40 | 108.17 | 115.92 |
| 17 | f | 4010 | BCR | C23-C22-C21 | 2.40 | 122.62 | 118.94 |
| 17 | v | 524 | BCR | C23-C24-C25 | -2.40 | 120.47 | 127.20 |
| 14 | 4 | 519 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 17 | 3 | 522 | BCR | C23-C24-C25 | -2.40 | 120.47 | 127.20 |
| 18 | G | 5006 | LHG | C11-C10-C9 | -2.40 | 102.25 | 114.42 |
| 17 | G | 4002 | BCR | C20-C19-C18 | -2.40 | 119.68 | 126.42 |
| 17 | u | 522 | BCR | C20-C21-C22 | -2.40 | 123.89 | 127.31 |
| 18 | e | 5006 | LHG | C11-C10-C9 | -2.40 | 102.26 | 114.42 |
| 14 | d | 502 | CLA | O2D-CGD-O1D | -2.40 | 119.15 | 123.84 |
| 14 | B | 1213 | CLA | C11-C10-C8 | -2.40 | 108.17 | 115.92 |
| 21 | c | 822 | SQD | C4-C3-C2 | 2.40 | 115.01 | 110.82 |
| 14 | H | 1240 | CLA | C1-C2-C3 | -2.40 | 121.90 | 126.04 |
| 17 | t | 522 | BCR | C33-C5-C4 | 2.40 | 118.22 | 113.62 |
| 17 | B | 4014 | BCR | C15-C14-C13 | -2.40 | 123.89 | 127.31 |
| 17 | L | 4020 | BCR | C15-C14-C13 | -2.40 | 123.89 | 127.31 |
| 17 | f | 4010 | BCR | C20-C19-C18 | -2.40 | 119.69 | 126.42 |
| 14 | 2 | 519 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 14 | 4 | 511 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 14 | f | 1240 | CLA | C1-C2-C3 | -2.40 | 121.90 | 126.04 |
| 17 | B | 4010 | BCR | C20-C19-C18 | -2.40 | 119.69 | 126.42 |
| 14 | G | 1134 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 14 | H | 1219 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | e | 1134 | CLA | C1B-CHB-C4A | -2.40 | 125.37 | 130.12 |
| 14 | f | 1236 | CLA | O2D-CGD-CBD | 2.40 | 115.52 | 111.27 |
| 17 | Z | 521 | BCR | C29-C30-C25 | 2.40 | 114.17 | 110.48 |
| 17 | f | 4010 | BCR | C28-C27-C26 | -2.39 | 109.80 | 114.08 |
| 17 | t | 524 | BCR | C3-C4-C5 | -2.39 | 109.80 | 114.08 |
| 17 | 1 | 522 | BCR | C30-C25-C26 | -2.39 | 119.24 | 122.61 |
| 17 | 5 | 522 | BCR | C20-C21-C22 | -2.39 | 123.89 | 127.31 |
| 14 | B | 1215 | CLA | C3C-C4C-NC | -2.39 | 107.89 | 110.57 |
| 18 | A | 5006 | LHG | C11-C10-C9 | -2.39 | 102.28 | 114.42 |
| 14 | 1 | 503 | CLA | C1B-CHB-C4A | -2.39 | 125.38 | 130.12 |
| 14 | s | 518 | CLA | C1B-CHB-C4A | -2.39 | 125.38 | 130.12 |
| 14 | H | 1230 | CLA | CHB-C4A-NA | 2.39 | 127.82 | 124.51 |
| 20 | f | 5002 | LMG | C38-C37-C36 | -2.39 | 102.28 | 114.42 |
| 14 | A | 1127 | CLA | CAA-CBA-CGA | -2.39 | 106.26 | 113.25 |
| 20 | H | 5002 | LMG | C38-C37-C36 | -2.39 | 102.28 | 114.42 |
| 14 | Y | 503 | CLA | C1B-CHB-C4A | -2.39 | 125.38 | 130.12 |
| 14 | A | 1129 | CLA | CHB-C4A-NA | 2.39 | 127.82 | 124.51 |
| 17 | A | 4001 | BCR | C35-C13-C12 | 2.39 | 121.84 | 118.08 |
| 17 | L | 4020 | BCR | C11-C10-C9 | -2.39 | 123.90 | 127.31 |
| 14 | s | 516 | CLA | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 14 | A | 1117 | CLA | C7-C6-C5 | -2.39 | 106.86 | 113.36 |
| 17 | B | 4006 | BCR | C37-C22-C21 | -2.39 | 119.57 | 122.92 |
| 17 | s | 522 | BCR | C23-C24-C25 | -2.39 | 120.49 | 127.20 |
| 17 | Z | 522 | BCR | C36-C18-C19 | 2.39 | 121.84 | 118.08 |
| 14 | 6 | 502 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 14 | B | 1236 | CLA | O2D-CGD-CBD | 2.39 | 115.51 | 111.27 |
| 17 | 4 | 522 | BCR | C1-C6-C5 | -2.39 | 119.25 | 122.61 |
| 17 | a | 524 | BCR | C27-C26-C25 | -2.39 | 119.26 | 122.73 |
| 14 | G | 1129 | CLA | CHB-C4A-NA | 2.39 | 127.82 | 124.51 |
| 17 | t | 522 | BCR | C33-C5-C6 | -2.39 | 121.84 | 124.53 |
| 17 | A | 4007 | BCR | C29-C30-C25 | 2.39 | 114.16 | 110.48 |
| 14 | q | 503 | CLA | C1B-CHB-C4A | -2.39 | 125.39 | 130.12 |
| 14 | A | 1102 | CLA | O2D-CGD-CBD | 2.39 | 115.51 | 111.27 |
| 17 | r | 521 | BCR | C29-C30-C25 | 2.39 | 114.16 | 110.48 |
| 14 | f | 1213 | CLA | C11-C10-C8 | -2.39 | 108.20 | 115.92 |
| 17 | 4 | 522 | BCR | C33-C5-C4 | 2.39 | 118.20 | 113.62 |
| 14 | 5 | 510 | CLA | C1B-CHB-C4A | -2.39 | 125.39 | 130.12 |
| 14 | u | 510 | CLA | C1B-CHB-C4A | -2.39 | 125.39 | 130.12 |
| 17 | k | 4018 | BCR | C4-C5-C6 | -2.39 | 119.27 | 122.73 |
| 17 | A | 4003 | BCR | C16-C15-C14 | -2.39 | 118.58 | 123.47 |
| 14 | K | 1105 | CLA | CHB-C4A-NA | 2.39 | 127.81 | 124.51 |
| 14 | 6 | 512 | CLA | CHB-C4A-NA | 2.39 | 127.81 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1107 | CLA | CHB-C4A-NA | 2.39 | 127.81 | 124.51 |
| 14 | G | 1103 | CLA | C1-C2-C3 | -2.39 | 121.92 | 126.04 |
| 17 | W | 4021 | BCR | C36-C18-C19 | 2.39 | 121.84 | 118.08 |
| 17 | V | 4019 | BCR | C33-C5-C6 | -2.39 | 121.85 | 124.53 |
| 14 | e | 1117 | CLA | C7-C6-C5 | -2.39 | 106.88 | 113.36 |
| 14 | c | 503 | CLA | C1B-CHB-C4A | -2.39 | 125.39 | 130.12 |
| 17 | d | 524 | BCR | C23-C24-C25 | -2.38 | 120.50 | 127.20 |
| 17 | S | 4018 | BCR | C4-C5-C6 | -2.38 | 119.27 | 122.73 |
| 17 | T | 4013 | BCR | C11-C10-C9 | -2.38 | 123.91 | 127.31 |
| 17 | b | 523 | BCR | C21-C20-C19 | -2.38 | 115.78 | 123.22 |
| 14 | e | 1129 | CLA | CHB-C4A-NA | 2.38 | 127.81 | 124.51 |
| 14 | H | 1225 | CLA | C2D-C1D-ND | -2.38 | 108.35 | 110.10 |
| 14 | r | 519 | CLA | C1B-CHB-C4A | -2.38 | 125.39 | 130.12 |
| 17 | e | 4007 | BCR | C29-C30-C25 | 2.38 | 114.15 | 110.48 |
| 14 | 3 | 516 | CLA | O2D-CGD-O1D | -2.38 | 119.18 | 123.84 |
| 14 | H | 1236 | CLA | O2A-CGA-O1A | -2.38 | 117.58 | 123.59 |
| 17 | 3 | 524 | BCR | C27-C26-C25 | -2.38 | 119.27 | 122.73 |
| 14 | a | 516 | CLA | O2D-CGD-O1D | -2.38 | 119.18 | 123.84 |
| 15 | A | 2001 | PQN | C2M-C2-C3 | -2.38 | 120.51 | 124.40 |
| 17 | l | 4015 | BCR | C16-C15-C14 | -2.38 | 118.59 | 123.47 |
| 14 | B | 1219 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 22 | P | 170 | FMN | O4-C4-C4A | -2.38 | 120.28 | 126.60 |
| 17 | b | 522 | BCR | C33-C5-C4 | 2.38 | 118.19 | 113.62 |
| 17 | 4 | 522 | BCR | C33-C5-C6 | -2.38 | 121.85 | 124.53 |
| 14 | b | 509 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 17 | t | 522 | BCR | C1-C6-C5 | -2.38 | 119.26 | 122.61 |
| 17 | 2 | 521 | BCR | C29-C30-C25 | 2.38 | 114.15 | 110.48 |
| 14 | G | 1801 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 17 | G | 4007 | BCR | C29-C30-C25 | 2.38 | 114.14 | 110.48 |
| 14 | 4 | 509 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 14 | R | 1301 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 14 | e | 1135 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 14 | e | 1117 | CLA | O2A-CGA-O1A | -2.38 | 117.59 | 123.59 |
| 14 | f | 1236 | CLA | O2A-CGA-O1A | -2.38 | 117.59 | 123.59 |
| 17 | n | 4020 | BCR | C11-C10-C9 | -2.38 | 123.91 | 127.31 |
| 14 | 4 | 503 | CLA | C1B-CHB-C4A | -2.38 | 125.40 | 130.12 |
| 17 | f | 4006 | BCR | C37-C22-C21 | -2.38 | 119.59 | 122.92 |
| 14 | A | 1135 | CLA | C1B-CHB-C4A | -2.38 | 125.41 | 130.12 |
| 14 | F | 1301 | CLA | C1B-CHB-C4A | -2.38 | 125.41 | 130.12 |
| 17 | A | 4002 | BCR | C33-C5-C6 | -2.38 | 121.86 | 124.53 |
| 17 | 2 | 522 | BCR | C36-C18-C19 | 2.38 | 121.82 | 118.08 |
| 14 | a | 501 | CLA | C1B-CHB-C4A | -2.38 | 125.41 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | B | 4010 | BCR | C28-C27-C26 | -2.38 | 109.83 | 114.08 |
| 14 | G | 1127 | CLA | CAA-CBA-CGA | -2.38 | 106.31 | 113.25 |
| 17 | e | 4003 | BCR | C16-C15-C14 | -2.37 | 118.61 | 123.47 |
| 14 | b | 513 | CLA | C1B-CHB-C4A | -2.37 | 125.41 | 130.12 |
| 17 | H | 4010 | BCR | C28-C27-C26 | -2.37 | 109.84 | 114.08 |
| 14 | T | 1303 | CLA | O2A-CGA-O1A | -2.37 | 117.38 | 123.30 |
| 14 | Y | 504 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 14 | e | 1130 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 14 | t | 513 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 21 | 3 | 822 | SQD | O5-C5-C4 | 2.37 | 114.00 | 109.69 |
| 14 | e | 1801 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 17 | J | 4013 | BCR | C11-C10-C9 | -2.37 | 123.92 | 127.31 |
| 17 | l | 4013 | BCR | C11-C10-C9 | -2.37 | 123.92 | 127.31 |
| 14 | e | 1111 | CLA | O2A-CGA-O1A | -2.37 | 117.61 | 123.59 |
| 21 | a | 822 | SQD | O5-C5-C4 | 2.37 | 114.00 | 109.69 |
| 14 | a | 507 | CLA | C2A-C1A-CHA | 2.37 | 128.01 | 123.86 |
| 14 | A | 1801 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 17 | c | 522 | BCR | C20-C21-C22 | -2.37 | 123.93 | 127.31 |
| 14 | 4 | 513 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 17 | J | 4015 | BCR | C16-C15-C14 | -2.37 | 118.62 | 123.47 |
| 14 | B | 1236 | CLA | O2A-CGA-O1A | -2.37 | 117.61 | 123.59 |
| 14 | s | 507 | CLA | C2A-C1A-CHA | 2.37 | 128.00 | 123.86 |
| 22 | p | 170 | FMN | O4-C4-C4A | -2.37 | 120.31 | 126.60 |
| 14 | c | 510 | CLA | C1B-CHB-C4A | -2.37 | 125.42 | 130.12 |
| 17 | f | 4010 | BCR | C33-C5-C6 | -2.37 | 121.87 | 124.53 |
| 17 | r | 522 | BCR | C36-C18-C19 | 2.37 | 121.81 | 118.08 |
| 14 | G | 1120 | CLA | CAA-C2A-C3A | -2.37 | 106.29 | 112.78 |
| 14 | m | 1105 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 14 | v | 512 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 14 | A | 1109 | CLA | O1D-CGD-CBD | 2.37 | 129.33 | 124.48 |
| 14 | H | 1236 | CLA | O2D-CGD-CBD | 2.37 | 115.48 | 111.27 |
| 17 | t | 524 | BCR | C1-C6-C7 | 2.37 | 122.48 | 115.78 |
| 14 | 6 | 518 | CLA | C1B-CHB-C4A | -2.37 | 125.43 | 130.12 |
| 14 | j | 1301 | CLA | C1B-CHB-C4A | -2.37 | 125.43 | 130.12 |
| 21 | s | 822 | SQD | O5-C5-C4 | 2.37 | 114.00 | 109.69 |
| 14 | b | 503 | CLA | C2D-C1D-ND | -2.37 | 108.36 | 110.10 |
| 14 | e | 1109 | CLA | O1D-CGD-CBD | 2.37 | 129.33 | 124.48 |
| 14 | f | 1219 | CLA | C1B-CHB-C4A | -2.37 | 125.43 | 130.12 |
| 17 | H | 4006 | BCR | C37-C22-C21 | -2.37 | 119.61 | 122.92 |
| 14 | e | 1103 | CLA | C1-C2-C3 | -2.37 | 121.95 | 126.04 |
| 14 | 5 | 503 | CLA | C1B-CHB-C4A | -2.37 | 125.43 | 130.12 |
| 19 | A | 1849 | LMU | O5'-C1'-C2' | 2.37 | 115.36 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19 | G | 1849 | LMU | O5'-C1'-C2' | 2.37 | 115.36 | 110.35 |
| 14 | A | 1111 | CLA | O2A-CGA-O1A | -2.37 | 117.62 | 123.59 |
| 14 | B | 1235 | CLA | CHD-C1D-ND | -2.37 | 122.28 | 124.45 |
| 14 | e | 1104 | CLA | CAA-C2A-C3A | -2.37 | 106.30 | 112.78 |
| 17 | n | 4020 | BCR | C15-C14-C13 | -2.37 | 123.93 | 127.31 |
| 17 | I | 4018 | BCR | C4-C5-C6 | -2.37 | 119.30 | 122.73 |
| 17 | a | 522 | BCR | C31-C1-C6 | -2.36 | 106.46 | 110.30 |
| 14 | G | 1108 | CLA | C1B-CHB-C4A | -2.36 | 125.43 | 130.12 |
| 14 | H | 1021 | CLA | C11-C12-C13 | -2.36 | 108.28 | 115.92 |
| 14 | c | 509 | CLA | C1B-CHB-C4A | -2.36 | 125.43 | 130.12 |
| 14 | J | 1303 | CLA | O2A-CGA-O1A | -2.36 | 117.41 | 123.30 |
| 14 | 3 | 501 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 17 | T | 4015 | BCR | C16-C15-C14 | -2.36 | 118.63 | 123.47 |
| 14 | s | 503 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 14 | A | 1103 | CLA | C1-C2-C3 | -2.36 | 121.96 | 126.04 |
| 14 | G | 1102 | CLA | O2D-CGD-CBD | 2.36 | 115.47 | 111.27 |
| 14 | q | 504 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 14 | v | 518 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 17 | V | 4020 | BCR | C11-C10-C9 | -2.36 | 123.94 | 127.31 |
| 14 | A | 1107 | CLA | CHB-C4A-NA | 2.36 | 127.78 | 124.51 |
| 17 | c | 521 | BCR | C27-C26-C25 | -2.36 | 119.30 | 122.73 |
| 15 | e | 2001 | PQN | C2M-C2-C3 | -2.36 | 120.55 | 124.40 |
| 14 | t | 503 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 17 | V | 4219 | BCR | C36-C18-C19 | 2.36 | 121.80 | 118.08 |
| 15 | B | 2002 | PQN | C2M-C2-C3 | -2.36 | 120.55 | 124.40 |
| 14 | G | 1111 | CLA | O2A-CGA-O1A | -2.36 | 117.63 | 123.59 |
| 17 | 3 | 522 | BCR | C31-C1-C6 | -2.36 | 106.47 | 110.30 |
| 14 | e | 1107 | CLA | CHB-C4A-NA | 2.36 | 127.78 | 124.51 |
| 18 | n | 5218 | LHG | O8-C23-C24 | 2.36 | 119.32 | 111.91 |
| 14 | u | 503 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 14 | u | 509 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 14 | G | 1117 | CLA | O2A-CGA-O1A | -2.36 | 117.64 | 123.59 |
| 14 | A | 1120 | CLA | CAA-C2A-C3A | -2.36 | 106.32 | 112.78 |
| 14 | d | 518 | CLA | C1B-CHB-C4A | -2.36 | 125.44 | 130.12 |
| 19 | e | 1849 | LMU | O5'-C1'-C2' | 2.36 | 115.34 | 110.35 |
| 17 | G | 4001 | BCR | C35-C13-C12 | 2.36 | 121.79 | 118.08 |
| 17 | 2 | 522 | BCR | C3-C4-C5 | -2.36 | 109.86 | 114.08 |
| 14 | n | 1503 | CLA | O2D-CGD-CBD | 2.36 | 115.46 | 111.27 |
| 14 | 5 | 509 | CLA | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 17 | s | 522 | BCR | C31-C1-C6 | -2.36 | 106.47 | 110.30 |
| 14 | q | 502 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 14 | A | 1104 | CLA | CAA-C2A-C3A | -2.36 | 106.32 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1108 | CLA | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 14 | f | 1223 | CLA | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 17 | B | 4014 | BCR | C12-C13-C14 | -2.36 | 115.33 | 118.94 |
| 14 | G | 1135 | CLA | C1B-CHB-C4A | -2.36 | 125.45 | 130.12 |
| 14 | G | 1104 | CLA | CAA-C2A-C3A | -2.36 | 106.33 | 112.78 |
| 14 | 1 | 502 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 14 | Y | 502 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 17 | 4 | 524 | BCR | C1-C6-C7 | 2.36 | 122.44 | 115.78 |
| 14 | A | 1117 | CLA | O2A-CGA-O1A | -2.36 | 117.65 | 123.59 |
| 14 | b | 503 | CLA | C1B-CHB-C4A | -2.35 | 125.45 | 130.12 |
| 14 | H | 1239 | CLA | C1B-CHB-C4A | -2.35 | 125.45 | 130.12 |
| 14 | B | 1021 | CLA | C11-C12-C13 | -2.35 | 108.31 | 115.92 |
| 17 | L | 4019 | BCR | C33-C5-C6 | -2.35 | 121.89 | 124.53 |
| 17 | b | 522 | BCR | C33-C5-C6 | -2.35 | 121.89 | 124.53 |
| 14 | 1 | 504 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 17 | b | 522 | BCR | C1-C6-C5 | -2.35 | 119.30 | 122.61 |
| 18 | L | 5218 | LHG | O8-C23-C24 | 2.35 | 119.29 | 111.91 |
| 17 | b | 524 | BCR | C1-C6-C7 | 2.35 | 122.43 | 115.78 |
| 14 | l | 1303 | CLA | O2A-CGA-O1A | -2.35 | 117.44 | 123.30 |
| 14 | e | 1120 | CLA | CAA-C2A-C3A | -2.35 | 106.34 | 112.78 |
| 17 | B | 4010 | BCR | C33-C5-C6 | -2.35 | 121.89 | 124.53 |
| 14 | 3 | 503 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 14 | H | 1223 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 14 | s | 501 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 14 | c | 506 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 17 | s | 523 | BCR | C8-C7-C6 | -2.35 | 120.60 | 127.20 |
| 17 | r | 522 | BCR | C3-C4-C5 | -2.35 | 109.88 | 114.08 |
| 14 | 3 | 507 | CLA | C2A-C1A-CHA | 2.35 | 127.97 | 123.86 |
| 14 | B | 1223 | CLA | C1B-CHB-C4A | -2.35 | 125.46 | 130.12 |
| 17 | v | 524 | BCR | C10-C11-C12 | -2.35 | 115.89 | 123.22 |
| 17 | Z | 522 | BCR | C23-C24-C25 | -2.35 | 120.60 | 127.20 |
| 21 | r | 822 | SQD | O6-C1-C2 | 2.35 | 111.97 | 108.30 |
| 14 | H | 1240 | CLA | C1B-CHB-C4A | -2.35 | 125.47 | 130.12 |
| 14 | d | 512 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 17 | v | 523 | BCR | C21-C20-C19 | -2.35 | 115.89 | 123.22 |
| 14 | 1 | 501 | CLA | C1B-CHB-C4A | -2.35 | 125.47 | 130.12 |
| 17 | L | 4219 | BCR | C36-C18-C19 | 2.35 | 121.78 | 118.08 |
| 14 | e | 1108 | CLA | C1B-CHB-C4A | -2.35 | 125.47 | 130.12 |
| 14 | B | 1204 | CLA | CHD-C1D-ND | -2.35 | 122.30 | 124.45 |
| 14 | G | 1013 | CLA | C3C-C4C-NC | -2.35 | 107.94 | 110.57 |
| 14 | G | 1109 | CLA | O1D-CGD-CBD | 2.35 | 129.29 | 124.48 |
| 14 | Y | 501 | CLA | C1B-CHB-C4A | -2.35 | 125.47 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | q | 501 | CLA | C1B-CHB-C4A | -2.35 | 125.47 | 130.12 |
| 14 | b | 508 | CLA | C2D-C1D-ND | -2.35 | 108.38 | 110.10 |
| 14 | f | 1021 | CLA | C11-C12-C13 | -2.35 | 108.34 | 115.92 |
| 17 | f | 4014 | BCR | C15-C16-C17 | -2.35 | 118.67 | 123.47 |
| 17 | Z | 522 | BCR | C3-C4-C5 | -2.35 | 109.89 | 114.08 |
| 18 | L | 5221 | LHG | O8-C23-C24 | 2.35 | 119.27 | 111.91 |
| 14 | 5 | 506 | CLA | C1B-CHB-C4A | -2.34 | 125.47 | 130.12 |
| 17 | 6 | 523 | BCR | C21-C20-C19 | -2.34 | 115.90 | 123.22 |
| 17 | d | 523 | BCR | C21-C20-C19 | -2.34 | 115.90 | 123.22 |
| 14 | 4 | 504 | CLA | C1B-CHB-C4A | -2.34 | 125.47 | 130.12 |
| 18 | V | 5218 | LHG | O8-C23-C24 | 2.34 | 119.26 | 111.91 |
| 14 | a | 502 | CLA | C1B-CHB-C4A | -2.34 | 125.47 | 130.12 |
| 14 | v | 510 | CLA | C1B-CHB-C4A | -2.34 | 125.47 | 130.12 |
| 21 | t | 822 | SQD | O5-C5-C4 | 2.34 | 113.95 | 109.69 |
| 14 | L | 1503 | CLA | O2D-CGD-CBD | 2.34 | 115.43 | 111.27 |
| 17 | 3 | 523 | BCR | C8-C7-C6 | -2.34 | 120.62 | 127.20 |
| 17 | a | 523 | BCR | C8-C7-C6 | -2.34 | 120.62 | 127.20 |
| 14 | B | 1225 | CLA | C2D-C1D-ND | -2.34 | 108.38 | 110.10 |
| 15 | f | 2002 | PQN | C2M-C2-C3 | -2.34 | 120.58 | 124.40 |
| 18 | V | 5221 | LHG | O8-C23-C24 | 2.34 | 119.26 | 111.91 |
| 18 | n | 5221 | LHG | O8-C23-C24 | 2.34 | 119.26 | 111.91 |
| 14 | H | 1235 | CLA | CHD-C1D-ND | -2.34 | 122.30 | 124.45 |
| 14 | v | 504 | CLA | C1B-CHB-C4A | -2.34 | 125.48 | 130.12 |
| 14 | f | 1240 | CLA | C1B-CHB-C4A | -2.34 | 125.48 | 130.12 |
| 14 | u | 501 | CLA | C1B-CHB-C4A | -2.34 | 125.48 | 130.12 |
| 14 | e | 1107 | CLA | O2A-CGA-O1A | -2.34 | 117.69 | 123.59 |
| 17 | B | 4014 | BCR | C15-C16-C17 | -2.34 | 118.68 | 123.47 |
| 14 | H | 1204 | CLA | CHD-C1D-ND | -2.34 | 122.31 | 124.45 |
| 14 | 4 | 508 | CLA | C2D-C1D-ND | -2.34 | 108.38 | 110.10 |
| 17 | 5 | 523 | BCR | C33-C5-C4 | 2.34 | 118.11 | 113.62 |
| 17 | M | 4021 | BCR | C3-C4-C5 | -2.34 | 109.90 | 114.08 |
| 17 | W | 4021 | BCR | C3-C4-C5 | -2.34 | 109.90 | 114.08 |
| 17 | 5 | 521 | BCR | C27-C26-C25 | -2.34 | 119.34 | 122.73 |
| 14 | B | 1240 | CLA | C1B-CHB-C4A | -2.34 | 125.49 | 130.12 |
| 14 | f | 1211 | CLA | O2D-CGD-CBD | 2.34 | 115.42 | 111.27 |
| 14 | e | 1127 | CLA | O2D-CGD-O1D | -2.34 | 119.27 | 123.84 |
| 14 | f | 1227 | CLA | CHD-C1D-ND | -2.34 | 122.31 | 124.45 |
| 17 | e | 4011 | BCR | C15-C14-C13 | -2.34 | 123.98 | 127.31 |
| 14 | H | 1226 | CLA | CAC-C3C-C4C | 2.34 | 127.84 | 124.81 |
| 17 | c | 523 | BCR | C33-C5-C4 | 2.34 | 118.10 | 113.62 |
| 17 | f | 4014 | BCR | C12-C13-C14 | -2.34 | 115.36 | 118.94 |
| 17 | H | 4014 | BCR | C12-C13-C14 | -2.33 | 115.36 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | u | 521 | BCR | C27-C26-C25 | -2.33 | 119.34 | 122.73 |
| 22 | P | 170 | FMN | C10-C4A-N5 | -2.33 | 119.90 | 124.86 |
| 17 | r | 522 | BCR | C23-C24-C25 | -2.33 | 120.64 | 127.20 |
| 14 | t | 504 | CLA | C1B-CHB-C4A | -2.33 | 125.49 | 130.12 |
| 17 | 6 | 524 | BCR | C10-C11-C12 | -2.33 | 115.93 | 123.22 |
| 17 | o | 4021 | BCR | C3-C4-C5 | -2.33 | 109.91 | 114.08 |
| 14 | G | 1107 | CLA | O2A-CGA-O1A | -2.33 | 117.70 | 123.59 |
| 14 | G | 1104 | CLA | C11-C12-C13 | -2.33 | 108.38 | 115.92 |
| 14 | H | 1215 | CLA | C16-C15-C13 | -2.33 | 108.38 | 115.92 |
| 20 | T | 5104 | LMG | O3-C3-C2 | -2.33 | 104.95 | 110.35 |
| 14 | 5 | 501 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 17 | H | 4014 | BCR | C15-C16-C17 | -2.33 | 118.69 | 123.47 |
| 14 | A | 1104 | CLA | C11-C12-C13 | -2.33 | 108.38 | 115.92 |
| 17 | c | 524 | BCR | C38-C26-C25 | -2.33 | 121.91 | 124.53 |
| 14 | B | 1239 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 14 | 1 | 510 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 14 | A | 1107 | CLA | O2A-CGA-O1A | -2.33 | 117.70 | 123.59 |
| 22 | X | 170 | FMN | C10-C4A-N5 | -2.33 | 119.91 | 124.86 |
| 14 | u | 506 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 17 | H | 4004 | BCR | C20-C19-C18 | -2.33 | 119.86 | 126.42 |
| 17 | A | 4011 | BCR | C15-C14-C13 | -2.33 | 123.98 | 127.31 |
| 17 | H | 4010 | BCR | C16-C17-C18 | -2.33 | 123.98 | 127.31 |
| 17 | a | 524 | BCR | C20-C21-C22 | -2.33 | 123.98 | 127.31 |
| 17 | n | 4219 | BCR | C36-C18-C19 | 2.33 | 121.75 | 118.08 |
| 17 | n | 4019 | BCR | C33-C5-C6 | -2.33 | 121.91 | 124.53 |
| 20 | H | 5002 | LMG | O3-C3-C2 | -2.33 | 104.96 | 110.35 |
| 14 | A | 1120 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 14 | Y | 511 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 14 | B | 1226 | CLA | CAC-C3C-C4C | 2.33 | 127.83 | 124.81 |
| 14 | r | 509 | CLA | O2A-CGA-O1A | -2.33 | 117.71 | 123.59 |
| 14 | f | 1239 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 17 | 2 | 522 | BCR | C23-C24-C25 | -2.33 | 120.66 | 127.20 |
| 14 | t | 511 | CLA | C2D-C1D-ND | -2.33 | 108.39 | 110.10 |
| 14 | e | 1120 | CLA | C1B-CHB-C4A | -2.33 | 125.50 | 130.12 |
| 17 | u | 523 | BCR | C33-C5-C4 | 2.33 | 118.09 | 113.62 |
| 14 | A | 1137 | CLA | C4-C3-C5 | 2.33 | 119.19 | 115.27 |
| 14 | e | 1104 | CLA | C11-C12-C13 | -2.33 | 108.39 | 115.92 |
| 14 | 3 | 502 | CLA | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 14 | f | 1021 | CLA | O2A-C1-C2 | -2.33 | 102.52 | 108.64 |
| 14 | B | 1215 | CLA | C16-C15-C13 | -2.33 | 108.40 | 115.92 |
| 14 | f | 1204 | CLA | CHD-C1D-ND | -2.33 | 122.32 | 124.45 |
| 14 | e | 1114 | CLA | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | u | 524 | BCR | C37-C22-C23 | 2.33 | 121.74 | 118.08 |
| 14 | f | 1221 | CLA | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 14 | u | 511 | CLA | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 17 | s | 524 | BCR | C20-C21-C22 | -2.33 | 123.99 | 127.31 |
| 14 | A | 1118 | CLA | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 17 | H | 4010 | BCR | C33-C5-C6 | -2.33 | 121.92 | 124.53 |
| 14 | b | 504 | CLA | C1B-CHB-C4A | -2.32 | 125.51 | 130.12 |
| 17 | 3 | 524 | BCR | C20-C21-C22 | -2.32 | 123.99 | 127.31 |
| 14 | A | 1127 | CLA | O2D-CGD-O1D | -2.32 | 119.29 | 123.84 |
| 14 | 6 | 510 | CLA | C1B-CHB-C4A | -2.32 | 125.51 | 130.12 |
| 14 | e | 1137 | CLA | C4-C3-C5 | 2.32 | 119.18 | 115.27 |
| 17 | d | 521 | BCR | C33-C5-C6 | -2.32 | 121.92 | 124.53 |
| 20 | B | 5002 | LMG | O3-C3-C2 | -2.32 | 104.98 | 110.35 |
| 14 | Y | 509 | CLA | C1B-CHB-C4A | -2.32 | 125.51 | 130.12 |
| 14 | a | 503 | CLA | C1B-CHB-C4A | -2.32 | 125.51 | 130.12 |
| 14 | e | 1118 | CLA | C1B-CHB-C4A | -2.32 | 125.51 | 130.12 |
| 21 | 2 | 822 | SQD | O6-C1-C2 | 2.32 | 111.93 | 108.30 |
| 14 | G | 1120 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | A | 1013 | CLA | C3C-C4C-NC | -2.32 | 107.97 | 110.57 |
| 14 | Y | 510 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | t | 502 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 20 | f | 5002 | LMG | O3-C3-C2 | -2.32 | 104.98 | 110.35 |
| 14 | Z | 519 | CLA | CMB-C2B-C3B | 2.32 | 129.02 | 124.68 |
| 14 | f | 1226 | CLA | CAC-C3C-C4C | 2.32 | 127.82 | 124.81 |
| 14 | A | 1114 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | c | 501 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | 1 | 511 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | 6 | 504 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | H | 1211 | CLA | O2D-CGD-CBD | 2.32 | 115.39 | 111.27 |
| 14 | V | 1503 | CLA | O2D-CGD-CBD | 2.32 | 115.39 | 111.27 |
| 17 | a | 524 | BCR | C1-C6-C5 | -2.32 | 119.34 | 122.61 |
| 14 | B | 1211 | CLA | O2D-CGD-CBD | 2.32 | 115.39 | 111.27 |
| 17 | Y | 524 | BCR | C16-C15-C14 | -2.32 | 118.72 | 123.47 |
| 17 | H | 4009 | BCR | C37-C22-C23 | 2.32 | 121.73 | 118.08 |
| 14 | s | 502 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 14 | B | 1202 | CLA | O2A-C1-C2 | -2.32 | 102.54 | 108.64 |
| 14 | G | 1137 | CLA | C4-C3-C5 | 2.32 | 119.17 | 115.27 |
| 21 | Z | 822 | SQD | O6-C1-C2 | 2.32 | 111.92 | 108.30 |
| 14 | 2 | 509 | CLA | O2A-CGA-O1A | -2.32 | 117.74 | 123.59 |
| 17 | d | 524 | BCR | C10-C11-C12 | -2.32 | 115.98 | 123.22 |
| 14 | G | 1114 | CLA | C1B-CHB-C4A | -2.32 | 125.52 | 130.12 |
| 21 | 4 | 822 | SQD | O5-C5-C4 | 2.32 | 113.91 | 109.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | c | 518 | CLA | C1B-CHB-C4A | -2.32 | 125.53 | 130.12 |
| 17 | B | 4014 | BCR | C38-C26-C25 | 2.32 | 127.13 | 124.53 |
| 14 | Z | 509 | CLA | O2D-CGD-O1D | -2.32 | 119.31 | 123.84 |
| 14 | d | 510 | CLA | C1B-CHB-C4A | -2.32 | 125.53 | 130.12 |
| 14 | B | 1021 | CLA | O2A-C1-C2 | -2.32 | 102.54 | 108.64 |
| 14 | 2 | 509 | CLA | O2D-CGD-O1D | -2.32 | 119.31 | 123.84 |
| 20 | J | 5104 | LMG | O3-C3-C2 | -2.32 | 104.99 | 110.35 |
| 14 | B | 1227 | CLA | CHD-C1D-ND | -2.32 | 122.33 | 124.45 |
| 14 | 1 | 509 | CLA | C1B-CHB-C4A | -2.32 | 125.53 | 130.12 |
| 17 | u | 524 | BCR | C38-C26-C25 | -2.32 | 121.93 | 124.53 |
| 17 | 3 | 524 | BCR | C34-C9-C8 | 2.32 | 121.73 | 118.08 |
| 14 | Z | 509 | CLA | O2A-CGA-O1A | -2.32 | 117.75 | 123.59 |
| 14 | f | 1219 | CLA | CHB-C4A-NA | 2.32 | 127.71 | 124.51 |
| 14 | q | 510 | CLA | C1B-CHB-C4A | -2.32 | 125.53 | 130.12 |
| 14 | H | 1021 | CLA | O2A-C1-C2 | -2.32 | 102.55 | 108.64 |
| 14 | B | 1221 | CLA | C1B-CHB-C4A | -2.31 | 125.53 | 130.12 |
| 14 | d | 504 | CLA | C1B-CHB-C4A | -2.31 | 125.53 | 130.12 |
| 14 | q | 509 | CLA | C1B-CHB-C4A | -2.31 | 125.53 | 130.12 |
| 14 | 2 | 519 | CLA | CMB-C2B-C3B | 2.31 | 129.01 | 124.68 |
| 14 | A | 1103 | CLA | CAA-C2A-C1A | -2.31 | 104.39 | 111.97 |
| 14 | A | 1117 | CLA | CHD-C1D-ND | -2.31 | 122.33 | 124.45 |
| 14 | B | 1219 | CLA | CHB-C4A-NA | 2.31 | 127.71 | 124.51 |
| 22 | p | 170 | FMN | C10-C4A-N5 | -2.31 | 119.95 | 124.86 |
| 17 | d | 522 | BCR | C23-C24-C25 | -2.31 | 120.70 | 127.20 |
| 14 | f | 1215 | CLA | C16-C15-C13 | -2.31 | 108.44 | 115.92 |
| 17 | B | 4009 | BCR | C37-C22-C23 | 2.31 | 121.72 | 118.08 |
| 14 | G | 1118 | CLA | C1B-CHB-C4A | -2.31 | 125.53 | 130.12 |
| 17 | B | 4004 | BCR | C20-C19-C18 | -2.31 | 119.92 | 126.42 |
| 14 | b | 502 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 17 | u | 521 | BCR | C20-C19-C18 | -2.31 | 119.92 | 126.42 |
| 14 | f | 1225 | CLA | C1-C2-C3 | -2.31 | 122.04 | 126.04 |
| 14 | H | 1221 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 14 | f | 1202 | CLA | O2A-C1-C2 | -2.31 | 102.56 | 108.64 |
| 17 | 6 | 522 | BCR | C36-C18-C19 | 2.31 | 121.72 | 118.08 |
| 14 | 6 | 512 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 17 | A | 4008 | BCR | C28-C27-C26 | -2.31 | 109.95 | 114.08 |
| 14 | f | 1225 | CLA | C2D-C1D-ND | -2.31 | 108.40 | 110.10 |
| 14 | t | 512 | CLA | C1B-CHB-C4A | -2.31 | 125.54 | 130.12 |
| 14 | r | 509 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 17 | c | 521 | BCR | C20-C19-C18 | -2.31 | 119.93 | 126.42 |
| 15 | H | 2002 | PQN | C2M-C2-C3 | -2.31 | 120.63 | 124.40 |
| 17 | c | 521 | BCR | C33-C5-C6 | -2.31 | 121.93 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | b | 822 | SQD | O5-C5-C4 | 2.31 | 113.89 | 109.69 |
| 17 | 3 | 524 | BCR | C1-C6-C5 | -2.31 | 119.36 | 122.61 |
| 14 | e | 1103 | CLA | CAA-C2A-C1A | -2.31 | 104.41 | 111.97 |
| 17 | 5 | 521 | BCR | C20-C19-C18 | -2.31 | 119.93 | 126.42 |
| 17 | 6 | 521 | BCR | C33-C5-C6 | -2.31 | 121.94 | 124.53 |
| 14 | G | 1103 | CLA | CAA-C2A-C1A | -2.31 | 104.41 | 111.97 |
| 17 | Y | 524 | BCR | C20-C21-C22 | -2.31 | 124.02 | 127.31 |
| 17 | q | 524 | BCR | C16-C15-C14 | -2.31 | 118.75 | 123.47 |
| 14 | 4 | 502 | CLA | C1B-CHB-C4A | -2.31 | 125.55 | 130.12 |
| 14 | 3 | 509 | CLA | O2D-CGD-O1D | -2.31 | 119.33 | 123.84 |
| 17 | f | 4014 | BCR | C38-C26-C25 | 2.31 | 127.12 | 124.53 |
| 14 | B | 1210 | CLA | C1B-CHB-C4A | -2.31 | 125.55 | 130.12 |
| 14 | 5 | 518 | CLA | C1B-CHB-C4A | -2.31 | 125.55 | 130.12 |
| 14 | G | 1127 | CLA | O2D-CGD-O1D | -2.31 | 119.33 | 123.84 |
| 21 | Y | 822 | SQD | O48-C23-O10 | -2.31 | 117.77 | 123.59 |
| 17 | e | 4008 | BCR | C28-C27-C26 | -2.31 | 109.96 | 114.08 |
| 14 | v | 512 | CLA | C1B-CHB-C4A | -2.31 | 125.55 | 130.12 |
| 17 | l | 524 | BCR | C16-C15-C14 | -2.31 | 118.75 | 123.47 |
| 14 | f | 1201 | CLA | O2A-CGA-O1A | -2.31 | 117.77 | 123.59 |
| 17 | B | 4010 | BCR | C16-C17-C18 | -2.31 | 124.02 | 127.31 |
| 17 | a | 524 | BCR | C34-C9-C8 | 2.31 | 121.71 | 118.08 |
| 17 | f | 4004 | BCR | C20-C19-C18 | -2.31 | 119.94 | 126.42 |
| 17 | 5 | 524 | BCR | C38-C26-C25 | -2.31 | 121.94 | 124.53 |
| 14 | A | 1123 | CLA | CHA-C1A-NA | -2.31 | 121.12 | 126.40 |
| 14 | H | 1219 | CLA | CHB-C4A-NA | 2.31 | 127.70 | 124.51 |
| 20 | l | 5104 | LMG | O3-C3-C2 | -2.31 | 105.02 | 110.35 |
| 17 | d | 522 | BCR | C36-C18-C19 | 2.30 | 121.71 | 118.08 |
| 21 | q | 822 | SQD | O48-C23-O10 | -2.30 | 117.78 | 123.59 |
| 17 | V | 4019 | BCR | C40-C30-C25 | -2.30 | 106.56 | 110.30 |
| 17 | v | 521 | BCR | C33-C5-C6 | -2.30 | 121.94 | 124.53 |
| 14 | l | 502 | CLA | C1B-CHB-C4A | -2.30 | 125.55 | 130.12 |
| 17 | v | 521 | BCR | C16-C15-C14 | -2.30 | 118.76 | 123.47 |
| 14 | G | 1137 | CLA | C2A-C1A-CHA | 2.30 | 127.89 | 123.86 |
| 17 | 6 | 522 | BCR | C23-C24-C25 | -2.30 | 120.73 | 127.20 |
| 14 | G | 1113 | CLA | O2A-CGA-O1A | -2.30 | 117.56 | 123.30 |
| 17 | G | 4011 | BCR | C15-C14-C13 | -2.30 | 124.02 | 127.31 |
| 14 | B | 1201 | CLA | O2A-CGA-O1A | -2.30 | 117.78 | 123.59 |
| 14 | e | 1123 | CLA | CHA-C1A-NA | -2.30 | 121.13 | 126.40 |
| 17 | s | 524 | BCR | C34-C9-C8 | 2.30 | 121.70 | 118.08 |
| 14 | r | 519 | CLA | CMB-C2B-C3B | 2.30 | 128.98 | 124.68 |
| 17 | G | 4008 | BCR | C28-C27-C26 | -2.30 | 109.97 | 114.08 |
| 17 | f | 4010 | BCR | C16-C17-C18 | -2.30 | 124.03 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | v | 522 | BCR | C23-C24-C25 | -2.30 | 120.74 | 127.20 |
| 17 | q | 524 | BCR | C20-C21-C22 | -2.30 | 124.03 | 127.31 |
| 14 | G | 1106 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 14 | G | 1123 | CLA | CHA-C1A-NA | -2.30 | 121.13 | 126.40 |
| 17 | u | 521 | BCR | C33-C5-C6 | -2.30 | 121.95 | 124.53 |
| 17 | 6 | 521 | BCR | C16-C15-C14 | -2.30 | 118.76 | 123.47 |
| 14 | 5 | 511 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 14 | Y | 502 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 14 | s | 509 | CLA | O2D-CGD-O1D | -2.30 | 119.34 | 123.84 |
| 14 | G | 1104 | CLA | C1-C2-C3 | -2.30 | 122.07 | 126.04 |
| 14 | J | 1302 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 14 | e | 1117 | CLA | CHD-C1D-ND | -2.30 | 122.34 | 124.45 |
| 14 | 6 | 517 | CLA | C1B-CHB-C4A | -2.30 | 125.56 | 130.12 |
| 17 | c | 524 | BCR | C37-C22-C23 | 2.30 | 121.70 | 118.08 |
| 17 | f | 4009 | BCR | C37-C22-C23 | 2.30 | 121.70 | 118.08 |
| 14 | H | 1201 | CLA | O2A-CGA-O1A | -2.30 | 117.79 | 123.59 |
| 14 | e | 1013 | CLA | C3C-C4C-NC | -2.30 | 107.99 | 110.57 |
| 14 | H | 1202 | CLA | O2A-C1-C2 | -2.30 | 102.60 | 108.64 |
| 14 | T | 1302 | CLA | O2A-CGA-O1A | -2.30 | 117.79 | 123.59 |
| 14 | j | 1302 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 14 | B | 1225 | CLA | C1-C2-C3 | -2.30 | 122.07 | 126.04 |
| 14 | H | 1225 | CLA | C1-C2-C3 | -2.30 | 122.07 | 126.04 |
| 17 | 5 | 521 | BCR | C33-C5-C6 | -2.30 | 121.95 | 124.53 |
| 20 | H | 5002 | LMG | O2-C2-C1 | -2.30 | 104.47 | 110.05 |
| 14 | a | 509 | CLA | O2D-CGD-O1D | -2.30 | 119.35 | 123.84 |
| 14 | q | 502 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 14 | a | 516 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 17 | H | 4014 | BCR | C23-C22-C21 | -2.30 | 115.42 | 118.94 |
| 14 | c | 511 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 14 | G | 1117 | CLA | CHD-C1D-ND | -2.29 | 122.34 | 124.45 |
| 18 | G | 5005 | LHG | C11-C10-C9 | -2.29 | 102.78 | 114.42 |
| 18 | A | 5005 | LHG | C11-C10-C9 | -2.29 | 102.78 | 114.42 |
| 17 | f | 4014 | BCR | C23-C22-C21 | -2.29 | 115.42 | 118.94 |
| 14 | e | 1113 | CLA | O2A-CGA-O1A | -2.29 | 117.58 | 123.30 |
| 17 | d | 521 | BCR | C16-C15-C14 | -2.29 | 118.77 | 123.47 |
| 17 | e | 4002 | BCR | C35-C13-C12 | 2.29 | 121.69 | 118.08 |
| 20 | B | 5002 | LMG | O2-C2-C1 | -2.29 | 104.47 | 110.05 |
| 17 | B | 4014 | BCR | C23-C22-C21 | -2.29 | 115.42 | 118.94 |
| 14 | A | 1137 | CLA | C2A-C1A-CHA | 2.29 | 127.87 | 123.86 |
| 17 | v | 522 | BCR | C36-C18-C19 | 2.29 | 121.69 | 118.08 |
| 14 | q | 511 | CLA | C1B-CHB-C4A | -2.29 | 125.57 | 130.12 |
| 14 | G | 1125 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | H | 1227 | CLA | CHD-C1D-ND | -2.29 | 122.35 | 124.45 |
| 14 | 4 | 512 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 14 | J | 1302 | CLA | O2A-CGA-O1A | -2.29 | 117.81 | 123.59 |
| 21 | f | 1852 | SQD | C4-C3-C2 | 2.29 | 114.82 | 110.82 |
| 17 | 5 | 524 | BCR | C37-C22-C23 | 2.29 | 121.69 | 118.08 |
| 17 | H | 4004 | BCR | C39-C30-C25 | -2.29 | 106.58 | 110.30 |
| 14 | e | 1237 | CLA | O2D-CGD-CBD | 2.29 | 115.34 | 111.27 |
| 18 | e | 5005 | LHG | C11-C10-C9 | -2.29 | 102.80 | 114.42 |
| 14 | d | 512 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 14 | f | 1231 | CLA | CHD-C1D-ND | -2.29 | 122.35 | 124.45 |
| 17 | f | 4004 | BCR | C39-C30-C25 | -2.29 | 106.59 | 110.30 |
| 18 | A | 5004 | LHG | C5-O7-C7 | -2.29 | 112.16 | 117.79 |
| 18 | e | 5004 | LHG | C5-O7-C7 | -2.29 | 112.16 | 117.79 |
| 14 | l | 1302 | CLA | O2A-CGA-O1A | -2.29 | 117.82 | 123.59 |
| 14 | A | 1125 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 14 | H | 1210 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 14 | f | 1210 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 14 | Y | 504 | CLA | CAA-C2A-C3A | -2.29 | 106.51 | 112.78 |
| 14 | A | 1104 | CLA | C1-C2-C3 | -2.29 | 122.08 | 126.04 |
| 21 | l | 822 | SQD | O48-C23-O10 | -2.29 | 117.82 | 123.59 |
| 14 | t | 510 | CLA | C1B-CHB-C4A | -2.29 | 125.58 | 130.12 |
| 14 | G | 1119 | CLA | C2D-C1D-ND | -2.29 | 108.42 | 110.10 |
| 14 | A | 1113 | CLA | O2A-CGA-O1A | -2.29 | 117.60 | 123.30 |
| 14 | e | 1104 | CLA | C1-C2-C3 | -2.29 | 122.09 | 126.04 |
| 21 | B | 1852 | SQD | C4-C3-C2 | 2.29 | 114.82 | 110.82 |
| 14 | A | 1106 | CLA | C1B-CHB-C4A | -2.29 | 125.59 | 130.12 |
| 14 | u | 518 | CLA | C1B-CHB-C4A | -2.29 | 125.59 | 130.12 |
| 14 | R | 1302 | CLA | C1B-CHB-C4A | -2.29 | 125.59 | 130.12 |
| 14 | q | 504 | CLA | CAA-C2A-C3A | -2.29 | 106.52 | 112.78 |
| 18 | G | 5007 | LHG | C27-C26-C25 | -2.29 | 102.82 | 114.42 |
| 20 | T | 5104 | LMG | O2-C2-C1 | -2.29 | 104.49 | 110.05 |
| 17 | t | 521 | BCR | C29-C30-C25 | 2.29 | 114.00 | 110.48 |
| 14 | H | 1204 | CLA | O2D-CGD-CBD | 2.29 | 115.33 | 111.27 |
| 14 | G | 1011 | CLA | CMD-C2D-C3D | 2.28 | 132.87 | 127.61 |
| 18 | G | 5007 | LHG | C18-C17-C16 | -2.28 | 102.83 | 114.42 |
| 14 | d | 517 | CLA | C1B-CHB-C4A | -2.28 | 125.59 | 130.12 |
| 14 | l | 1302 | CLA | C1B-CHB-C4A | -2.28 | 125.59 | 130.12 |
| 14 | t | 508 | CLA | C2D-C1D-ND | -2.28 | 108.42 | 110.10 |
| 18 | B | 1842 | LHG | O8-C23-C24 | 2.28 | 119.07 | 111.91 |
| 18 | G | 5004 | LHG | C5-O7-C7 | -2.28 | 112.17 | 117.79 |
| 17 | l | 524 | BCR | C20-C21-C22 | -2.28 | 124.05 | 127.31 |
| 14 | l | 504 | CLA | CAA-C2A-C3A | -2.28 | 106.53 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | b | 510 | CLA | C1B-CHB-C4A | -2.28 | 125.59 | 130.12 |
| 14 | 2 | 502 | CLA | CAA-C2A-C3A | -2.28 | 106.53 | 112.78 |
| 14 | r | 502 | CLA | CAA-C2A-C3A | -2.28 | 106.53 | 112.78 |
| 18 | A | 5007 | LHG | C18-C17-C16 | -2.28 | 102.83 | 114.42 |
| 17 | G | 4002 | BCR | C35-C13-C12 | 2.28 | 121.67 | 118.08 |
| 14 | H | 1012 | CLA | CAA-CBA-CGA | -2.28 | 106.58 | 113.25 |
| 17 | q | 522 | BCR | C1-C6-C7 | 2.28 | 122.24 | 115.78 |
| 18 | e | 5007 | LHG | C18-C17-C16 | -2.28 | 102.84 | 114.42 |
| 14 | b | 512 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 14 | b | 518 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 14 | e | 1129 | CLA | C2D-C1D-ND | -2.28 | 108.42 | 110.10 |
| 17 | d | 523 | BCR | C33-C5-C4 | 2.28 | 118.00 | 113.62 |
| 14 | 4 | 508 | CLA | CHC-C1C-NC | 2.28 | 127.66 | 124.20 |
| 14 | T | 1302 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 14 | f | 1207 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 14 | 3 | 510 | CLA | O2A-CGA-O1A | -2.28 | 117.61 | 123.30 |
| 18 | e | 5007 | LHG | C27-C26-C25 | -2.28 | 102.85 | 114.42 |
| 14 | B | 1207 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 14 | B | 1012 | CLA | CAA-CBA-CGA | -2.28 | 106.59 | 113.25 |
| 17 | B | 4004 | BCR | C39-C30-C25 | -2.28 | 106.60 | 110.30 |
| 17 | s | 524 | BCR | C1-C6-C5 | -2.28 | 119.40 | 122.61 |
| 17 | n | 4019 | BCR | C40-C30-C25 | -2.28 | 106.60 | 110.30 |
| 14 | 4 | 510 | CLA | C1B-CHB-C4A | -2.28 | 125.60 | 130.12 |
| 14 | f | 1012 | CLA | CAA-CBA-CGA | -2.28 | 106.59 | 113.25 |
| 14 | 4 | 511 | CLA | C2D-C1D-ND | -2.28 | 108.42 | 110.10 |
| 14 | e | 1108 | CLA | O2D-CGD-CBD | 2.28 | 115.32 | 111.27 |
| 14 | t | 508 | CLA | CHC-C1C-NC | 2.28 | 127.66 | 124.20 |
| 14 | r | 512 | CLA | CHB-C4A-NA | 2.28 | 127.66 | 124.51 |
| 17 | Y | 522 | BCR | C1-C6-C7 | 2.28 | 122.22 | 115.78 |
| 14 | F | 1302 | CLA | C1B-CHB-C4A | -2.28 | 125.61 | 130.12 |
| 17 | 1 | 521 | BCR | C2-C1-C6 | 2.28 | 113.99 | 110.48 |
| 14 | A | 1103 | CLA | CAA-CBA-CGA | -2.28 | 106.60 | 113.25 |
| 20 | f | 5002 | LMG | O2-C2-C1 | -2.28 | 104.51 | 110.05 |
| 17 | L | 4019 | BCR | C40-C30-C25 | -2.28 | 106.61 | 110.30 |
| 17 | s | 522 | BCR | C21-C20-C19 | -2.28 | 116.11 | 123.22 |
| 19 | G | 1849 | LMU | C3'-C4'-C5' | 2.28 | 114.30 | 110.24 |
| 17 | 1 | 522 | BCR | C1-C6-C7 | 2.28 | 122.22 | 115.78 |
| 17 | q | 521 | BCR | C2-C1-C6 | 2.28 | 113.98 | 110.48 |
| 17 | Z | 521 | BCR | C20-C19-C18 | -2.28 | 120.02 | 126.42 |
| 14 | s | 502 | CLA | CMB-C2B-C3B | 2.28 | 128.94 | 124.68 |
| 18 | H | 1842 | LHG | O8-C23-C24 | 2.28 | 119.05 | 111.91 |
| 14 | H | 1207 | CLA | C1B-CHB-C4A | -2.28 | 125.61 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | A | 4008 | BCR | C20-C19-C18 | -2.28 | 120.03 | 126.42 |
| 17 | 2 | 521 | BCR | C20-C19-C18 | -2.28 | 120.03 | 126.42 |
| 18 | A | 5007 | LHG | C27-C26-C25 | -2.27 | 102.88 | 114.42 |
| 17 | 3 | 522 | BCR | C21-C20-C19 | -2.27 | 116.12 | 123.22 |
| 14 | e | 1125 | CLA | C1B-CHB-C4A | -2.27 | 125.61 | 130.12 |
| 18 | f | 1842 | LHG | O8-C23-C24 | 2.27 | 119.05 | 111.91 |
| 14 | G | 1103 | CLA | CAA-CBA-CGA | -2.27 | 106.61 | 113.25 |
| 20 | J | 5104 | LMG | O2-C2-C1 | -2.27 | 104.52 | 110.05 |
| 14 | e | 1110 | CLA | C1B-CHB-C4A | -2.27 | 125.61 | 130.12 |
| 14 | Z | 501 | CLA | CAA-C2A-C3A | -2.27 | 106.55 | 112.78 |
| 14 | e | 1106 | CLA | C1B-CHB-C4A | -2.27 | 125.61 | 130.12 |
| 14 | v | 517 | CLA | C1B-CHB-C4A | -2.27 | 125.61 | 130.12 |
| 17 | e | 4008 | BCR | C20-C19-C18 | -2.27 | 120.03 | 126.42 |
| 14 | Z | 502 | CLA | CAA-C2A-C3A | -2.27 | 106.56 | 112.78 |
| 14 | a | 510 | CLA | O2A-CGA-O1A | -2.27 | 117.64 | 123.30 |
| 14 | e | 1137 | CLA | C2A-C1A-CHA | 2.27 | 127.83 | 123.86 |
| 14 | G | 1108 | CLA | O2D-CGD-CBD | 2.27 | 115.30 | 111.27 |
| 17 | 4 | 521 | BCR | C29-C30-C25 | 2.27 | 113.98 | 110.48 |
| 14 | 3 | 516 | CLA | C1B-CHB-C4A | -2.27 | 125.62 | 130.12 |
| 14 | B | 1012 | CLA | C11-C12-C13 | -2.27 | 108.58 | 115.92 |
| 14 | 4 | 518 | CLA | C1B-CHB-C4A | -2.27 | 125.62 | 130.12 |
| 14 | H | 1239 | CLA | O2A-CGA-O1A | -2.27 | 117.86 | 123.59 |
| 14 | A | 1119 | CLA | C2D-C1D-ND | -2.27 | 108.43 | 110.10 |
| 14 | b | 511 | CLA | C2D-C1D-ND | -2.27 | 108.43 | 110.10 |
| 17 | 6 | 523 | BCR | C33-C5-C4 | 2.27 | 117.98 | 113.62 |
| 14 | H | 1239 | CLA | O2D-CGD-CBD | 2.27 | 115.30 | 111.27 |
| 14 | Z | 511 | CLA | C1B-CHB-C4A | -2.27 | 125.62 | 130.12 |
| 14 | H | 1012 | CLA | C11-C12-C13 | -2.27 | 108.59 | 115.92 |
| 17 | A | 4002 | BCR | C35-C13-C12 | 2.27 | 121.65 | 118.08 |
| 14 | f | 1012 | CLA | C11-C12-C13 | -2.27 | 108.59 | 115.92 |
| 19 | A | 1849 | LMU | C3'-C4'-C5' | 2.27 | 114.28 | 110.24 |
| 14 | f | 1236 | CLA | CHB-C4A-NA | 2.27 | 127.65 | 124.51 |
| 17 | Y | 521 | BCR | C2-C1-C6 | 2.27 | 113.97 | 110.48 |
| 14 | e | 1130 | CLA | O2A-CGA-O1A | -2.27 | 117.87 | 123.59 |
| 17 | r | 521 | BCR | C20-C19-C18 | -2.27 | 120.05 | 126.42 |
| 14 | b | 508 | CLA | CHC-C1C-NC | 2.27 | 127.64 | 124.20 |
| 14 | Z | 503 | CLA | C1B-CHB-C4A | -2.27 | 125.63 | 130.12 |
| 14 | B | 1221 | CLA | C2A-C1A-CHA | 2.27 | 127.82 | 123.86 |
| 14 | G | 1130 | CLA | O2A-CGA-O1A | -2.27 | 117.87 | 123.59 |
| 17 | r | 524 | BCR | C1-C6-C5 | -2.27 | 119.42 | 122.61 |
| 17 | c | 521 | BCR | C15-C16-C17 | -2.27 | 118.83 | 123.47 |
| 14 | 2 | 511 | CLA | C1B-CHB-C4A | -2.27 | 125.63 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1204 | CLA | O2D-CGD-CBD | 2.27 | 115.30 | 111.27 |
| 14 | G | 1237 | CLA | O2D-CGD-CBD | 2.27 | 115.30 | 111.27 |
| 20 | l | 5104 | LMG | O2-C2-C1 | -2.27 | 104.54 | 110.05 |
| 14 | A | 1129 | CLA | C2D-C1D-ND | -2.27 | 108.43 | 110.10 |
| 17 | 2 | 524 | BCR | C1-C6-C5 | -2.27 | 119.42 | 122.61 |
| 14 | s | 516 | CLA | C1B-CHB-C4A | -2.27 | 125.63 | 130.12 |
| 14 | 3 | 502 | CLA | CMB-C2B-C3B | 2.27 | 128.92 | 124.68 |
| 14 | 2 | 501 | CLA | CAA-C2A-C3A | -2.27 | 106.57 | 112.78 |
| 17 | H | 4014 | BCR | C38-C26-C25 | 2.27 | 127.07 | 124.53 |
| 17 | B | 4006 | BCR | C28-C27-C26 | -2.26 | 110.03 | 114.08 |
| 14 | G | 1011 | CLA | OBD-CAD-C3D | 2.26 | 133.97 | 128.52 |
| 21 | B | 1852 | SQD | O48-C23-O10 | -2.26 | 117.88 | 123.59 |
| 14 | A | 1011 | CLA | CMD-C2D-C3D | 2.26 | 132.82 | 127.61 |
| 17 | G | 4008 | BCR | C20-C19-C18 | -2.26 | 120.06 | 126.42 |
| 14 | r | 501 | CLA | CAA-C2A-C3A | -2.26 | 106.58 | 112.78 |
| 14 | A | 1108 | CLA | O2D-CGD-CBD | 2.26 | 115.29 | 111.27 |
| 14 | B | 1239 | CLA | O2D-CGD-CBD | 2.26 | 115.29 | 111.27 |
| 14 | e | 1101 | CLA | C1B-CHB-C4A | -2.26 | 125.63 | 130.12 |
| 17 | b | 521 | BCR | C29-C30-C25 | 2.26 | 113.97 | 110.48 |
| 14 | e | 1103 | CLA | CAA-CBA-CGA | -2.26 | 106.64 | 113.25 |
| 14 | F | 1302 | CLA | CMB-C2B-C3B | 2.26 | 128.91 | 124.68 |
| 17 | a | 522 | BCR | C21-C20-C19 | -2.26 | 116.16 | 123.22 |
| 14 | t | 516 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 14 | f | 1239 | CLA | O2D-CGD-CBD | 2.26 | 115.29 | 111.27 |
| 14 | s | 510 | CLA | O2A-CGA-O1A | -2.26 | 117.66 | 123.30 |
| 14 | H | 1231 | CLA | CHD-C1D-ND | -2.26 | 122.38 | 124.45 |
| 14 | G | 1110 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 14 | b | 516 | CLA | C1B-CHB-C4A | -2.26 | 125.64 | 130.12 |
| 14 | G | 1022 | CLA | CAA-CBA-CGA | -2.26 | 106.65 | 113.25 |
| 14 | e | 1022 | CLA | CAA-CBA-CGA | -2.26 | 106.65 | 113.25 |
| 18 | f | 1855 | LHG | C11-C10-C9 | -2.26 | 102.95 | 114.42 |
| 14 | H | 1221 | CLA | C2A-C1A-CHA | 2.26 | 127.81 | 123.86 |
| 14 | e | 1011 | CLA | CMD-C2D-C3D | 2.26 | 132.81 | 127.61 |
| 14 | A | 1237 | CLA | O2D-CGD-CBD | 2.26 | 115.28 | 111.27 |
| 17 | 5 | 521 | BCR | C15-C16-C17 | -2.26 | 118.85 | 123.47 |
| 19 | e | 1849 | LMU | C3'-C4'-C5' | 2.26 | 114.27 | 110.24 |
| 14 | f | 1023 | CLA | CMD-C2D-C3D | 2.26 | 132.81 | 127.61 |
| 14 | A | 1022 | CLA | CAA-CBA-CGA | -2.26 | 106.65 | 113.25 |
| 17 | f | 4006 | BCR | C28-C27-C26 | -2.26 | 110.05 | 114.08 |
| 14 | t | 507 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 14 | R | 1302 | CLA | CMB-C2B-C3B | 2.26 | 128.90 | 124.68 |
| 14 | H | 1208 | CLA | CHB-C4A-NA | 2.26 | 127.63 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | H | 1852 | SQD | O48-C23-O10 | -2.26 | 117.90 | 123.59 |
| 14 | T | 1303 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 14 | r | 511 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 14 | f | 1221 | CLA | C2A-C1A-CHA | 2.26 | 127.81 | 123.86 |
| 18 | B | 1855 | LHG | C11-C10-C9 | -2.26 | 102.97 | 114.42 |
| 17 | v | 523 | BCR | C33-C5-C4 | 2.26 | 117.95 | 113.62 |
| 21 | f | 1852 | SQD | O48-C23-O10 | -2.26 | 117.90 | 123.59 |
| 17 | u | 521 | BCR | C15-C16-C17 | -2.26 | 118.85 | 123.47 |
| 14 | 4 | 516 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 14 | f | 1224 | CLA | C1-C2-C3 | -2.26 | 122.14 | 126.04 |
| 14 | a | 502 | CLA | CMB-C2B-C3B | 2.26 | 128.90 | 124.68 |
| 21 | H | 1852 | SQD | O6-C1-C2 | 2.26 | 111.83 | 108.30 |
| 14 | 2 | 503 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 17 | e | 4002 | BCR | C38-C26-C27 | 2.26 | 117.95 | 113.62 |
| 17 | T | 4012 | BCR | C28-C27-C26 | -2.26 | 110.05 | 114.08 |
| 14 | A | 1101 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 14 | H | 1208 | CLA | C1B-CHB-C4A | -2.26 | 125.65 | 130.12 |
| 14 | f | 1202 | CLA | C1B-CHB-C4A | -2.25 | 125.65 | 130.12 |
| 14 | G | 1129 | CLA | C2D-C1D-ND | -2.25 | 108.44 | 110.10 |
| 14 | H | 1224 | CLA | C1-C2-C3 | -2.25 | 122.14 | 126.04 |
| 14 | G | 1107 | CLA | CAA-CBA-CGA | -2.25 | 106.67 | 113.25 |
| 14 | f | 1204 | CLA | O2D-CGD-CBD | 2.25 | 115.27 | 111.27 |
| 14 | d | 502 | CLA | CAA-C2A-C3A | -2.25 | 106.61 | 112.78 |
| 21 | H | 1852 | SQD | C4-C3-C2 | 2.25 | 114.76 | 110.82 |
| 14 | b | 507 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 14 | t | 518 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 14 | 2 | 512 | CLA | CHB-C4A-NA | 2.25 | 127.63 | 124.51 |
| 14 | V | 1501 | CLA | CAA-C2A-C3A | -2.25 | 106.61 | 112.78 |
| 14 | H | 1226 | CLA | CHC-C1C-NC | 2.25 | 127.62 | 124.20 |
| 14 | B | 1208 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 14 | A | 1134 | CLA | C4-C3-C5 | 2.25 | 119.06 | 115.27 |
| 14 | Z | 518 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 18 | H | 1855 | LHG | C11-C10-C9 | -2.25 | 102.99 | 114.42 |
| 17 | J | 4012 | BCR | C28-C27-C26 | -2.25 | 110.06 | 114.08 |
| 15 | e | 2001 | PQN | C21-C20-C18 | -2.25 | 108.64 | 115.92 |
| 14 | B | 1239 | CLA | O2A-CGA-O1A | -2.25 | 117.91 | 123.59 |
| 14 | B | 1224 | CLA | C1-C2-C3 | -2.25 | 122.15 | 126.04 |
| 17 | l | 4012 | BCR | C28-C27-C26 | -2.25 | 110.06 | 114.08 |
| 17 | L | 4219 | BCR | C24-C23-C22 | -2.25 | 122.83 | 126.23 |
| 14 | B | 1231 | CLA | CHD-C1D-ND | -2.25 | 122.39 | 124.45 |
| 14 | m | 1401 | CLA | O2A-CGA-O1A | -2.25 | 117.91 | 123.59 |
| 14 | 2 | 502 | CLA | CMB-C2B-C3B | 2.25 | 128.89 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1023 | CLA | CMD-C2D-C3D | 2.25 | 132.79 | 127.61 |
| 14 | L | 1501 | CLA | CAA-C2A-C3A | -2.25 | 106.62 | 112.78 |
| 14 | H | 1023 | CLA | CMD-C2D-C3D | 2.25 | 132.79 | 127.61 |
| 17 | n | 4219 | BCR | C24-C23-C22 | -2.25 | 122.84 | 126.23 |
| 14 | 6 | 502 | CLA | CAA-C2A-C3A | -2.25 | 106.62 | 112.78 |
| 14 | f | 1208 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 14 | r | 502 | CLA | CMB-C2B-C3B | 2.25 | 128.89 | 124.68 |
| 15 | A | 2001 | PQN | C21-C20-C18 | -2.25 | 108.65 | 115.92 |
| 17 | n | 4020 | BCR | C21-C20-C19 | -2.25 | 116.20 | 123.22 |
| 14 | n | 1501 | CLA | CAA-C2A-C3A | -2.25 | 106.62 | 112.78 |
| 14 | 4 | 507 | CLA | C1B-CHB-C4A | -2.25 | 125.66 | 130.12 |
| 14 | G | 1103 | CLA | C3C-C4C-NC | -2.25 | 108.05 | 110.57 |
| 14 | f | 1239 | CLA | O2A-CGA-O1A | -2.25 | 117.92 | 123.59 |
| 21 | q | 822 | SQD | O48-C23-C24 | 2.25 | 118.96 | 111.91 |
| 14 | A | 1107 | CLA | CAA-CBA-CGA | -2.25 | 106.69 | 113.25 |
| 18 | H | 1855 | LHG | C18-C17-C16 | -2.25 | 103.02 | 114.42 |
| 14 | l | 1303 | CLA | C1B-CHB-C4A | -2.25 | 125.67 | 130.12 |
| 14 | r | 503 | CLA | C1B-CHB-C4A | -2.25 | 125.67 | 130.12 |
| 14 | G | 1134 | CLA | C4-C3-C5 | 2.25 | 119.05 | 115.27 |
| 14 | e | 1011 | CLA | OBD-CAD-C3D | 2.25 | 133.93 | 128.52 |
| 17 | L | 4020 | BCR | C21-C20-C19 | -2.25 | 116.21 | 123.22 |
| 14 | L | 1501 | CLA | C2A-C1A-CHA | 2.25 | 127.79 | 123.86 |
| 17 | A | 4002 | BCR | C38-C26-C27 | 2.25 | 117.93 | 113.62 |
| 14 | A | 1011 | CLA | OBD-CAD-C3D | 2.25 | 133.92 | 128.52 |
| 17 | V | 4020 | BCR | C21-C20-C19 | -2.24 | 116.21 | 123.22 |
| 14 | A | 1130 | CLA | O2A-CGA-O1A | -2.24 | 117.93 | 123.59 |
| 17 | G | 4002 | BCR | C38-C26-C27 | 2.24 | 117.93 | 113.62 |
| 20 | f | 5002 | LMG | C35-C34-C33 | -2.24 | 103.03 | 114.42 |
| 14 | A | 1110 | CLA | C1B-CHB-C4A | -2.24 | 125.67 | 130.12 |
| 14 | B | 1202 | CLA | C1B-CHB-C4A | -2.24 | 125.67 | 130.12 |
| 21 | Y | 822 | SQD | O48-C23-C24 | 2.24 | 118.95 | 111.91 |
| 14 | m | 1105 | CLA | O2D-CGD-CBD | 2.24 | 115.25 | 111.27 |
| 18 | f | 1855 | LHG | C18-C17-C16 | -2.24 | 103.04 | 114.42 |
| 20 | B | 5002 | LMG | C35-C34-C33 | -2.24 | 103.04 | 114.42 |
| 18 | B | 1855 | LHG | C18-C17-C16 | -2.24 | 103.04 | 114.42 |
| 14 | G | 1101 | CLA | C1B-CHB-C4A | -2.24 | 125.68 | 130.12 |
| 14 | A | 1121 | CLA | C2D-C1D-ND | -2.24 | 108.45 | 110.10 |
| 14 | J | 1303 | CLA | C1B-CHB-C4A | -2.24 | 125.68 | 130.12 |
| 14 | e | 1107 | CLA | CAA-CBA-CGA | -2.24 | 106.70 | 113.25 |
| 17 | V | 4219 | BCR | C24-C23-C22 | -2.24 | 122.85 | 126.23 |
| 15 | G | 2001 | PQN | C21-C20-C18 | -2.24 | 108.68 | 115.92 |
| 17 | H | 4014 | BCR | C8-C9-C10 | -2.24 | 115.50 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | H | 4006 | BCR | C28-C27-C26 | -2.24 | 110.08 | 114.08 |
| 14 | s | 503 | CLA | CAA-CBA-CGA | -2.24 | 106.56 | 112.51 |
| 14 | B | 1236 | CLA | CHB-C4A-NA | 2.24 | 127.61 | 124.51 |
| 22 | p | 170 | FMN | C9A-C5A-N5 | -2.24 | 120.00 | 122.43 |
| 14 | e | 1134 | CLA | C4-C3-C5 | 2.24 | 119.04 | 115.27 |
| 17 | d | 522 | BCR | C21-C20-C19 | -2.24 | 116.23 | 123.22 |
| 14 | U | 1105 | CLA | O2D-CGD-CBD | 2.24 | 115.25 | 111.27 |
| 21 | B | 1852 | SQD | O6-C1-C2 | 2.24 | 111.80 | 108.30 |
| 14 | H | 1202 | CLA | C1B-CHB-C4A | -2.24 | 125.69 | 130.12 |
| 17 | B | 4009 | BCR | C1-C6-C5 | -2.24 | 119.46 | 122.61 |
| 14 | H | 1220 | CLA | O2A-CGA-O1A | -2.24 | 117.94 | 123.59 |
| 22 | P | 170 | FMN | C9A-C5A-N5 | -2.24 | 120.00 | 122.43 |
| 14 | B | 1226 | CLA | CHC-C1C-NC | 2.24 | 127.60 | 124.20 |
| 17 | e | 4011 | BCR | C23-C24-C25 | -2.24 | 120.92 | 127.20 |
| 20 | H | 5002 | LMG | C35-C34-C33 | -2.24 | 103.07 | 114.42 |
| 17 | v | 522 | BCR | C21-C20-C19 | -2.24 | 116.24 | 123.22 |
| 17 | Z | 524 | BCR | C1-C6-C5 | -2.24 | 119.47 | 122.61 |
| 17 | 6 | 522 | BCR | C21-C20-C19 | -2.23 | 116.24 | 123.22 |
| 14 | 3 | 503 | CLA | CAA-CBA-CGA | -2.23 | 106.58 | 112.51 |
| 14 | Z | 507 | CLA | CAA-C2A-C3A | -2.23 | 106.66 | 112.78 |
| 14 | n | 1501 | CLA | C2A-C1A-CHA | 2.23 | 127.77 | 123.86 |
| 14 | Y | 508 | CLA | CHC-C1C-NC | 2.23 | 127.59 | 124.20 |
| 14 | K | 1105 | CLA | O2D-CGD-CBD | 2.23 | 115.24 | 111.27 |
| 14 | r | 504 | CLA | C1B-CHB-C4A | -2.23 | 125.69 | 130.12 |
| 14 | t | 509 | CLA | C2A-C1A-CHA | 2.23 | 127.76 | 123.86 |
| 17 | H | 4009 | BCR | C1-C6-C5 | -2.23 | 119.47 | 122.61 |
| 14 | 2 | 518 | CLA | C1B-CHB-C4A | -2.23 | 125.69 | 130.12 |
| 14 | d | 511 | CLA | C1B-CHB-C4A | -2.23 | 125.69 | 130.12 |
| 14 | v | 502 | CLA | CAA-C2A-C3A | -2.23 | 106.67 | 112.78 |
| 14 | e | 1121 | CLA | C2A-C1A-CHA | 2.23 | 127.76 | 123.86 |
| 14 | j | 1302 | CLA | CMB-C2B-C3B | 2.23 | 128.85 | 124.68 |
| 21 | l | 822 | SQD | O48-C23-C24 | 2.23 | 118.91 | 111.91 |
| 14 | v | 511 | CLA | C1B-CHB-C4A | -2.23 | 125.70 | 130.12 |
| 14 | G | 1121 | CLA | C2D-C1D-ND | -2.23 | 108.46 | 110.10 |
| 17 | s | 524 | BCR | C38-C26-C27 | 2.23 | 117.90 | 113.62 |
| 14 | d | 502 | CLA | CMB-C2B-C3B | 2.23 | 128.85 | 124.68 |
| 14 | H | 1211 | CLA | O2A-CGA-O1A | -2.23 | 117.97 | 123.59 |
| 14 | f | 1220 | CLA | O2A-CGA-O1A | -2.23 | 117.97 | 123.59 |
| 14 | A | 1132 | CLA | C2D-C1D-ND | -2.23 | 108.46 | 110.10 |
| 14 | A | 1121 | CLA | C2A-C1A-CHA | 2.23 | 127.76 | 123.86 |
| 14 | f | 1226 | CLA | CHC-C1C-NC | 2.23 | 127.58 | 124.20 |
| 14 | 2 | 507 | CLA | CAA-C2A-C3A | -2.23 | 106.67 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | G | 4011 | BCR | C23-C24-C25 | -2.23 | 120.94 | 127.20 |
| 17 | c | 522 | BCR | C3-C4-C5 | -2.23 | 110.10 | 114.08 |
| 17 | B | 4005 | BCR | C21-C20-C19 | -2.23 | 116.26 | 123.22 |
| 17 | B | 4006 | BCR | C29-C30-C25 | 2.23 | 113.91 | 110.48 |
| 14 | B | 1220 | CLA | O2A-CGA-O1A | -2.23 | 117.97 | 123.59 |
| 17 | H | 4005 | BCR | C21-C20-C19 | -2.23 | 116.27 | 123.22 |
| 14 | 6 | 511 | CLA | C1B-CHB-C4A | -2.23 | 125.71 | 130.12 |
| 14 | b | 509 | CLA | C2A-C1A-CHA | 2.23 | 127.75 | 123.86 |
| 17 | A | 4011 | BCR | C23-C24-C25 | -2.23 | 120.95 | 127.20 |
| 22 | X | 170 | FMN | C9A-C5A-N5 | -2.23 | 120.01 | 122.43 |
| 21 | H | 1852 | SQD | C44-O6-C1 | 2.23 | 118.09 | 113.74 |
| 14 | r | 518 | CLA | C1B-CHB-C4A | -2.23 | 125.71 | 130.12 |
| 14 | s | 507 | CLA | O2A-CGA-O1A | -2.23 | 117.75 | 123.30 |
| 14 | V | 1501 | CLA | C2A-C1A-CHA | 2.23 | 127.75 | 123.86 |
| 14 | v | 502 | CLA | CMB-C2B-C3B | 2.23 | 128.84 | 124.68 |
| 14 | r | 507 | CLA | CAA-C2A-C3A | -2.23 | 106.68 | 112.78 |
| 14 | d | 511 | CLA | CHD-C1D-ND | -2.23 | 122.41 | 124.45 |
| 14 | f | 1211 | CLA | O2A-CGA-O1A | -2.23 | 117.98 | 123.59 |
| 14 | u | 502 | CLA | CMB-C2B-C3B | 2.22 | 128.84 | 124.68 |
| 17 | o | 4021 | BCR | C8-C7-C6 | -2.22 | 120.96 | 127.20 |
| 17 | f | 4014 | BCR | C8-C9-C10 | -2.22 | 115.53 | 118.94 |
| 14 | l | 1302 | CLA | O2D-CGD-CBD | 2.22 | 115.22 | 111.27 |
| 14 | Z | 502 | CLA | CMB-C2B-C3B | 2.22 | 128.84 | 124.68 |
| 17 | Y | 522 | BCR | C1-C6-C5 | -2.22 | 119.48 | 122.61 |
| 17 | 5 | 521 | BCR | C31-C1-C6 | -2.22 | 106.69 | 110.30 |
| 17 | u | 521 | BCR | C31-C1-C6 | -2.22 | 106.69 | 110.30 |
| 14 | f | 1208 | CLA | CHB-C4A-NA | 2.22 | 127.59 | 124.51 |
| 14 | u | 512 | CLA | CHB-C4A-NA | 2.22 | 127.59 | 124.51 |
| 14 | K | 1401 | CLA | O2A-CGA-O1A | -2.22 | 117.98 | 123.59 |
| 14 | e | 1119 | CLA | C2D-C1D-ND | -2.22 | 108.47 | 110.10 |
| 17 | Y | 522 | BCR | C21-C20-C19 | -2.22 | 116.28 | 123.22 |
| 18 | G | 5006 | LHG | C27-C26-C25 | -2.22 | 103.14 | 114.42 |
| 17 | B | 4014 | BCR | C8-C9-C10 | -2.22 | 115.53 | 118.94 |
| 20 | J | 5104 | LMG | C1-C2-C3 | -2.22 | 105.37 | 110.00 |
| 20 | T | 5104 | LMG | C1-C2-C3 | -2.22 | 105.37 | 110.00 |
| 14 | l | 508 | CLA | CHC-C1C-NC | 2.22 | 127.57 | 124.20 |
| 17 | f | 4005 | BCR | C21-C20-C19 | -2.22 | 116.29 | 123.22 |
| 17 | H | 4006 | BCR | C29-C30-C25 | 2.22 | 113.90 | 110.48 |
| 14 | H | 1236 | CLA | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 17 | c | 521 | BCR | C31-C1-C6 | -2.22 | 106.70 | 110.30 |
| 14 | 4 | 509 | CLA | C2A-C1A-CHA | 2.22 | 127.74 | 123.86 |
| 17 | f | 4009 | BCR | C1-C6-C5 | -2.22 | 119.49 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1121 | CLA | C2A-C1A-CHA | 2.22 | 127.74 | 123.86 |
| 14 | G | 1104 | CLA | CHD-C1D-ND | -2.22 | 122.41 | 124.45 |
| 14 | a | 503 | CLA | CAA-CBA-CGA | -2.22 | 106.62 | 112.51 |
| 18 | e | 5006 | LHG | C27-C26-C25 | -2.22 | 103.16 | 114.42 |
| 17 | f | 4009 | BCR | C36-C18-C19 | 2.22 | 121.57 | 118.08 |
| 14 | 6 | 511 | CLA | CHD-C1D-ND | -2.22 | 122.42 | 124.45 |
| 17 | M | 4021 | BCR | C8-C7-C6 | -2.22 | 120.97 | 127.20 |
| 17 | b | 522 | BCR | C11-C12-C13 | -2.22 | 120.19 | 126.42 |
| 14 | Z | 504 | CLA | C1B-CHB-C4A | -2.22 | 125.72 | 130.12 |
| 18 | A | 5006 | LHG | C27-C26-C25 | -2.22 | 103.17 | 114.42 |
| 17 | a | 523 | BCR | C11-C12-C13 | -2.22 | 120.19 | 126.42 |
| 17 | H | 4009 | BCR | C36-C18-C19 | 2.22 | 121.57 | 118.08 |
| 14 | s | 505 | CLA | C2D-C1D-ND | -2.22 | 108.47 | 110.10 |
| 14 | c | 512 | CLA | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 17 | l | 522 | BCR | C21-C20-C19 | -2.22 | 116.30 | 123.22 |
| 17 | q | 522 | BCR | C21-C20-C19 | -2.22 | 116.30 | 123.22 |
| 20 | l | 5104 | LMG | C1-C2-C3 | -2.22 | 105.38 | 110.00 |
| 14 | q | 508 | CLA | CHC-C1C-NC | 2.22 | 127.57 | 124.20 |
| 14 | U | 1401 | CLA | O2A-CGA-O1A | -2.22 | 118.00 | 123.59 |
| 14 | 6 | 502 | CLA | CMB-C2B-C3B | 2.22 | 128.82 | 124.68 |
| 14 | B | 1208 | CLA | CHB-C4A-NA | 2.22 | 127.58 | 124.51 |
| 14 | 2 | 504 | CLA | C1B-CHB-C4A | -2.22 | 125.73 | 130.12 |
| 17 | t | 522 | BCR | C11-C12-C13 | -2.22 | 120.19 | 126.42 |
| 21 | f | 1852 | SQD | O6-C1-C2 | 2.22 | 111.76 | 108.30 |
| 17 | 5 | 522 | BCR | C3-C4-C5 | -2.22 | 110.12 | 114.08 |
| 17 | t | 523 | BCR | C7-C8-C9 | -2.22 | 122.89 | 126.23 |
| 14 | t | 503 | CLA | C2A-C1A-CHA | 2.21 | 127.73 | 123.86 |
| 14 | e | 1103 | CLA | C3C-C4C-NC | -2.21 | 108.09 | 110.57 |
| 14 | B | 1211 | CLA | O2A-CGA-O1A | -2.21 | 118.00 | 123.59 |
| 17 | u | 522 | BCR | C3-C4-C5 | -2.21 | 110.12 | 114.08 |
| 14 | B | 1209 | CLA | C1B-CHB-C4A | -2.21 | 125.73 | 130.12 |
| 21 | q | 822 | SQD | O6-C1-C2 | 2.21 | 111.76 | 108.30 |
| 14 | f | 1209 | CLA | C1B-CHB-C4A | -2.21 | 125.73 | 130.12 |
| 17 | 4 | 522 | BCR | C11-C12-C13 | -2.21 | 120.20 | 126.42 |
| 14 | H | 1213 | CLA | C1B-CHB-C4A | -2.21 | 125.73 | 130.12 |
| 14 | G | 1130 | CLA | C2D-C1D-ND | -2.21 | 108.47 | 110.10 |
| 14 | A | 1103 | CLA | C3C-C4C-NC | -2.21 | 108.09 | 110.57 |
| 14 | 3 | 516 | CLA | O2A-CGA-O1A | -2.21 | 117.78 | 123.30 |
| 14 | r | 508 | CLA | O2A-CGA-O1A | -2.21 | 117.78 | 123.30 |
| 17 | V | 4219 | BCR | C4-C5-C6 | -2.21 | 119.52 | 122.73 |
| 17 | B | 4009 | BCR | C36-C18-C19 | 2.21 | 121.56 | 118.08 |
| 14 | Y | 518 | CLA | C1B-CHB-C4A | -2.21 | 125.74 | 130.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1213 | CLA | C1B-CHB-C4A | -2.21 | 125.74 | 130.12 |
| 14 | A | 1104 | CLA | CHD-C1D-ND | -2.21 | 122.42 | 124.45 |
| 14 | a | 516 | CLA | O2A-CGA-O1A | -2.21 | 117.79 | 123.30 |
| 17 | A | 4011 | BCR | C8-C9-C10 | 2.21 | 122.33 | 118.94 |
| 14 | b | 503 | CLA | C2A-C1A-CHA | 2.21 | 127.72 | 123.86 |
| 17 | 3 | 523 | BCR | C11-C12-C13 | -2.21 | 120.21 | 126.42 |
| 14 | c | 502 | CLA | CMB-C2B-C3B | 2.21 | 128.81 | 124.68 |
| 18 | e | 5008 | LHG | C11-C10-C9 | -2.21 | 103.22 | 114.42 |
| 17 | V | 4019 | BCR | C15-C16-C17 | -2.21 | 118.95 | 123.47 |
| 14 | 5 | 502 | CLA | CMB-C2B-C3B | 2.21 | 128.81 | 124.68 |
| 17 | b | 523 | BCR | C7-C8-C9 | -2.21 | 122.90 | 126.23 |
| 14 | e | 1104 | CLA | CHD-C1D-ND | -2.21 | 122.43 | 124.45 |
| 18 | A | 5008 | LHG | C11-C10-C9 | -2.21 | 103.23 | 114.42 |
| 14 | v | 511 | CLA | CHD-C1D-ND | -2.20 | 122.43 | 124.45 |
| 18 | G | 5008 | LHG | C11-C10-C9 | -2.20 | 103.23 | 114.42 |
| 17 | q | 523 | BCR | C8-C7-C6 | -2.20 | 121.01 | 127.20 |
| 17 | 4 | 523 | BCR | C7-C8-C9 | -2.20 | 122.91 | 126.23 |
| 14 | Z | 512 | CLA | CHB-C4A-NA | 2.20 | 127.56 | 124.51 |
| 17 | b | 523 | BCR | C36-C18-C19 | 2.20 | 121.55 | 118.08 |
| 14 | s | 516 | CLA | O2A-CGA-O1A | -2.20 | 117.81 | 123.30 |
| 17 | 3 | 524 | BCR | C38-C26-C27 | 2.20 | 117.85 | 113.62 |
| 14 | e | 1121 | CLA | C2D-C1D-ND | -2.20 | 108.48 | 110.10 |
| 14 | B | 1221 | CLA | O2A-CGA-O1A | -2.20 | 118.03 | 123.59 |
| 14 | f | 1221 | CLA | O2A-CGA-O1A | -2.20 | 118.03 | 123.59 |
| 14 | m | 1103 | CLA | C1B-CHB-C4A | -2.20 | 125.75 | 130.12 |
| 21 | 1 | 822 | SQD | O6-C1-C2 | 2.20 | 111.74 | 108.30 |
| 14 | 5 | 502 | CLA | C1B-CHB-C4A | -2.20 | 125.76 | 130.12 |
| 14 | u | 502 | CLA | C1B-CHB-C4A | -2.20 | 125.76 | 130.12 |
| 14 | G | 1132 | CLA | C2D-C1D-ND | -2.20 | 108.48 | 110.10 |
| 14 | B | 1021 | CLA | C1B-CHB-C4A | -2.20 | 125.76 | 130.12 |
| 14 | 4 | 503 | CLA | C2A-C1A-CHA | 2.20 | 127.71 | 123.86 |
| 14 | 3 | 507 | CLA | O2A-CGA-O1A | -2.20 | 117.81 | 123.30 |
| 14 | 5 | 512 | CLA | CHB-C4A-NA | 2.20 | 127.56 | 124.51 |
| 14 | A | 1104 | CLA | O1D-CGD-CBD | 2.20 | 128.99 | 124.48 |
| 17 | d | 521 | BCR | C2-C1-C6 | 2.20 | 113.87 | 110.48 |
| 17 | e | 4011 | BCR | C8-C9-C10 | 2.20 | 122.32 | 118.94 |
| 17 | q | 522 | BCR | C1-C6-C5 | -2.20 | 119.52 | 122.61 |
| 17 | 4 | 523 | BCR | C36-C18-C19 | 2.20 | 121.54 | 118.08 |
| 17 | H | 4014 | BCR | C31-C1-C6 | -2.20 | 106.73 | 110.30 |
| 14 | H | 1209 | CLA | C2A-C1A-CHA | 2.20 | 127.70 | 123.86 |
| 17 | G | 4011 | BCR | C8-C9-C10 | 2.20 | 122.32 | 118.94 |
| 17 | G | 4003 | BCR | C8-C7-C6 | -2.20 | 121.03 | 127.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | t | 523 | BCR | C36-C18-C19 | 2.20 | 121.54 | 118.08 |
| 14 | f | 1223 | CLA | C1-C2-C3 | -2.20 | 122.24 | 126.04 |
| 17 | s | 523 | BCR | C11-C12-C13 | -2.20 | 120.24 | 126.42 |
| 17 | 2 | 521 | BCR | C15-C16-C17 | -2.20 | 118.97 | 123.47 |
| 17 | l | 4012 | BCR | C23-C24-C25 | -2.20 | 121.03 | 127.20 |
| 17 | W | 4021 | BCR | C8-C7-C6 | -2.20 | 121.03 | 127.20 |
| 21 | Y | 822 | SQD | O6-C1-C2 | 2.20 | 111.73 | 108.30 |
| 14 | J | 1302 | CLA | O2D-CGD-CBD | 2.20 | 115.17 | 111.27 |
| 14 | A | 1011 | CLA | CHA-C1A-NA | -2.20 | 121.36 | 126.40 |
| 17 | a | 524 | BCR | C38-C26-C27 | 2.20 | 117.84 | 113.62 |
| 14 | U | 1103 | CLA | C1B-CHB-C4A | -2.20 | 125.76 | 130.12 |
| 21 | B | 1852 | SQD | C44-O6-C1 | 2.20 | 118.03 | 113.74 |
| 14 | e | 1104 | CLA | O1D-CGD-CBD | 2.20 | 128.98 | 124.48 |
| 17 | 4 | 522 | BCR | C3-C4-C5 | -2.20 | 110.15 | 114.08 |
| 14 | Z | 508 | CLA | O2A-CGA-O1A | -2.20 | 117.82 | 123.30 |
| 17 | f | 4006 | BCR | C29-C30-C25 | 2.20 | 113.86 | 110.48 |
| 14 | c | 502 | CLA | C1B-CHB-C4A | -2.20 | 125.77 | 130.12 |
| 19 | H | 1843 | LMU | O1'-C1'-C2' | 2.20 | 111.73 | 108.30 |
| 14 | f | 1021 | CLA | C1B-CHB-C4A | -2.20 | 125.77 | 130.12 |
| 18 | L | 5221 | LHG | C27-C26-C25 | -2.20 | 103.28 | 114.42 |
| 14 | f | 1209 | CLA | C2A-C1A-CHA | 2.20 | 127.70 | 123.86 |
| 17 | J | 4012 | BCR | C23-C24-C25 | -2.20 | 121.04 | 127.20 |
| 17 | e | 4003 | BCR | C8-C7-C6 | -2.20 | 121.04 | 127.20 |
| 14 | f | 1213 | CLA | C1B-CHB-C4A | -2.19 | 125.77 | 130.12 |
| 14 | G | 1136 | CLA | C7-C6-C5 | -2.19 | 107.40 | 113.36 |
| 18 | S | 5001 | LHG | C11-C10-C9 | -2.19 | 103.29 | 114.42 |
| 18 | n | 5221 | LHG | C27-C26-C25 | -2.19 | 103.29 | 114.42 |
| 19 | B | 1843 | LMU | O1'-C1'-C2' | 2.19 | 111.73 | 108.30 |
| 17 | Y | 523 | BCR | C8-C7-C6 | -2.19 | 121.04 | 127.20 |
| 17 | r | 521 | BCR | C15-C16-C17 | -2.19 | 118.98 | 123.47 |
| 17 | 1 | 522 | BCR | C1-C6-C5 | -2.19 | 119.53 | 122.61 |
| 17 | b | 522 | BCR | C3-C4-C5 | -2.19 | 110.16 | 114.08 |
| 14 | A | 1136 | CLA | C7-C6-C5 | -2.19 | 107.41 | 113.36 |
| 17 | Z | 523 | BCR | C37-C22-C23 | 2.19 | 121.53 | 118.08 |
| 14 | 1 | 518 | CLA | C1B-CHB-C4A | -2.19 | 125.78 | 130.12 |
| 14 | G | 1118 | CLA | C2A-C1A-CHA | 2.19 | 127.69 | 123.86 |
| 14 | G | 1104 | CLA | O1D-CGD-CBD | 2.19 | 128.97 | 124.48 |
| 14 | A | 1013 | CLA | O2D-CGD-CBD | 2.19 | 115.16 | 111.27 |
| 14 | T | 1302 | CLA | O2D-CGD-CBD | 2.19 | 115.16 | 111.27 |
| 14 | 2 | 502 | CLA | C1B-CHB-C4A | -2.19 | 125.78 | 130.12 |
| 14 | H | 1021 | CLA | C1B-CHB-C4A | -2.19 | 125.78 | 130.12 |
| 17 | 1 | 523 | BCR | C8-C7-C6 | -2.19 | 121.05 | 127.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | T | 4012 | BCR | C23-C24-C25 | -2.19 | 121.05 | 127.20 |
| 17 | B | 4014 | BCR | C31-C1-C6 | -2.19 | 106.75 | 110.30 |
| 17 | l | 4013 | BCR | C23-C22-C21 | 2.19 | 122.30 | 118.94 |
| 14 | B | 1209 | CLA | C2A-C1A-CHA | 2.19 | 127.69 | 123.86 |
| 14 | B | 1223 | CLA | C1-C2-C3 | -2.19 | 122.26 | 126.04 |
| 17 | G | 4007 | BCR | C4-C5-C6 | -2.19 | 119.55 | 122.73 |
| 17 | A | 4003 | BCR | C8-C7-C6 | -2.19 | 121.05 | 127.20 |
| 14 | e | 1013 | CLA | O2D-CGD-CBD | 2.19 | 115.16 | 111.27 |
| 14 | H | 1209 | CLA | C1B-CHB-C4A | -2.19 | 125.78 | 130.12 |
| 17 | B | 4004 | BCR | C8-C7-C6 | -2.19 | 121.06 | 127.20 |
| 17 | G | 4007 | BCR | C2-C1-C6 | 2.19 | 113.85 | 110.48 |
| 14 | q | 518 | CLA | C1B-CHB-C4A | -2.19 | 125.78 | 130.12 |
| 14 | s | 511 | CLA | C1B-CHB-C4A | -2.19 | 125.78 | 130.12 |
| 14 | H | 1221 | CLA | O2A-CGA-O1A | -2.19 | 118.07 | 123.59 |
| 17 | e | 4007 | BCR | C33-C5-C4 | 2.19 | 117.82 | 113.62 |
| 17 | Z | 521 | BCR | C15-C16-C17 | -2.19 | 118.99 | 123.47 |
| 17 | t | 522 | BCR | C3-C4-C5 | -2.19 | 110.17 | 114.08 |
| 14 | 2 | 508 | CLA | O2A-CGA-O1A | -2.19 | 117.85 | 123.30 |
| 17 | L | 4219 | BCR | C4-C5-C6 | -2.19 | 119.56 | 122.73 |
| 17 | d | 523 | BCR | C16-C15-C14 | -2.19 | 119.00 | 123.47 |
| 17 | q | 522 | BCR | C36-C18-C19 | 2.19 | 121.52 | 118.08 |
| 17 | J | 4013 | BCR | C23-C22-C21 | 2.19 | 122.30 | 118.94 |
| 14 | e | 1136 | CLA | C7-C6-C5 | -2.19 | 107.42 | 113.36 |
| 14 | 4 | 517 | CLA | C1B-CHB-C4A | -2.19 | 125.79 | 130.12 |
| 17 | J | 4012 | BCR | C10-C11-C12 | -2.19 | 116.40 | 123.22 |
| 17 | l | 4012 | BCR | C10-C11-C12 | -2.19 | 116.40 | 123.22 |
| 14 | b | 517 | CLA | C1B-CHB-C4A | -2.19 | 125.79 | 130.12 |
| 14 | c | 507 | CLA | O2A-CGA-O1A | -2.18 | 117.85 | 123.30 |
| 17 | f | 4014 | BCR | C31-C1-C6 | -2.18 | 106.75 | 110.30 |
| 14 | e | 1132 | CLA | C2D-C1D-ND | -2.18 | 108.49 | 110.10 |
| 14 | K | 1103 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 14 | a | 511 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 18 | V | 5221 | LHG | C27-C26-C25 | -2.18 | 103.33 | 114.42 |
| 17 | t | 523 | BCR | C8-C7-C6 | -2.18 | 121.07 | 127.20 |
| 18 | I | 5001 | LHG | C11-C10-C9 | -2.18 | 103.34 | 114.42 |
| 20 | f | 5002 | LMG | O7-C10-O9 | -2.18 | 118.42 | 123.70 |
| 17 | T | 4013 | BCR | C23-C22-C21 | 2.18 | 122.29 | 118.94 |
| 17 | 6 | 523 | BCR | C16-C15-C14 | -2.18 | 119.00 | 123.47 |
| 14 | G | 1013 | CLA | O2D-CGD-CBD | 2.18 | 115.15 | 111.27 |
| 14 | a | 507 | CLA | O2A-CGA-O1A | -2.18 | 117.86 | 123.30 |
| 14 | a | 512 | CLA | CHB-C4A-NA | 2.18 | 127.53 | 124.51 |
| 17 | V | 4219 | BCR | C19-C18-C17 | -2.18 | 115.59 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | v | 509 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 18 | G | 5004 | LHG | C11-C10-C9 | -2.18 | 103.34 | 114.42 |
| 14 | B | 1226 | CLA | CHA-C4D-ND | 2.18 | 137.06 | 132.50 |
| 14 | G | 1121 | CLA | C1B-CHB-C4A | -2.18 | 125.79 | 130.12 |
| 17 | 4 | 523 | BCR | C8-C7-C6 | -2.18 | 121.07 | 127.20 |
| 17 | 6 | 521 | BCR | C2-C1-C6 | 2.18 | 113.84 | 110.48 |
| 17 | G | 4002 | BCR | C31-C1-C6 | -2.18 | 106.76 | 110.30 |
| 14 | u | 507 | CLA | O2A-CGA-O1A | -2.18 | 117.86 | 123.30 |
| 18 | k | 5001 | LHG | C11-C10-C9 | -2.18 | 103.35 | 114.42 |
| 14 | e | 1011 | CLA | CHA-C1A-NA | -2.18 | 121.40 | 126.40 |
| 14 | e | 1127 | CLA | C2A-C1A-CHA | 2.18 | 127.67 | 123.86 |
| 14 | r | 502 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 17 | v | 522 | BCR | C2-C3-C4 | -2.18 | 106.50 | 111.38 |
| 14 | 5 | 507 | CLA | O2A-CGA-O1A | -2.18 | 117.86 | 123.30 |
| 14 | A | 1118 | CLA | O2A-CGA-O1A | -2.18 | 118.09 | 123.59 |
| 14 | u | 501 | CLA | CAA-C2A-C3A | -2.18 | 106.81 | 112.78 |
| 17 | T | 4012 | BCR | C10-C11-C12 | -2.18 | 116.41 | 123.22 |
| 14 | 3 | 511 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 17 | A | 4002 | BCR | C31-C1-C6 | -2.18 | 106.76 | 110.30 |
| 14 | Z | 502 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 14 | d | 502 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 14 | A | 1127 | CLA | C2A-C1A-CHA | 2.18 | 127.67 | 123.86 |
| 14 | e | 1122 | CLA | C2A-C1A-CHA | 2.18 | 127.67 | 123.86 |
| 21 | f | 1852 | SQD | C44-O6-C1 | 2.18 | 117.99 | 113.74 |
| 17 | H | 4004 | BCR | C8-C7-C6 | -2.18 | 121.08 | 127.20 |
| 14 | f | 1238 | CLA | C2D-C1D-ND | -2.18 | 108.50 | 110.10 |
| 17 | A | 4007 | BCR | C30-C25-C26 | -2.18 | 119.55 | 122.61 |
| 17 | n | 4219 | BCR | C4-C5-C6 | -2.18 | 119.57 | 122.73 |
| 14 | 6 | 509 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 14 | H | 1217 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 17 | A | 4007 | BCR | C33-C5-C4 | 2.18 | 117.80 | 113.62 |
| 20 | B | 5002 | LMG | O7-C10-O9 | -2.18 | 118.44 | 123.70 |
| 14 | G | 1137 | CLA | C3A-C2A-C1A | 2.18 | 104.60 | 101.34 |
| 17 | 5 | 522 | BCR | C27-C26-C25 | -2.18 | 119.57 | 122.73 |
| 14 | H | 1216 | CLA | CMB-C2B-C3B | 2.18 | 128.75 | 124.68 |
| 14 | A | 1117 | CLA | CHB-C4A-NA | 2.18 | 127.52 | 124.51 |
| 14 | A | 1128 | CLA | C2D-C1D-ND | -2.18 | 108.50 | 110.10 |
| 17 | b | 523 | BCR | C8-C7-C6 | -2.17 | 121.09 | 127.20 |
| 14 | t | 507 | CLA | O2D-CGD-CBD | 2.17 | 115.13 | 111.27 |
| 18 | A | 5004 | LHG | C11-C10-C9 | -2.17 | 103.39 | 114.42 |
| 17 | n | 4219 | BCR | C29-C28-C27 | -2.17 | 106.52 | 111.38 |
| 17 | q | 522 | BCR | C15-C16-C17 | -2.17 | 119.02 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | e | 5004 | LHG | C11-C10-C9 | -2.17 | 103.39 | 114.42 |
| 17 | G | 4007 | BCR | C16-C15-C14 | -2.17 | 119.02 | 123.47 |
| 17 | V | 4219 | BCR | C29-C28-C27 | -2.17 | 106.52 | 111.38 |
| 14 | 5 | 501 | CLA | CAA-C2A-C3A | -2.17 | 106.83 | 112.78 |
| 14 | A | 1101 | CLA | C1-C2-C3 | -2.17 | 122.28 | 126.04 |
| 14 | e | 1101 | CLA | C1-C2-C3 | -2.17 | 122.28 | 126.04 |
| 17 | u | 522 | BCR | C27-C26-C25 | -2.17 | 119.58 | 122.73 |
| 17 | v | 523 | BCR | C16-C15-C14 | -2.17 | 119.02 | 123.47 |
| 14 | G | 1011 | CLA | CHA-C1A-NA | -2.17 | 121.42 | 126.40 |
| 14 | f | 1226 | CLA | CHA-C4D-ND | 2.17 | 137.04 | 132.50 |
| 17 | A | 4007 | BCR | C2-C1-C6 | 2.17 | 113.83 | 110.48 |
| 14 | A | 1121 | CLA | C1B-CHB-C4A | -2.17 | 125.81 | 130.12 |
| 14 | B | 1217 | CLA | C1B-CHB-C4A | -2.17 | 125.81 | 130.12 |
| 14 | A | 1121 | CLA | CHA-C1A-NA | -2.17 | 121.42 | 126.40 |
| 14 | G | 1121 | CLA | CHA-C1A-NA | -2.17 | 121.42 | 126.40 |
| 14 | v | 502 | CLA | C1B-CHB-C4A | -2.17 | 125.82 | 130.12 |
| 17 | 6 | 522 | BCR | C2-C3-C4 | -2.17 | 106.53 | 111.38 |
| 20 | H | 5002 | LMG | O7-C10-O9 | -2.17 | 118.45 | 123.70 |
| 14 | H | 1223 | CLA | C1-C2-C3 | -2.17 | 122.29 | 126.04 |
| 17 | U | 4104 | BCR | C30-C25-C24 | 2.17 | 121.92 | 115.78 |
| 17 | L | 4019 | BCR | C15-C16-C17 | -2.17 | 119.03 | 123.47 |
| 17 | n | 4019 | BCR | C15-C16-C17 | -2.17 | 119.03 | 123.47 |
| 17 | H | 4006 | BCR | C10-C11-C12 | -2.17 | 116.44 | 123.22 |
| 14 | t | 517 | CLA | C1B-CHB-C4A | -2.17 | 125.82 | 130.12 |
| 17 | e | 4002 | BCR | C31-C1-C6 | -2.17 | 106.78 | 110.30 |
| 17 | 2 | 523 | BCR | C37-C22-C23 | 2.17 | 121.50 | 118.08 |
| 14 | A | 1122 | CLA | C2A-C1A-CHA | 2.17 | 127.65 | 123.86 |
| 14 | G | 1118 | CLA | O2A-CGA-O1A | -2.17 | 118.12 | 123.59 |
| 14 | G | 1117 | CLA | CHB-C4A-NA | 2.17 | 127.51 | 124.51 |
| 17 | e | 4007 | BCR | C30-C25-C26 | -2.17 | 119.56 | 122.61 |
| 14 | 6 | 502 | CLA | C1B-CHB-C4A | -2.17 | 125.82 | 130.12 |
| 14 | H | 1226 | CLA | CMC-C2C-C1C | -2.17 | 121.74 | 125.04 |
| 14 | c | 501 | CLA | CAA-C2A-C3A | -2.17 | 106.84 | 112.78 |
| 18 | G | 5005 | LHG | C27-C26-C25 | -2.17 | 103.42 | 114.42 |
| 18 | G | 5003 | LHG | C27-C26-C25 | -2.17 | 103.42 | 114.42 |
| 18 | A | 5005 | LHG | C27-C26-C25 | -2.17 | 103.42 | 114.42 |
| 17 | q | 522 | BCR | C16-C17-C18 | -2.17 | 124.22 | 127.31 |
| 18 | e | 5003 | LHG | C27-C26-C25 | -2.17 | 103.43 | 114.42 |
| 17 | A | 4007 | BCR | C4-C5-C6 | -2.17 | 119.59 | 122.73 |
| 18 | n | 5221 | LHG | C18-C17-C16 | -2.17 | 103.43 | 114.42 |
| 17 | f | 4004 | BCR | C8-C7-C6 | -2.17 | 121.12 | 127.20 |
| 14 | G | 1127 | CLA | C2A-C1A-CHA | 2.17 | 127.65 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | v | 521 | BCR | C2-C1-C6 | 2.17 | 113.81 | 110.48 |
| 14 | B | 1238 | CLA | C2D-C1D-ND | -2.17 | 108.51 | 110.10 |
| 14 | d | 505 | CLA | C2D-C1D-ND | -2.17 | 108.51 | 110.10 |
| 14 | B | 1226 | CLA | CMC-C2C-C1C | -2.17 | 121.74 | 125.04 |
| 14 | A | 1137 | CLA | C3A-C2A-C1A | 2.16 | 104.58 | 101.34 |
| 14 | A | 1130 | CLA | C2D-C1D-ND | -2.16 | 108.51 | 110.10 |
| 18 | A | 5003 | LHG | C27-C26-C25 | -2.16 | 103.44 | 114.42 |
| 17 | c | 522 | BCR | C27-C26-C25 | -2.16 | 119.59 | 122.73 |
| 17 | B | 4006 | BCR | C10-C11-C12 | -2.16 | 116.46 | 123.22 |
| 18 | e | 5005 | LHG | C27-C26-C25 | -2.16 | 103.44 | 114.42 |
| 14 | e | 1013 | CLA | C2C-C1C-NC | -2.16 | 107.94 | 109.97 |
| 14 | l | 507 | CLA | CHA-C1A-NA | -2.16 | 121.44 | 126.40 |
| 17 | s | 522 | BCR | C27-C26-C25 | -2.16 | 119.59 | 122.73 |
| 14 | A | 1107 | CLA | O2D-CGD-O1D | -2.16 | 119.61 | 123.84 |
| 14 | e | 1128 | CLA | C2D-C1D-ND | -2.16 | 108.51 | 110.10 |
| 14 | q | 503 | CLA | C2A-C1A-CHA | 2.16 | 127.64 | 123.86 |
| 17 | G | 4007 | BCR | C33-C5-C4 | 2.16 | 117.77 | 113.62 |
| 14 | G | 1112 | CLA | C2A-C1A-CHA | 2.16 | 127.64 | 123.86 |
| 14 | H | 1226 | CLA | CHA-C4D-ND | 2.16 | 137.02 | 132.50 |
| 17 | l | 522 | BCR | C36-C18-C19 | 2.16 | 121.48 | 118.08 |
| 17 | m | 4104 | BCR | C30-C25-C24 | 2.16 | 121.89 | 115.78 |
| 14 | U | 1401 | CLA | CAA-CBA-CGA | -2.16 | 106.94 | 113.25 |
| 14 | e | 1118 | CLA | O2A-CGA-O1A | -2.16 | 118.14 | 123.59 |
| 14 | e | 1121 | CLA | CHA-C1A-NA | -2.16 | 121.45 | 126.40 |
| 14 | B | 1023 | CLA | CAC-C3C-C2C | -2.16 | 123.83 | 127.53 |
| 14 | d | 509 | CLA | C1B-CHB-C4A | -2.16 | 125.84 | 130.12 |
| 14 | m | 1401 | CLA | CAA-CBA-CGA | -2.16 | 106.94 | 113.25 |
| 14 | A | 1118 | CLA | C2A-C1A-CHA | 2.16 | 127.64 | 123.86 |
| 14 | K | 1401 | CLA | CAA-CBA-CGA | -2.16 | 106.94 | 113.25 |
| 17 | d | 522 | BCR | C2-C3-C4 | -2.16 | 106.55 | 111.38 |
| 17 | G | 4007 | BCR | C30-C25-C26 | -2.16 | 119.57 | 122.61 |
| 17 | K | 4104 | BCR | C30-C25-C24 | 2.16 | 121.89 | 115.78 |
| 19 | f | 1843 | LMU | O1'-C1'-C2' | 2.16 | 111.67 | 108.30 |
| 14 | H | 1023 | CLA | CAC-C3C-C2C | -2.16 | 123.84 | 127.53 |
| 14 | B | 1219 | CLA | C2D-C1D-ND | -2.16 | 108.51 | 110.10 |
| 17 | e | 4007 | BCR | C4-C5-C6 | -2.16 | 119.60 | 122.73 |
| 17 | e | 4007 | BCR | C2-C1-C6 | 2.16 | 113.80 | 110.48 |
| 17 | r | 523 | BCR | C37-C22-C23 | 2.16 | 121.48 | 118.08 |
| 18 | L | 5221 | LHG | C18-C17-C16 | -2.16 | 103.47 | 114.42 |
| 18 | V | 5221 | LHG | C18-C17-C16 | -2.16 | 103.47 | 114.42 |
| 14 | f | 1023 | CLA | CAC-C3C-C2C | -2.16 | 123.84 | 127.53 |
| 14 | G | 1107 | CLA | O2D-CGD-O1D | -2.16 | 119.62 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1226 | CLA | CMC-C2C-C1C | -2.16 | 121.75 | 125.04 |
| 14 | 2 | 510 | CLA | C1B-CHB-C4A | -2.16 | 125.84 | 130.12 |
| 17 | f | 4006 | BCR | C10-C11-C12 | -2.16 | 116.48 | 123.22 |
| 14 | A | 1112 | CLA | C2A-C1A-CHA | 2.16 | 127.63 | 123.86 |
| 14 | s | 512 | CLA | CHB-C4A-NA | 2.16 | 127.50 | 124.51 |
| 14 | f | 1216 | CLA | CMB-C2B-C3B | 2.16 | 128.71 | 124.68 |
| 14 | B | 1216 | CLA | CMB-C2B-C3B | 2.16 | 128.71 | 124.68 |
| 14 | m | 1103 | CLA | O2A-CGA-O1A | -2.16 | 118.15 | 123.59 |
| 14 | H | 1219 | CLA | C2D-C1D-ND | -2.16 | 108.52 | 110.10 |
| 14 | q | 507 | CLA | CHA-C1A-NA | -2.16 | 121.46 | 126.40 |
| 14 | e | 1118 | CLA | C2A-C1A-CHA | 2.16 | 127.63 | 123.86 |
| 14 | 5 | 508 | CLA | CHC-C1C-NC | 2.16 | 127.47 | 124.20 |
| 14 | H | 1228 | CLA | O2A-CGA-O1A | -2.16 | 118.15 | 123.59 |
| 17 | J | 4013 | BCR | C29-C30-C25 | 2.16 | 113.80 | 110.48 |
| 14 | K | 1103 | CLA | O2A-CGA-O1A | -2.15 | 118.15 | 123.59 |
| 17 | t | 524 | BCR | C28-C27-C26 | -2.15 | 110.23 | 114.08 |
| 14 | u | 508 | CLA | CHC-C1C-NC | 2.15 | 127.47 | 124.20 |
| 17 | L | 4219 | BCR | C29-C28-C27 | -2.15 | 106.56 | 111.38 |
| 14 | 4 | 507 | CLA | O2D-CGD-CBD | 2.15 | 115.09 | 111.27 |
| 17 | u | 523 | BCR | C34-C9-C8 | 2.15 | 121.47 | 118.08 |
| 17 | a | 523 | BCR | C3-C4-C5 | -2.15 | 110.23 | 114.08 |
| 17 | L | 4219 | BCR | C19-C18-C17 | -2.15 | 115.64 | 118.94 |
| 14 | e | 1121 | CLA | C1B-CHB-C4A | -2.15 | 125.86 | 130.12 |
| 17 | 3 | 523 | BCR | C3-C4-C5 | -2.15 | 110.23 | 114.08 |
| 14 | H | 1226 | CLA | C3D-C2D-C1D | 2.15 | 108.77 | 105.83 |
| 14 | G | 1022 | CLA | CHD-C1D-ND | -2.15 | 122.48 | 124.45 |
| 14 | f | 1217 | CLA | C1B-CHB-C4A | -2.15 | 125.86 | 130.12 |
| 14 | Y | 507 | CLA | CHA-C1A-NA | -2.15 | 121.47 | 126.40 |
| 14 | G | 1013 | CLA | C2C-C1C-NC | -2.15 | 107.96 | 109.97 |
| 14 | B | 1234 | CLA | C2A-C1A-CHA | 2.15 | 127.62 | 123.86 |
| 17 | f | 4014 | BCR | C29-C30-C25 | 2.15 | 113.79 | 110.48 |
| 14 | e | 1117 | CLA | CHB-C4A-NA | 2.15 | 127.49 | 124.51 |
| 17 | s | 523 | BCR | C3-C4-C5 | -2.15 | 110.24 | 114.08 |
| 14 | Y | 507 | CLA | O2A-CGA-O1A | -2.15 | 117.94 | 123.30 |
| 14 | G | 1122 | CLA | C2A-C1A-CHA | 2.15 | 127.62 | 123.86 |
| 14 | f | 1234 | CLA | C2A-C1A-CHA | 2.15 | 127.62 | 123.86 |
| 14 | G | 1101 | CLA | C1-C2-C3 | -2.15 | 122.32 | 126.04 |
| 14 | d | 501 | CLA | O2D-CGD-CBD | 2.15 | 115.09 | 111.27 |
| 14 | A | 1013 | CLA | C2C-C1C-NC | -2.15 | 107.96 | 109.97 |
| 17 | Y | 522 | BCR | C16-C17-C18 | -2.15 | 124.24 | 127.31 |
| 14 | d | 508 | CLA | O2A-CGA-O1A | -2.15 | 117.94 | 123.30 |
| 17 | A | 4007 | BCR | C16-C15-C14 | -2.15 | 119.07 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | Z | 510 | CLA | C1B-CHB-C4A | -2.15 | 125.86 | 130.12 |
| 14 | H | 1216 | CLA | C2D-C1D-ND | -2.15 | 108.52 | 110.10 |
| 14 | G | 1013 | CLA | CHD-C1D-ND | -2.15 | 122.48 | 124.45 |
| 14 | H | 1218 | CLA | CHD-C1D-ND | -2.15 | 122.48 | 124.45 |
| 14 | u | 503 | CLA | CHD-C1D-ND | -2.15 | 122.48 | 124.45 |
| 14 | v | 507 | CLA | CHA-C1A-NA | -2.15 | 121.48 | 126.40 |
| 17 | T | 4012 | BCR | C2-C1-C6 | 2.15 | 113.79 | 110.48 |
| 17 | 1 | 522 | BCR | C15-C16-C17 | -2.15 | 119.08 | 123.47 |
| 14 | r | 510 | CLA | C1B-CHB-C4A | -2.15 | 125.86 | 130.12 |
| 17 | L | 4219 | BCR | C16-C15-C14 | -2.15 | 119.08 | 123.47 |
| 14 | 6 | 508 | CLA | O2A-CGA-O1A | -2.15 | 117.95 | 123.30 |
| 14 | f | 1218 | CLA | CHD-C1D-ND | -2.15 | 122.48 | 124.45 |
| 14 | Z | 502 | CLA | C2A-C1A-CHA | 2.15 | 127.61 | 123.86 |
| 14 | G | 1128 | CLA | C2D-C1D-ND | -2.15 | 108.52 | 110.10 |
| 14 | a | 505 | CLA | C2D-C1D-ND | -2.15 | 108.52 | 110.10 |
| 17 | B | 4014 | BCR | C19-C18-C17 | -2.15 | 115.65 | 118.94 |
| 14 | l | 1302 | CLA | C2A-C1A-CHA | 2.15 | 127.61 | 123.86 |
| 14 | f | 1226 | CLA | C3D-C2D-C1D | 2.14 | 108.76 | 105.83 |
| 17 | f | 4014 | BCR | C19-C18-C17 | -2.14 | 115.65 | 118.94 |
| 14 | 6 | 507 | CLA | CHA-C1A-NA | -2.14 | 121.49 | 126.40 |
| 17 | Y | 522 | BCR | C36-C18-C19 | 2.14 | 121.45 | 118.08 |
| 14 | B | 1218 | CLA | CHD-C1D-ND | -2.14 | 122.48 | 124.45 |
| 17 | l | 4013 | BCR | C29-C30-C25 | 2.14 | 113.78 | 110.48 |
| 17 | V | 4219 | BCR | C16-C15-C14 | -2.14 | 119.08 | 123.47 |
| 17 | r | 524 | BCR | C15-C16-C17 | -2.14 | 119.08 | 123.47 |
| 14 | v | 501 | CLA | O2D-CGD-CBD | 2.14 | 115.08 | 111.27 |
| 14 | H | 1234 | CLA | C2A-C1A-CHA | 2.14 | 127.61 | 123.86 |
| 17 | H | 4014 | BCR | C19-C18-C17 | -2.14 | 115.65 | 118.94 |
| 14 | d | 509 | CLA | O2A-CGA-O1A | -2.14 | 117.96 | 123.30 |
| 17 | 1 | 524 | BCR | C3-C4-C5 | -2.14 | 110.25 | 114.08 |
| 17 | B | 4014 | BCR | C29-C30-C25 | 2.14 | 113.78 | 110.48 |
| 17 | e | 4007 | BCR | C16-C15-C14 | -2.14 | 119.09 | 123.47 |
| 14 | e | 1104 | CLA | C1B-CHB-C4A | -2.14 | 125.88 | 130.12 |
| 17 | Y | 524 | BCR | C3-C4-C5 | -2.14 | 110.25 | 114.08 |
| 14 | U | 1103 | CLA | O2A-CGA-O1A | -2.14 | 118.19 | 123.59 |
| 17 | n | 4019 | BCR | C38-C26-C27 | 2.14 | 117.73 | 113.62 |
| 17 | T | 4013 | BCR | C29-C30-C25 | 2.14 | 113.78 | 110.48 |
| 17 | Y | 522 | BCR | C15-C16-C17 | -2.14 | 119.09 | 123.47 |
| 14 | c | 508 | CLA | CHC-C1C-NC | 2.14 | 127.45 | 124.20 |
| 14 | J | 1302 | CLA | C2A-C1A-CHA | 2.14 | 127.60 | 123.86 |
| 14 | G | 1122 | CLA | O2A-CGA-O1A | -2.14 | 118.19 | 123.59 |
| 14 | H | 1238 | CLA | O2A-CGA-O1A | -2.14 | 118.19 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | r | 522 | BCR | C30-C25-C26 | -2.14 | 119.60 | 122.61 |
| 14 | q | 504 | CLA | CAC-C3C-C4C | 2.14 | 127.58 | 124.81 |
| 17 | Y | 524 | BCR | C10-C11-C12 | -2.14 | 116.55 | 123.22 |
| 17 | v | 524 | BCR | C23-C22-C21 | -2.14 | 115.66 | 118.94 |
| 17 | L | 4019 | BCR | C38-C26-C27 | 2.14 | 117.72 | 113.62 |
| 17 | 3 | 522 | BCR | C27-C26-C25 | -2.14 | 119.63 | 122.73 |
| 14 | Z | 508 | CLA | C2D-C1D-ND | -2.14 | 108.53 | 110.10 |
| 14 | c | 504 | CLA | C2A-C1A-CHA | 2.14 | 127.60 | 123.86 |
| 19 | e | 1848 | LMU | C2'-C3'-C4' | 2.14 | 114.56 | 109.68 |
| 15 | B | 2002 | PQN | C9-C10-C5 | 2.14 | 121.64 | 119.26 |
| 17 | Z | 524 | BCR | C15-C16-C17 | -2.14 | 119.10 | 123.47 |
| 17 | G | 4002 | BCR | C27-C26-C25 | -2.14 | 119.63 | 122.73 |
| 17 | t | 522 | BCR | C27-C26-C25 | -2.14 | 119.63 | 122.73 |
| 14 | v | 509 | CLA | O2A-CGA-O1A | -2.14 | 117.97 | 123.30 |
| 14 | B | 1224 | CLA | C2A-C1A-CHA | 2.14 | 127.59 | 123.86 |
| 14 | e | 1107 | CLA | O2D-CGD-O1D | -2.14 | 119.66 | 123.84 |
| 17 | V | 4019 | BCR | C38-C26-C27 | 2.14 | 117.72 | 113.62 |
| 17 | L | 4019 | BCR | C21-C20-C19 | -2.14 | 116.55 | 123.22 |
| 17 | T | 4012 | BCR | C15-C14-C13 | -2.14 | 124.26 | 127.31 |
| 14 | 6 | 501 | CLA | O2D-CGD-CBD | 2.14 | 115.06 | 111.27 |
| 17 | b | 523 | BCR | C8-C9-C10 | -2.14 | 115.66 | 118.94 |
| 17 | n | 4219 | BCR | C19-C18-C17 | -2.14 | 115.66 | 118.94 |
| 14 | e | 1112 | CLA | C2A-C1A-CHA | 2.14 | 127.59 | 123.86 |
| 17 | Z | 522 | BCR | C30-C25-C26 | -2.13 | 119.61 | 122.61 |
| 14 | 3 | 505 | CLA | C2D-C1D-ND | -2.13 | 108.53 | 110.10 |
| 14 | e | 1130 | CLA | C2D-C1D-ND | -2.13 | 108.53 | 110.10 |
| 17 | 2 | 524 | BCR | C15-C16-C17 | -2.13 | 119.10 | 123.47 |
| 17 | Y | 524 | BCR | C1-C6-C7 | 2.13 | 121.82 | 115.78 |
| 14 | 1 | 504 | CLA | CAC-C3C-C4C | 2.13 | 127.58 | 124.81 |
| 14 | A | 1013 | CLA | CHD-C1D-ND | -2.13 | 122.49 | 124.45 |
| 14 | B | 1226 | CLA | C3D-C2D-C1D | 2.13 | 108.74 | 105.83 |
| 17 | 4 | 522 | BCR | C27-C26-C25 | -2.13 | 119.63 | 122.73 |
| 14 | c | 503 | CLA | CHD-C1D-ND | -2.13 | 122.49 | 124.45 |
| 18 | f | 1855 | LHG | C29-C28-C27 | -2.13 | 103.60 | 114.42 |
| 14 | A | 1101 | CLA | CAC-C3C-C4C | 2.13 | 127.58 | 124.81 |
| 17 | n | 4019 | BCR | C21-C20-C19 | -2.13 | 116.56 | 123.22 |
| 14 | 1 | 503 | CLA | C2A-C1A-CHA | 2.13 | 127.59 | 123.86 |
| 14 | f | 1206 | CLA | C3C-C4C-NC | -2.13 | 108.18 | 110.57 |
| 14 | e | 1101 | CLA | CAC-C3C-C4C | 2.13 | 127.58 | 124.81 |
| 14 | a | 503 | CLA | C2D-C1D-ND | -2.13 | 108.53 | 110.10 |
| 14 | H | 1219 | CLA | O2D-CGD-CBD | 2.13 | 115.06 | 111.27 |
| 17 | q | 524 | BCR | C3-C4-C5 | -2.13 | 110.27 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 5 | 523 | BCR | C34-C9-C8 | 2.13 | 121.43 | 118.08 |
| 14 | b | 507 | CLA | O2D-CGD-CBD | 2.13 | 115.05 | 111.27 |
| 14 | B | 1228 | CLA | O2A-CGA-O1A | -2.13 | 118.22 | 123.59 |
| 14 | 1 | 507 | CLA | O2A-CGA-O1A | -2.13 | 117.99 | 123.30 |
| 17 | q | 524 | BCR | C10-C11-C12 | -2.13 | 116.57 | 123.22 |
| 14 | f | 1228 | CLA | O2A-CGA-O1A | -2.13 | 118.22 | 123.59 |
| 14 | Z | 506 | CLA | O2A-CGA-O1A | -2.13 | 117.99 | 123.30 |
| 17 | 1 | 524 | BCR | C10-C11-C12 | -2.13 | 116.57 | 123.22 |
| 14 | G | 1108 | CLA | C1-C2-C3 | -2.13 | 122.36 | 126.04 |
| 14 | 5 | 504 | CLA | C1B-CHB-C4A | -2.13 | 125.90 | 130.12 |
| 17 | V | 4019 | BCR | C21-C20-C19 | -2.13 | 116.57 | 123.22 |
| 17 | q | 524 | BCR | C1-C6-C7 | 2.13 | 121.80 | 115.78 |
| 14 | 6 | 509 | CLA | O2A-CGA-O1A | -2.13 | 117.99 | 123.30 |
| 18 | B | 1855 | LHG | C29-C28-C27 | -2.13 | 103.62 | 114.42 |
| 14 | 3 | 512 | CLA | CHB-C4A-NA | 2.13 | 127.45 | 124.51 |
| 14 | e | 1110 | CLA | O2A-CGA-O1A | -2.13 | 118.22 | 123.59 |
| 14 | A | 1126 | CLA | C2A-C1A-CHA | 2.13 | 127.58 | 123.86 |
| 14 | 5 | 504 | CLA | C2A-C1A-CHA | 2.13 | 127.58 | 123.86 |
| 14 | Z | 507 | CLA | CHA-C1A-NA | -2.13 | 121.53 | 126.40 |
| 17 | n | 4022 | BCR | C28-C27-C26 | -2.13 | 110.28 | 114.08 |
| 14 | H | 1206 | CLA | C3C-C4C-NC | -2.13 | 108.19 | 110.57 |
| 14 | 1 | 516 | CLA | CHD-C1D-ND | -2.13 | 122.50 | 124.45 |
| 14 | Y | 504 | CLA | CAC-C3C-C4C | 2.13 | 127.57 | 124.81 |
| 14 | G | 1115 | CLA | C4-C3-C5 | 2.13 | 118.85 | 115.27 |
| 17 | 1 | 524 | BCR | C1-C6-C7 | 2.13 | 121.80 | 115.78 |
| 17 | c | 523 | BCR | C34-C9-C8 | 2.13 | 121.43 | 118.08 |
| 17 | H | 4014 | BCR | C29-C30-C25 | 2.13 | 113.75 | 110.48 |
| 14 | A | 1140 | CLA | O2D-CGD-CBD | 2.13 | 115.05 | 111.27 |
| 14 | 3 | 503 | CLA | C2D-C1D-ND | -2.13 | 108.54 | 110.10 |
| 14 | f | 1238 | CLA | O2A-CGA-O1A | -2.13 | 118.23 | 123.59 |
| 14 | e | 1121 | CLA | C1-C2-C3 | -2.13 | 122.37 | 126.04 |
| 14 | v | 508 | CLA | O2A-CGA-O1A | -2.13 | 118.00 | 123.30 |
| 14 | A | 1104 | CLA | C1B-CHB-C4A | -2.13 | 125.91 | 130.12 |
| 17 | l | 4012 | BCR | C15-C14-C13 | -2.13 | 124.28 | 127.31 |
| 17 | 6 | 524 | BCR | C36-C18-C19 | 2.13 | 121.43 | 118.08 |
| 14 | u | 504 | CLA | C1B-CHB-C4A | -2.13 | 125.91 | 130.12 |
| 14 | d | 507 | CLA | CHA-C1A-NA | -2.13 | 121.53 | 126.40 |
| 19 | A | 1848 | LMU | C2'-C3'-C4' | 2.13 | 114.53 | 109.68 |
| 14 | B | 1219 | CLA | O2D-CGD-CBD | 2.12 | 115.04 | 111.27 |
| 17 | d | 524 | BCR | C36-C18-C19 | 2.12 | 121.42 | 118.08 |
| 14 | f | 1224 | CLA | C2A-C1A-CHA | 2.12 | 127.57 | 123.86 |
| 14 | A | 1122 | CLA | O2A-CGA-O1A | -2.12 | 118.23 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | G | 1110 | CLA | O2A-CGA-O1A | -2.12 | 118.23 | 123.59 |
| 14 | q | 507 | CLA | O2A-CGA-O1A | -2.12 | 118.00 | 123.30 |
| 14 | A | 1108 | CLA | C1-C2-C3 | -2.12 | 122.37 | 126.04 |
| 14 | G | 1140 | CLA | O2D-CGD-CBD | 2.12 | 115.04 | 111.27 |
| 17 | 6 | 524 | BCR | C23-C22-C21 | -2.12 | 115.68 | 118.94 |
| 14 | A | 1110 | CLA | O2A-CGA-O1A | -2.12 | 118.23 | 123.59 |
| 14 | f | 1219 | CLA | C2D-C1D-ND | -2.12 | 108.54 | 110.10 |
| 14 | A | 1104 | CLA | O2D-CGD-O1D | -2.12 | 119.69 | 123.84 |
| 14 | B | 1234 | CLA | CHA-C1A-NA | -2.12 | 121.53 | 126.40 |
| 14 | e | 1122 | CLA | O2A-CGA-O1A | -2.12 | 118.23 | 123.59 |
| 17 | t | 523 | BCR | C8-C9-C10 | -2.12 | 115.68 | 118.94 |
| 14 | T | 1302 | CLA | C2A-C1A-CHA | 2.12 | 127.57 | 123.86 |
| 18 | H | 1855 | LHG | C29-C28-C27 | -2.12 | 103.65 | 114.42 |
| 15 | H | 2002 | PQN | C9-C10-C5 | 2.12 | 121.62 | 119.26 |
| 17 | d | 524 | BCR | C33-C5-C4 | 2.12 | 117.69 | 113.62 |
| 14 | B | 1206 | CLA | C3C-C4C-NC | -2.12 | 108.19 | 110.57 |
| 14 | B | 1201 | CLA | C6-C7-C8 | -2.12 | 109.06 | 115.92 |
| 14 | e | 1137 | CLA | C3A-C2A-C1A | 2.12 | 104.52 | 101.34 |
| 14 | H | 1224 | CLA | C2A-C1A-CHA | 2.12 | 127.57 | 123.86 |
| 14 | e | 1119 | CLA | O2A-CGA-O1A | -2.12 | 118.24 | 123.59 |
| 14 | e | 1108 | CLA | C1-C2-C3 | -2.12 | 122.37 | 126.04 |
| 14 | r | 506 | CLA | O2A-CGA-O1A | -2.12 | 118.01 | 123.30 |
| 14 | 1 | 517 | CLA | O2A-CGA-O1A | -2.12 | 118.01 | 123.30 |
| 18 | A | 5001 | LHG | O10-C23-C24 | -2.12 | 115.46 | 123.73 |
| 14 | 3 | 502 | CLA | CAA-C2A-C3A | -2.12 | 106.97 | 112.78 |
| 14 | 2 | 507 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 14 | f | 1219 | CLA | O2D-CGD-CBD | 2.12 | 115.03 | 111.27 |
| 17 | v | 524 | BCR | C36-C18-C19 | 2.12 | 121.42 | 118.08 |
| 14 | Z | 503 | CLA | C2D-C1D-ND | -2.12 | 108.54 | 110.10 |
| 14 | f | 1201 | CLA | C6-C7-C8 | -2.12 | 109.07 | 115.92 |
| 17 | b | 522 | BCR | C27-C26-C25 | -2.12 | 119.65 | 122.73 |
| 18 | G | 5001 | LHG | O10-C23-C24 | -2.12 | 115.46 | 123.73 |
| 17 | d | 524 | BCR | C23-C22-C21 | -2.12 | 115.69 | 118.94 |
| 14 | 2 | 506 | CLA | O2A-CGA-O1A | -2.12 | 118.02 | 123.30 |
| 19 | G | 1848 | LMU | C2'-C3'-C4' | 2.12 | 114.52 | 109.68 |
| 17 | J | 4012 | BCR | C2-C1-C6 | 2.12 | 113.74 | 110.48 |
| 17 | J | 4012 | BCR | C15-C14-C13 | -2.12 | 124.29 | 127.31 |
| 14 | Y | 503 | CLA | C2A-C1A-CHA | 2.12 | 127.56 | 123.86 |
| 14 | b | 502 | CLA | CMB-C2B-C3B | 2.12 | 128.64 | 124.68 |
| 14 | 6 | 508 | CLA | CHD-C1D-ND | -2.12 | 122.51 | 124.45 |
| 14 | B | 1238 | CLA | O2A-CGA-O1A | -2.12 | 118.25 | 123.59 |
| 14 | 5 | 502 | CLA | C2A-C1A-CHA | 2.12 | 127.56 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | e | 4002 | BCR | C27-C26-C25 | -2.12 | 119.66 | 122.73 |
| 14 | c | 501 | CLA | C2A-C1A-CHA | 2.12 | 127.56 | 123.86 |
| 14 | u | 504 | CLA | C2A-C1A-CHA | 2.12 | 127.56 | 123.86 |
| 17 | 4 | 523 | BCR | C8-C9-C10 | -2.12 | 115.69 | 118.94 |
| 14 | 3 | 502 | CLA | C2A-C1A-CHA | 2.12 | 127.56 | 123.86 |
| 17 | n | 4219 | BCR | C16-C15-C14 | -2.12 | 119.14 | 123.47 |
| 14 | r | 507 | CLA | CHA-C1A-NA | -2.12 | 121.55 | 126.40 |
| 14 | s | 509 | CLA | O1A-CGA-CBA | 2.12 | 129.88 | 123.08 |
| 14 | c | 504 | CLA | C1B-CHB-C4A | -2.12 | 125.93 | 130.12 |
| 17 | r | 522 | BCR | C33-C5-C4 | 2.12 | 117.68 | 113.62 |
| 17 | l | 522 | BCR | C16-C17-C18 | -2.12 | 124.29 | 127.31 |
| 17 | b | 524 | BCR | C28-C27-C26 | -2.12 | 110.30 | 114.08 |
| 14 | f | 1231 | CLA | CMA-C3A-C2A | -2.12 | 105.30 | 113.83 |
| 17 | 6 | 524 | BCR | C33-C5-C4 | 2.12 | 117.68 | 113.62 |
| 14 | e | 1126 | CLA | C2A-C1A-CHA | 2.11 | 127.56 | 123.86 |
| 14 | B | 1231 | CLA | CMA-C3A-C2A | -2.11 | 105.30 | 113.83 |
| 14 | G | 1121 | CLA | C1-C2-C3 | -2.11 | 122.39 | 126.04 |
| 15 | f | 2002 | PQN | C9-C10-C5 | 2.11 | 121.61 | 119.26 |
| 14 | a | 502 | CLA | CAA-C2A-C3A | -2.11 | 106.99 | 112.78 |
| 14 | s | 502 | CLA | CAA-C2A-C3A | -2.11 | 106.99 | 112.78 |
| 14 | H | 1234 | CLA | CHA-C1A-NA | -2.11 | 121.56 | 126.40 |
| 14 | H | 1235 | CLA | O2D-CGD-CBD | 2.11 | 115.02 | 111.27 |
| 14 | H | 1231 | CLA | CMA-C3A-C2A | -2.11 | 105.30 | 113.83 |
| 14 | e | 1140 | CLA | O2D-CGD-CBD | 2.11 | 115.02 | 111.27 |
| 17 | A | 4002 | BCR | C27-C26-C25 | -2.11 | 119.66 | 122.73 |
| 17 | 4 | 524 | BCR | C28-C27-C26 | -2.11 | 110.30 | 114.08 |
| 14 | H | 1201 | CLA | C6-C7-C8 | -2.11 | 109.09 | 115.92 |
| 14 | f | 1235 | CLA | O2D-CGD-CBD | 2.11 | 115.02 | 111.27 |
| 17 | v | 524 | BCR | C33-C5-C4 | 2.11 | 117.67 | 113.62 |
| 14 | A | 1022 | CLA | CHD-C1D-ND | -2.11 | 122.51 | 124.45 |
| 14 | e | 1013 | CLA | CHD-C1D-ND | -2.11 | 122.51 | 124.45 |
| 14 | r | 502 | CLA | C2A-C1A-CHA | 2.11 | 127.55 | 123.86 |
| 14 | Y | 517 | CLA | O2A-CGA-O1A | -2.11 | 118.03 | 123.30 |
| 14 | B | 1235 | CLA | O2D-CGD-CBD | 2.11 | 115.02 | 111.27 |
| 14 | B | 1216 | CLA | C2D-C1D-ND | -2.11 | 108.55 | 110.10 |
| 14 | s | 502 | CLA | C2A-C1A-CHA | 2.11 | 127.55 | 123.86 |
| 14 | e | 1104 | CLA | O2D-CGD-O1D | -2.11 | 119.71 | 123.84 |
| 14 | 5 | 503 | CLA | CHD-C1D-ND | -2.11 | 122.51 | 124.45 |
| 14 | e | 1112 | CLA | O2D-CGD-CBD | 2.11 | 115.02 | 111.27 |
| 14 | 5 | 501 | CLA | C2A-C1A-CHA | 2.11 | 127.55 | 123.86 |
| 14 | 2 | 519 | CLA | O2A-CGA-O1A | -2.11 | 118.04 | 123.30 |
| 17 | 2 | 522 | BCR | C30-C25-C26 | -2.11 | 119.64 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | b | 504 | CLA | CHD-C1D-ND | -2.11 | 122.52 | 124.45 |
| 14 | Y | 513 | CLA | O2A-CGA-O1A | -2.11 | 118.04 | 123.30 |
| 14 | q | 502 | CLA | CAA-C2A-C3A | -2.11 | 107.00 | 112.78 |
| 14 | A | 1119 | CLA | O2A-CGA-O1A | -2.11 | 118.27 | 123.59 |
| 14 | B | 1224 | CLA | O2A-CGA-O1A | -2.11 | 118.27 | 123.59 |
| 14 | G | 1022 | CLA | C4D-C3D-CAD | -2.11 | 105.61 | 108.10 |
| 14 | G | 1101 | CLA | CAC-C3C-C4C | 2.11 | 127.55 | 124.81 |
| 14 | 3 | 509 | CLA | O1A-CGA-CBA | 2.11 | 129.85 | 123.08 |
| 14 | q | 517 | CLA | O2A-CGA-O1A | -2.11 | 118.04 | 123.30 |
| 14 | H | 1224 | CLA | O2A-CGA-O1A | -2.11 | 118.27 | 123.59 |
| 14 | f | 1234 | CLA | CHA-C1A-NA | -2.11 | 121.57 | 126.40 |
| 14 | v | 508 | CLA | CHD-C1D-ND | -2.11 | 122.52 | 124.45 |
| 18 | e | 5001 | LHG | O10-C23-C24 | -2.11 | 115.51 | 123.73 |
| 14 | u | 503 | CLA | C2A-C1A-CHA | 2.11 | 127.54 | 123.86 |
| 17 | G | 4001 | BCR | C37-C22-C21 | -2.11 | 119.97 | 122.92 |
| 14 | f | 1012 | CLA | C4-C3-C5 | 2.11 | 118.82 | 115.27 |
| 17 | 2 | 522 | BCR | C33-C5-C4 | 2.11 | 117.66 | 113.62 |
| 17 | A | 4001 | BCR | C37-C22-C21 | -2.11 | 119.97 | 122.92 |
| 14 | s | 511 | CLA | CAA-C2A-C3A | -2.11 | 107.01 | 112.78 |
| 14 | Y | 512 | CLA | CHB-C4A-NA | 2.11 | 127.42 | 124.51 |
| 14 | f | 1218 | CLA | C1B-CHB-C4A | -2.11 | 125.94 | 130.12 |
| 14 | H | 1238 | CLA | C2D-C1D-ND | -2.11 | 108.55 | 110.10 |
| 14 | Z | 519 | CLA | O2A-CGA-O1A | -2.11 | 118.05 | 123.30 |
| 17 | a | 523 | BCR | C21-C20-C19 | -2.11 | 116.64 | 123.22 |
| 14 | a | 502 | CLA | C2A-C1A-CHA | 2.11 | 127.54 | 123.86 |
| 14 | e | 1122 | CLA | CHD-C1D-ND | -2.11 | 122.52 | 124.45 |
| 14 | G | 1104 | CLA | O2D-CGD-O1D | -2.11 | 119.72 | 123.84 |
| 14 | a | 511 | CLA | CAA-C2A-C3A | -2.11 | 107.01 | 112.78 |
| 14 | B | 1226 | CLA | O2A-CGA-O1A | -2.11 | 118.28 | 123.59 |
| 14 | f | 1222 | CLA | O2A-CGA-O1A | -2.11 | 118.28 | 123.59 |
| 14 | G | 1126 | CLA | C2A-C1A-CHA | 2.11 | 127.54 | 123.86 |
| 14 | r | 502 | CLA | O2A-CGA-O1A | -2.10 | 118.05 | 123.30 |
| 17 | 3 | 523 | BCR | C21-C20-C19 | -2.10 | 116.65 | 123.22 |
| 14 | H | 1218 | CLA | C1B-CHB-C4A | -2.10 | 125.95 | 130.12 |
| 18 | A | 5002 | LHG | C27-C26-C25 | -2.10 | 103.74 | 114.42 |
| 17 | Z | 522 | BCR | C33-C5-C4 | 2.10 | 117.66 | 113.62 |
| 18 | e | 5002 | LHG | C27-C26-C25 | -2.10 | 103.74 | 114.42 |
| 14 | r | 519 | CLA | O2A-CGA-O1A | -2.10 | 118.06 | 123.30 |
| 14 | f | 1226 | CLA | O2A-CGA-O1A | -2.10 | 118.28 | 123.59 |
| 14 | u | 503 | CLA | O2A-CGA-O1A | -2.10 | 118.06 | 123.30 |
| 17 | 5 | 523 | BCR | C8-C7-C6 | -2.10 | 121.30 | 127.20 |
| 17 | L | 4022 | BCR | C28-C27-C26 | -2.10 | 110.32 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | 5 | 511 | CLA | O2A-CGA-O1A | -2.10 | 118.06 | 123.30 |
| 14 | Z | 519 | CLA | CHD-C1D-ND | -2.10 | 122.52 | 124.45 |
| 17 | a | 522 | BCR | C27-C26-C25 | -2.10 | 119.68 | 122.73 |
| 17 | t | 522 | BCR | C36-C18-C19 | 2.10 | 121.39 | 118.08 |
| 14 | r | 508 | CLA | C2D-C1D-ND | -2.10 | 108.56 | 110.10 |
| 17 | b | 522 | BCR | C30-C25-C26 | -2.10 | 119.65 | 122.61 |
| 19 | H | 1843 | LMU | C3-C2-C1 | -2.10 | 104.17 | 113.49 |
| 17 | s | 523 | BCR | C21-C20-C19 | -2.10 | 116.66 | 123.22 |
| 14 | A | 1121 | CLA | C1-C2-C3 | -2.10 | 122.41 | 126.04 |
| 14 | H | 1232 | CLA | O2A-CGA-O1A | -2.10 | 118.29 | 123.59 |
| 14 | T | 1303 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 14 | 1 | 513 | CLA | O2A-CGA-O1A | -2.10 | 118.06 | 123.30 |
| 14 | G | 1104 | CLA | C1B-CHB-C4A | -2.10 | 125.96 | 130.12 |
| 14 | q | 516 | CLA | CHD-C1D-ND | -2.10 | 122.52 | 124.45 |
| 14 | t | 504 | CLA | CHD-C1D-ND | -2.10 | 122.52 | 124.45 |
| 14 | H | 1226 | CLA | O2A-CGA-O1A | -2.10 | 118.29 | 123.59 |
| 14 | 2 | 502 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 14 | c | 502 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 14 | t | 517 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 14 | c | 511 | CLA | O2A-CGA-O1A | -2.10 | 118.06 | 123.30 |
| 14 | A | 1140 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 14 | G | 1119 | CLA | O2A-CGA-O1A | -2.10 | 118.29 | 123.59 |
| 14 | a | 509 | CLA | O1A-CGA-CBA | 2.10 | 129.82 | 123.08 |
| 14 | 3 | 501 | CLA | CHD-C1D-ND | -2.10 | 122.53 | 124.45 |
| 17 | u | 523 | BCR | C8-C7-C6 | -2.10 | 121.31 | 127.20 |
| 14 | Z | 508 | CLA | CHC-C1C-NC | 2.10 | 127.39 | 124.20 |
| 17 | k | 4018 | BCR | C31-C1-C6 | -2.10 | 106.89 | 110.30 |
| 17 | A | 4011 | BCR | C16-C15-C14 | -2.10 | 119.17 | 123.47 |
| 17 | 4 | 524 | BCR | C16-C15-C14 | -2.10 | 119.17 | 123.47 |
| 14 | H | 1222 | CLA | O2A-CGA-O1A | -2.10 | 118.30 | 123.59 |
| 21 | H | 1852 | SQD | C3-C4-C5 | 2.10 | 113.98 | 110.24 |
| 14 | A | 1115 | CLA | C4-C3-C5 | 2.10 | 118.80 | 115.27 |
| 14 | u | 501 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 17 | t | 522 | BCR | C30-C25-C26 | -2.10 | 119.66 | 122.61 |
| 14 | A | 1129 | CLA | O2A-CGA-O1A | -2.10 | 118.30 | 123.59 |
| 14 | f | 1224 | CLA | O2A-CGA-O1A | -2.10 | 118.30 | 123.59 |
| 14 | 1 | 502 | CLA | CAA-C2A-C3A | -2.10 | 107.03 | 112.78 |
| 14 | V | 1501 | CLA | O2A-CGA-O1A | -2.10 | 118.30 | 123.59 |
| 14 | 5 | 503 | CLA | C2A-C1A-CHA | 2.10 | 127.53 | 123.86 |
| 14 | 3 | 511 | CLA | CAA-C2A-C3A | -2.10 | 107.03 | 112.78 |
| 20 | f | 5002 | LMG | C31-C30-C29 | -2.10 | 105.65 | 113.19 |
| 17 | 4 | 522 | BCR | C30-C25-C26 | -2.10 | 119.66 | 122.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19 | f | 1843 | LMU | C3-C2-C1 | -2.10 | 104.20 | 113.49 |
| 20 | B | 5002 | LMG | C31-C30-C29 | -2.10 | 105.65 | 113.19 |
| 14 | 2 | 502 | CLA | O2A-CGA-O1A | -2.10 | 118.07 | 123.30 |
| 17 | H | 4005 | BCR | C16-C15-C14 | -2.10 | 119.18 | 123.47 |
| 18 | G | 5002 | LHG | C27-C26-C25 | -2.10 | 103.78 | 114.42 |
| 14 | q | 513 | CLA | O2A-CGA-O1A | -2.10 | 118.08 | 123.30 |
| 14 | e | 1115 | CLA | C4-C3-C5 | 2.10 | 118.80 | 115.27 |
| 14 | 4 | 507 | CLA | C2A-C1A-CHA | 2.10 | 127.52 | 123.86 |
| 14 | c | 503 | CLA | C2A-C1A-CHA | 2.10 | 127.52 | 123.86 |
| 14 | e | 1125 | CLA | C11-C12-C13 | -2.10 | 109.15 | 115.92 |
| 14 | G | 1112 | CLA | O2D-CGD-CBD | 2.10 | 114.99 | 111.27 |
| 14 | 2 | 507 | CLA | O2A-CGA-O1A | -2.10 | 118.08 | 123.30 |
| 14 | e | 1022 | CLA | CHD-C1D-ND | -2.09 | 122.53 | 124.45 |
| 14 | B | 1222 | CLA | O2A-CGA-O1A | -2.09 | 118.31 | 123.59 |
| 14 | G | 1140 | CLA | C2A-C1A-CHA | 2.09 | 127.52 | 123.86 |
| 20 | H | 5002 | LMG | C31-C30-C29 | -2.09 | 105.67 | 113.19 |
| 14 | A | 1125 | CLA | C11-C12-C13 | -2.09 | 109.16 | 115.92 |
| 17 | c | 523 | BCR | C8-C7-C6 | -2.09 | 121.33 | 127.20 |
| 14 | 4 | 502 | CLA | CMB-C2B-C3B | 2.09 | 128.59 | 124.68 |
| 17 | B | 4005 | BCR | C16-C15-C14 | -2.09 | 119.19 | 123.47 |
| 14 | f | 1206 | CLA | O1D-CGD-CBD | 2.09 | 128.76 | 124.48 |
| 14 | l | 1303 | CLA | C2A-C1A-CHA | 2.09 | 127.52 | 123.86 |
| 14 | H | 1219 | CLA | C1-O2A-CGA | 2.09 | 121.93 | 116.44 |
| 19 | B | 1843 | LMU | C3-C2-C1 | -2.09 | 104.22 | 113.49 |
| 14 | u | 511 | CLA | O2A-CGA-O1A | -2.09 | 118.09 | 123.30 |
| 14 | A | 1122 | CLA | CHD-C1D-ND | -2.09 | 122.53 | 124.45 |
| 14 | 2 | 508 | CLA | CHC-C1C-NC | 2.09 | 127.38 | 124.20 |
| 14 | e | 1120 | CLA | O2A-CGA-O1A | -2.09 | 118.31 | 123.59 |
| 17 | l | 4012 | BCR | C2-C1-C6 | 2.09 | 113.70 | 110.48 |
| 14 | B | 1216 | CLA | CAA-CBA-CGA | -2.09 | 107.14 | 113.25 |
| 14 | H | 1226 | CLA | CHB-C4A-NA | 2.09 | 127.40 | 124.51 |
| 14 | f | 1216 | CLA | CAA-CBA-CGA | -2.09 | 107.15 | 113.25 |
| 14 | A | 1112 | CLA | O2D-CGD-CBD | 2.09 | 114.98 | 111.27 |
| 14 | a | 504 | CLA | CAA-C2A-C3A | -2.09 | 107.06 | 112.78 |
| 14 | B | 1219 | CLA | C1-O2A-CGA | 2.09 | 121.93 | 116.44 |
| 17 | f | 4017 | BCR | C8-C7-C6 | -2.09 | 121.33 | 127.20 |
| 14 | 4 | 517 | CLA | C2A-C1A-CHA | 2.09 | 127.51 | 123.86 |
| 14 | b | 517 | CLA | C2A-C1A-CHA | 2.09 | 127.51 | 123.86 |
| 14 | A | 1013 | CLA | C11-C12-C13 | -2.09 | 109.17 | 115.92 |
| 17 | f | 4004 | BCR | C34-C9-C8 | 2.09 | 121.37 | 118.08 |
| 18 | n | 5220 | LHG | C27-C26-C25 | -2.09 | 103.82 | 114.42 |
| 17 | f | 4004 | BCR | C11-C12-C13 | -2.09 | 120.55 | 126.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | B | 1208 | CLA | CHD-C1D-ND | -2.09 | 122.53 | 124.45 |
| 14 | H | 1216 | CLA | CAA-CBA-CGA | -2.09 | 107.15 | 113.25 |
| 14 | t | 507 | CLA | C2A-C1A-CHA | 2.09 | 127.51 | 123.86 |
| 14 | Z | 507 | CLA | O2A-CGA-O1A | -2.09 | 118.09 | 123.30 |
| 14 | B | 1218 | CLA | C1B-CHB-C4A | -2.09 | 125.98 | 130.12 |
| 18 | L | 5220 | LHG | C27-C26-C25 | -2.09 | 103.83 | 114.42 |
| 18 | V | 5220 | LHG | C27-C26-C25 | -2.09 | 103.83 | 114.42 |
| 14 | 1 | 512 | CLA | CHB-C4A-NA | 2.09 | 127.40 | 124.51 |
| 14 | 6 | 505 | CLA | C2D-C1D-ND | -2.09 | 108.57 | 110.10 |
| 14 | G | 1129 | CLA | O2A-CGA-O1A | -2.09 | 118.33 | 123.59 |
| 14 | J | 1303 | CLA | C2A-C1A-CHA | 2.09 | 127.51 | 123.86 |
| 14 | f | 1219 | CLA | C1-O2A-CGA | 2.09 | 121.92 | 116.44 |
| 14 | Z | 502 | CLA | O2A-CGA-O1A | -2.09 | 118.10 | 123.30 |
| 17 | B | 4017 | BCR | C8-C7-C6 | -2.09 | 121.34 | 127.20 |
| 14 | f | 1232 | CLA | O2A-CGA-O1A | -2.09 | 118.33 | 123.59 |
| 17 | a | 524 | BCR | C23-C22-C21 | -2.09 | 115.74 | 118.94 |
| 14 | H | 1208 | CLA | CHD-C1D-ND | -2.09 | 122.54 | 124.45 |
| 14 | e | 1101 | CLA | C1-O2A-CGA | -2.09 | 110.97 | 116.44 |
| 14 | Y | 502 | CLA | CAA-C2A-C3A | -2.09 | 107.07 | 112.78 |
| 14 | 4 | 504 | CLA | CHD-C1D-ND | -2.08 | 122.54 | 124.45 |
| 14 | e | 1130 | CLA | CHD-C1D-ND | -2.08 | 122.54 | 124.45 |
| 17 | 3 | 524 | BCR | C23-C22-C21 | -2.08 | 115.74 | 118.94 |
| 18 | e | 5003 | LHG | C18-C17-C16 | -2.08 | 103.84 | 114.42 |
| 14 | B | 1238 | CLA | O2A-C1-C2 | -2.08 | 103.16 | 108.64 |
| 14 | B | 1012 | CLA | C4-C3-C5 | 2.08 | 118.78 | 115.27 |
| 14 | G | 1101 | CLA | C1-O2A-CGA | -2.08 | 110.98 | 116.44 |
| 14 | r | 503 | CLA | CHD-C1D-ND | -2.08 | 122.54 | 124.45 |
| 14 | B | 1232 | CLA | O2A-CGA-O1A | -2.08 | 118.33 | 123.59 |
| 14 | r | 507 | CLA | O2A-CGA-O1A | -2.08 | 118.11 | 123.30 |
| 18 | A | 5003 | LHG | C18-C17-C16 | -2.08 | 103.85 | 114.42 |
| 14 | G | 1013 | CLA | C11-C12-C13 | -2.08 | 109.19 | 115.92 |
| 17 | T | 4015 | BCR | C37-C22-C23 | 2.08 | 121.36 | 118.08 |
| 17 | V | 4022 | BCR | C28-C27-C26 | -2.08 | 110.36 | 114.08 |
| 17 | n | 4219 | BCR | C32-C1-C6 | -2.08 | 106.92 | 110.30 |
| 17 | b | 524 | BCR | C16-C15-C14 | -2.08 | 119.21 | 123.47 |
| 17 | e | 4001 | BCR | C37-C22-C21 | -2.08 | 120.01 | 122.92 |
| 14 | G | 1120 | CLA | O2A-CGA-O1A | -2.08 | 118.34 | 123.59 |
| 14 | G | 1125 | CLA | C11-C12-C13 | -2.08 | 109.19 | 115.92 |
| 14 | e | 1013 | CLA | C11-C12-C13 | -2.08 | 109.19 | 115.92 |
| 14 | H | 1238 | CLA | O2A-C1-C2 | -2.08 | 103.16 | 108.64 |
| 14 | B | 1021 | CLA | O1D-CGD-CBD | 2.08 | 128.74 | 124.48 |
| 14 | b | 507 | CLA | C2A-C1A-CHA | 2.08 | 127.50 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1238 | CLA | O2A-C1-C2 | -2.08 | 103.16 | 108.64 |
| 14 | Y | 516 | CLA | CHD-C1D-ND | -2.08 | 122.54 | 124.45 |
| 14 | 2 | 503 | CLA | C2D-C1D-ND | -2.08 | 108.57 | 110.10 |
| 17 | b | 522 | BCR | C36-C18-C19 | 2.08 | 121.36 | 118.08 |
| 14 | H | 1206 | CLA | O1D-CGD-CBD | 2.08 | 128.74 | 124.48 |
| 14 | e | 1129 | CLA | O2A-CGA-O1A | -2.08 | 118.34 | 123.59 |
| 14 | 3 | 504 | CLA | CAA-C2A-C3A | -2.08 | 107.08 | 112.78 |
| 14 | H | 1226 | CLA | CMC-C2C-C3C | 2.08 | 131.76 | 126.12 |
| 14 | u | 502 | CLA | C2A-C1A-CHA | 2.08 | 127.50 | 123.86 |
| 17 | H | 4004 | BCR | C11-C12-C13 | -2.08 | 120.57 | 126.42 |
| 14 | c | 503 | CLA | O2A-CGA-O1A | -2.08 | 118.11 | 123.30 |
| 14 | A | 1120 | CLA | O2A-CGA-O1A | -2.08 | 118.34 | 123.59 |
| 14 | 5 | 503 | CLA | O2A-CGA-O1A | -2.08 | 118.11 | 123.30 |
| 17 | Z | 523 | BCR | C8-C7-C6 | -2.08 | 121.36 | 127.20 |
| 14 | s | 504 | CLA | CAA-C2A-C3A | -2.08 | 107.08 | 112.78 |
| 17 | T | 4012 | BCR | C23-C22-C21 | 2.08 | 122.13 | 118.94 |
| 17 | r | 523 | BCR | C8-C7-C6 | -2.08 | 121.36 | 127.20 |
| 14 | 2 | 517 | CLA | O2A-CGA-O1A | -2.08 | 118.12 | 123.30 |
| 17 | B | 4004 | BCR | C11-C12-C13 | -2.08 | 120.58 | 126.42 |
| 14 | q | 502 | CLA | O2A-CGA-O1A | -2.08 | 118.12 | 123.30 |
| 14 | v | 508 | CLA | CHC-C1C-NC | 2.08 | 127.36 | 124.20 |
| 14 | B | 1221 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 14 | f | 1221 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 17 | f | 4005 | BCR | C16-C15-C14 | -2.08 | 119.22 | 123.47 |
| 17 | H | 4017 | BCR | C8-C7-C6 | -2.08 | 121.37 | 127.20 |
| 17 | d | 522 | BCR | C30-C25-C26 | -2.08 | 119.69 | 122.61 |
| 14 | r | 508 | CLA | CHC-C1C-NC | 2.08 | 127.35 | 124.20 |
| 14 | Y | 502 | CLA | O2A-CGA-O1A | -2.08 | 118.12 | 123.30 |
| 14 | G | 1104 | CLA | C2A-C1A-CHA | 2.08 | 127.49 | 123.86 |
| 18 | G | 5003 | LHG | C18-C17-C16 | -2.08 | 103.89 | 114.42 |
| 17 | t | 524 | BCR | C16-C15-C14 | -2.08 | 119.22 | 123.47 |
| 18 | e | 5008 | LHG | C27-C26-C25 | -2.08 | 103.89 | 114.42 |
| 14 | t | 511 | CLA | CHD-C1D-ND | -2.08 | 122.55 | 124.45 |
| 18 | A | 5008 | LHG | C27-C26-C25 | -2.07 | 103.89 | 114.42 |
| 14 | f | 1236 | CLA | CAA-CBA-CGA | -2.07 | 107.19 | 113.25 |
| 14 | n | 1501 | CLA | O2A-CGA-O1A | -2.07 | 118.36 | 123.59 |
| 14 | r | 517 | CLA | O2A-CGA-O1A | -2.07 | 118.13 | 123.30 |
| 17 | l | 4012 | BCR | C23-C22-C21 | 2.07 | 122.12 | 118.94 |
| 14 | e | 1140 | CLA | C2A-C1A-CHA | 2.07 | 127.49 | 123.86 |
| 17 | v | 522 | BCR | C30-C25-C26 | -2.07 | 119.69 | 122.61 |
| 17 | I | 4018 | BCR | C33-C5-C6 | -2.07 | 122.20 | 124.53 |
| 17 | I | 4018 | BCR | C31-C1-C6 | -2.07 | 106.94 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | e | 4011 | BCR | C16-C15-C14 | -2.07 | 119.23 | 123.47 |
| 14 | e | 1131 | CLA | C7-C6-C5 | -2.07 | 107.73 | 113.36 |
| 14 | f | 1226 | CLA | CHB-C4A-NA | 2.07 | 127.38 | 124.51 |
| 14 | 1 | 502 | CLA | O2A-CGA-O1A | -2.07 | 118.13 | 123.30 |
| 14 | a | 501 | CLA | CHD-C1D-ND | -2.07 | 122.55 | 124.45 |
| 17 | 4 | 522 | BCR | C36-C18-C19 | 2.07 | 121.34 | 118.08 |
| 14 | t | 502 | CLA | CMB-C2B-C3B | 2.07 | 128.56 | 124.68 |
| 14 | B | 1206 | CLA | O1D-CGD-CBD | 2.07 | 128.72 | 124.48 |
| 14 | Z | 518 | CLA | O2A-CGA-O1A | -2.07 | 118.36 | 123.59 |
| 17 | 2 | 523 | BCR | C34-C9-C8 | 2.07 | 121.34 | 118.08 |
| 14 | A | 1101 | CLA | C1-O2A-CGA | -2.07 | 111.01 | 116.44 |
| 14 | c | 507 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 14 | f | 1220 | CLA | CHD-C1D-ND | -2.07 | 122.55 | 124.45 |
| 14 | f | 1021 | CLA | O1D-CGD-CBD | 2.07 | 128.72 | 124.48 |
| 17 | J | 4015 | BCR | C37-C22-C23 | 2.07 | 121.34 | 118.08 |
| 18 | G | 5008 | LHG | C27-C26-C25 | -2.07 | 103.91 | 114.42 |
| 14 | L | 1501 | CLA | O2A-CGA-O1A | -2.07 | 118.36 | 123.59 |
| 14 | 6 | 508 | CLA | CHC-C1C-NC | 2.07 | 127.34 | 124.20 |
| 17 | 2 | 523 | BCR | C8-C7-C6 | -2.07 | 121.39 | 127.20 |
| 14 | 2 | 508 | CLA | C2D-C1D-ND | -2.07 | 108.58 | 110.10 |
| 14 | A | 1119 | CLA | C16-C15-C13 | -2.07 | 109.23 | 115.92 |
| 17 | G | 4011 | BCR | C16-C15-C14 | -2.07 | 119.23 | 123.47 |
| 17 | d | 523 | BCR | C15-C16-C17 | -2.07 | 119.23 | 123.47 |
| 17 | d | 524 | BCR | C16-C15-C14 | -2.07 | 119.23 | 123.47 |
| 14 | u | 518 | CLA | O2A-CGA-O1A | -2.07 | 118.14 | 123.30 |
| 14 | f | 1208 | CLA | CHD-C1D-ND | -2.07 | 122.55 | 124.45 |
| 14 | s | 503 | CLA | C2D-C1D-ND | -2.07 | 108.58 | 110.10 |
| 21 | B | 1852 | SQD | C3-C4-C5 | 2.07 | 113.93 | 110.24 |
| 14 | f | 1226 | CLA | CMC-C2C-C3C | 2.07 | 131.73 | 126.12 |
| 14 | H | 1221 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 14 | r | 505 | CLA | C2D-C1D-ND | -2.07 | 108.58 | 110.10 |
| 14 | u | 519 | CLA | O2A-CGA-O1A | -2.07 | 118.14 | 123.30 |
| 14 | G | 1120 | CLA | CHD-C1D-ND | -2.07 | 122.55 | 124.45 |
| 14 | 5 | 518 | CLA | O2A-CGA-O1A | -2.07 | 118.15 | 123.30 |
| 17 | d | 523 | BCR | C8-C7-C6 | -2.07 | 121.40 | 127.20 |
| 17 | v | 521 | BCR | C10-C11-C12 | -2.07 | 116.77 | 123.22 |
| 17 | V | 4020 | BCR | C33-C5-C4 | -2.07 | 109.65 | 113.62 |
| 17 | r | 521 | BCR | C39-C30-C25 | -2.07 | 106.95 | 110.30 |
| 17 | B | 4004 | BCR | C34-C9-C8 | 2.07 | 121.33 | 118.08 |
| 14 | j | 1302 | CLA | CAA-C2A-C3A | -2.07 | 107.12 | 112.78 |
| 14 | 2 | 519 | CLA | CHD-C1D-ND | -2.07 | 122.56 | 124.45 |
| 14 | B | 1226 | CLA | CMC-C2C-C3C | 2.07 | 131.73 | 126.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | A | 1022 | CLA | C4D-C3D-CAD | -2.07 | 105.66 | 108.10 |
| 14 | H | 1021 | CLA | O1D-CGD-CBD | 2.07 | 128.71 | 124.48 |
| 14 | A | 1127 | CLA | CHA-C1A-NA | -2.07 | 121.67 | 126.40 |
| 14 | G | 1114 | CLA | CAA-CBA-CGA | -2.07 | 107.03 | 112.51 |
| 14 | 2 | 503 | CLA | CHD-C1D-ND | -2.07 | 122.56 | 124.45 |
| 14 | t | 501 | CLA | CHD-C1D-ND | -2.07 | 122.56 | 124.45 |
| 14 | F | 1302 | CLA | CAA-C2A-C3A | -2.06 | 107.12 | 112.78 |
| 14 | G | 1127 | CLA | CHA-C1A-NA | -2.06 | 121.67 | 126.40 |
| 14 | B | 1236 | CLA | CAA-CBA-CGA | -2.06 | 107.22 | 113.25 |
| 17 | f | 4005 | BCR | C33-C5-C4 | 2.06 | 117.58 | 113.62 |
| 17 | J | 4012 | BCR | C23-C22-C21 | 2.06 | 122.11 | 118.94 |
| 17 | Y | 521 | BCR | C29-C30-C25 | 2.06 | 113.66 | 110.48 |
| 14 | A | 1119 | CLA | O2D-CGD-CBD | 2.06 | 114.94 | 111.27 |
| 14 | G | 1119 | CLA | O2D-CGD-CBD | 2.06 | 114.94 | 111.27 |
| 14 | Z | 508 | CLA | O1A-CGA-CBA | 2.06 | 129.71 | 123.08 |
| 19 | J | 5105 | LMU | C6'-C5'-C4' | -2.06 | 108.17 | 113.00 |
| 14 | c | 519 | CLA | O2A-CGA-O1A | -2.06 | 118.16 | 123.30 |
| 14 | G | 1119 | CLA | C16-C15-C13 | -2.06 | 109.25 | 115.92 |
| 17 | 6 | 524 | BCR | C16-C15-C14 | -2.06 | 119.25 | 123.47 |
| 14 | H | 1203 | CLA | CAA-C2A-C1A | -2.06 | 105.21 | 111.97 |
| 14 | 5 | 519 | CLA | O2A-CGA-O1A | -2.06 | 118.16 | 123.30 |
| 14 | H | 1206 | CLA | CHC-C1C-NC | 2.06 | 127.33 | 124.20 |
| 14 | q | 509 | CLA | O2A-CGA-O1A | -2.06 | 118.16 | 123.30 |
| 14 | G | 1107 | CLA | C2A-C1A-CHA | 2.06 | 127.47 | 123.86 |
| 18 | L | 5221 | LHG | C15-C14-C13 | -2.06 | 103.95 | 114.42 |
| 14 | B | 1226 | CLA | CHB-C4A-NA | 2.06 | 127.36 | 124.51 |
| 14 | G | 1122 | CLA | CHD-C1D-ND | -2.06 | 122.56 | 124.45 |
| 14 | H | 1226 | CLA | CHD-C1D-C2D | 2.06 | 129.81 | 125.48 |
| 14 | H | 1236 | CLA | CAA-CBA-CGA | -2.06 | 107.23 | 113.25 |
| 14 | B | 1206 | CLA | CHC-C1C-NC | 2.06 | 127.33 | 124.20 |
| 17 | L | 4219 | BCR | C32-C1-C6 | -2.06 | 106.95 | 110.30 |
| 14 | f | 1216 | CLA | C2D-C1D-ND | -2.06 | 108.58 | 110.10 |
| 14 | e | 1011 | CLA | O2A-CGA-O1A | -2.06 | 118.39 | 123.59 |
| 14 | B | 1226 | CLA | CHD-C1D-C2D | 2.06 | 129.80 | 125.48 |
| 14 | 5 | 507 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 14 | e | 1119 | CLA | C16-C15-C13 | -2.06 | 109.26 | 115.92 |
| 14 | e | 1114 | CLA | CAA-CBA-CGA | -2.06 | 107.04 | 112.51 |
| 14 | G | 1011 | CLA | O2A-CGA-O1A | -2.06 | 118.39 | 123.59 |
| 14 | e | 1104 | CLA | C2A-C1A-CHA | 2.06 | 127.46 | 123.86 |
| 14 | s | 511 | CLA | C2A-C1A-CHA | 2.06 | 127.46 | 123.86 |
| 17 | s | 524 | BCR | C23-C22-C21 | -2.06 | 115.78 | 118.94 |
| 14 | 4 | 511 | CLA | CHD-C1D-ND | -2.06 | 122.56 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | n | 4020 | BCR | C33-C5-C4 | -2.06 | 109.66 | 113.62 |
| 14 | H | 1021 | CLA | CBA-CAA-C2A | -2.06 | 107.78 | 113.86 |
| 14 | e | 1127 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 17 | l | 4015 | BCR | C37-C22-C23 | 2.06 | 121.32 | 118.08 |
| 14 | t | 516 | CLA | CAA-C2A-C3A | -2.06 | 107.14 | 112.78 |
| 17 | d | 521 | BCR | C10-C11-C12 | -2.06 | 116.79 | 123.22 |
| 14 | B | 1203 | CLA | CAA-C2A-C1A | -2.06 | 105.23 | 111.97 |
| 14 | r | 504 | CLA | CAA-C2A-C3A | -2.06 | 107.14 | 112.78 |
| 14 | s | 504 | CLA | O2D-CGD-CBD | 2.06 | 114.93 | 111.27 |
| 14 | B | 1021 | CLA | CBA-CAA-C2A | -2.06 | 107.78 | 113.86 |
| 18 | f | 1842 | LHG | C27-C26-C25 | -2.06 | 103.97 | 114.42 |
| 14 | Z | 517 | CLA | O2A-CGA-O1A | -2.06 | 118.17 | 123.30 |
| 14 | e | 1132 | CLA | C3A-C2A-C1A | 2.06 | 104.42 | 101.34 |
| 18 | V | 5221 | LHG | C15-C14-C13 | -2.06 | 103.97 | 114.42 |
| 17 | G | 4011 | BCR | C36-C18-C17 | -2.06 | 120.04 | 122.92 |
| 14 | 2 | 504 | CLA | CAA-C2A-C3A | -2.06 | 107.14 | 112.78 |
| 18 | B | 1842 | LHG | C27-C26-C25 | -2.06 | 103.97 | 114.42 |
| 17 | v | 524 | BCR | C16-C15-C14 | -2.06 | 119.26 | 123.47 |
| 14 | A | 1131 | CLA | C7-C6-C5 | -2.06 | 107.77 | 113.36 |
| 17 | V | 4019 | BCR | C29-C30-C25 | 2.06 | 113.65 | 110.48 |
| 14 | B | 1217 | CLA | O2A-CGA-O1A | -2.06 | 118.40 | 123.59 |
| 18 | H | 1842 | LHG | C27-C26-C25 | -2.06 | 103.98 | 114.42 |
| 17 | H | 4009 | BCR | C19-C18-C17 | -2.06 | 115.78 | 118.94 |
| 17 | L | 4019 | BCR | C29-C30-C25 | 2.06 | 113.65 | 110.48 |
| 17 | n | 4019 | BCR | C29-C30-C25 | 2.06 | 113.65 | 110.48 |
| 14 | f | 1206 | CLA | CHC-C1C-NC | 2.06 | 127.33 | 124.20 |
| 14 | v | 508 | CLA | CAA-C2A-C3A | -2.06 | 107.14 | 112.78 |
| 14 | G | 1132 | CLA | C3A-C2A-C1A | 2.06 | 104.42 | 101.34 |
| 17 | 6 | 523 | BCR | C8-C7-C6 | -2.06 | 121.42 | 127.20 |
| 14 | 2 | 518 | CLA | O2A-CGA-O1A | -2.06 | 118.40 | 123.59 |
| 14 | f | 1021 | CLA | CBA-CAA-C2A | -2.06 | 107.79 | 113.86 |
| 14 | f | 1217 | CLA | O2A-CGA-O1A | -2.06 | 118.40 | 123.59 |
| 18 | n | 5220 | LHG | O8-C23-O10 | -2.06 | 118.40 | 123.59 |
| 14 | A | 1114 | CLA | CAA-CBA-CGA | -2.06 | 107.05 | 112.51 |
| 14 | 4 | 501 | CLA | CHD-C1D-ND | -2.06 | 122.56 | 124.45 |
| 14 | b | 501 | CLA | CHD-C1D-ND | -2.06 | 122.56 | 124.45 |
| 14 | b | 511 | CLA | CHD-C1D-ND | -2.06 | 122.56 | 124.45 |
| 14 | e | 1120 | CLA | CHD-C1D-ND | -2.06 | 122.56 | 124.45 |
| 14 | b | 508 | CLA | CMC-C2C-C1C | -2.06 | 121.91 | 125.04 |
| 14 | r | 508 | CLA | O1A-CGA-CBA | 2.06 | 129.69 | 123.08 |
| 14 | A | 1101 | CLA | C3A-C2A-C1A | 2.06 | 104.42 | 101.34 |
| 20 | f | 5002 | LMG | C3-C4-C5 | -2.06 | 106.57 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | L | 5218 | LHG | C5-O7-C7 | -2.06 | 112.73 | 117.79 |
| 14 | H | 1240 | CLA | O2A-CGA-O1A | -2.06 | 118.40 | 123.59 |
| 17 | V | 4219 | BCR | C32-C1-C6 | -2.06 | 106.97 | 110.30 |
| 14 | v | 519 | CLA | O2A-CGA-O1A | -2.06 | 118.18 | 123.30 |
| 14 | r | 501 | CLA | C2A-C1A-CHA | 2.06 | 127.45 | 123.86 |
| 14 | A | 1011 | CLA | O2A-CGA-O1A | -2.06 | 118.41 | 123.59 |
| 14 | B | 1240 | CLA | O2A-CGA-O1A | -2.06 | 118.41 | 123.59 |
| 14 | s | 501 | CLA | O2D-CGD-CBD | 2.06 | 114.92 | 111.27 |
| 18 | n | 5221 | LHG | C15-C14-C13 | -2.06 | 103.99 | 114.42 |
| 17 | s | 523 | BCR | C1-C6-C5 | -2.06 | 119.72 | 122.61 |
| 14 | A | 1125 | CLA | CAA-CBA-CGA | -2.05 | 107.25 | 113.25 |
| 14 | f | 1226 | CLA | CHD-C1D-C2D | 2.05 | 129.79 | 125.48 |
| 17 | Y | 523 | BCR | C7-C8-C9 | -2.05 | 123.13 | 126.23 |
| 19 | T | 5105 | LMU | C6'-C5'-C4' | -2.05 | 108.19 | 113.00 |
| 14 | r | 504 | CLA | C2A-C1A-CHA | 2.05 | 127.45 | 123.86 |
| 17 | 6 | 521 | BCR | C10-C11-C12 | -2.05 | 116.81 | 123.22 |
| 14 | 3 | 502 | CLA | O2A-CGA-O1A | -2.05 | 118.18 | 123.30 |
| 17 | v | 522 | BCR | C27-C26-C25 | -2.05 | 119.75 | 122.73 |
| 17 | c | 523 | BCR | C37-C22-C23 | 2.05 | 121.31 | 118.08 |
| 14 | e | 1022 | CLA | C4D-C3D-CAD | -2.05 | 105.67 | 108.10 |
| 14 | H | 1012 | CLA | C4-C3-C5 | 2.05 | 118.73 | 115.27 |
| 17 | Z | 523 | BCR | C34-C9-C8 | 2.05 | 121.31 | 118.08 |
| 14 | R | 1302 | CLA | CAA-C2A-C3A | -2.05 | 107.15 | 112.78 |
| 18 | L | 5220 | LHG | O8-C23-O10 | -2.05 | 118.41 | 123.59 |
| 14 | d | 508 | CLA | CHC-C1C-NC | 2.05 | 127.32 | 124.20 |
| 14 | a | 511 | CLA | C2A-C1A-CHA | 2.05 | 127.45 | 123.86 |
| 14 | a | 502 | CLA | O2A-CGA-O1A | -2.05 | 118.18 | 123.30 |
| 20 | B | 5002 | LMG | C3-C4-C5 | -2.05 | 106.58 | 110.24 |
| 17 | 6 | 523 | BCR | C15-C16-C17 | -2.05 | 119.27 | 123.47 |
| 14 | G | 1022 | CLA | O1D-CGD-CBD | 2.05 | 128.68 | 124.48 |
| 14 | q | 511 | CLA | O2A-CGA-O1A | -2.05 | 118.18 | 123.30 |
| 17 | B | 4005 | BCR | C33-C5-C4 | 2.05 | 117.56 | 113.62 |
| 14 | A | 1104 | CLA | C2A-C1A-CHA | 2.05 | 127.45 | 123.86 |
| 14 | 5 | 509 | CLA | O2A-CGA-O1A | -2.05 | 118.41 | 123.59 |
| 17 | 2 | 521 | BCR | C39-C30-C25 | -2.05 | 106.97 | 110.30 |
| 14 | A | 1116 | CLA | O2A-CGA-O1A | -2.05 | 118.41 | 123.59 |
| 17 | u | 523 | BCR | C37-C22-C23 | 2.05 | 121.31 | 118.08 |
| 14 | b | 516 | CLA | CAA-C2A-C3A | -2.05 | 107.16 | 112.78 |
| 14 | u | 507 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 14 | A | 1132 | CLA | C3A-C2A-C1A | 2.05 | 104.41 | 101.34 |
| 14 | G | 1101 | CLA | C3A-C2A-C1A | 2.05 | 104.41 | 101.34 |
| 14 | G | 1131 | CLA | C7-C6-C5 | -2.05 | 107.79 | 113.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | L | 4020 | BCR | C33-C5-C4 | -2.05 | 109.67 | 113.62 |
| 17 | l | 521 | BCR | C29-C30-C25 | 2.05 | 113.64 | 110.48 |
| 17 | H | 4005 | BCR | C33-C5-C4 | 2.05 | 117.56 | 113.62 |
| 17 | c | 522 | BCR | C30-C25-C26 | -2.05 | 119.72 | 122.61 |
| 17 | G | 4003 | BCR | C15-C16-C17 | -2.05 | 119.27 | 123.47 |
| 14 | l | 511 | CLA | O2A-CGA-O1A | -2.05 | 118.19 | 123.30 |
| 14 | a | 511 | CLA | O2A-CGA-O1A | -2.05 | 118.19 | 123.30 |
| 14 | e | 1101 | CLA | C3A-C2A-C1A | 2.05 | 104.41 | 101.34 |
| 19 | l | 5105 | LMU | C6'-C5'-C4' | -2.05 | 108.20 | 113.00 |
| 21 | f | 1852 | SQD | C3-C4-C5 | 2.05 | 113.90 | 110.24 |
| 17 | b | 521 | BCR | C38-C26-C25 | -2.05 | 122.23 | 124.53 |
| 17 | Z | 521 | BCR | C39-C30-C25 | -2.05 | 106.97 | 110.30 |
| 14 | 3 | 501 | CLA | O2D-CGD-CBD | 2.05 | 114.91 | 111.27 |
| 14 | e | 1119 | CLA | O2D-CGD-CBD | 2.05 | 114.91 | 111.27 |
| 14 | f | 1203 | CLA | CAA-C2A-C1A | -2.05 | 105.26 | 111.97 |
| 14 | G | 1125 | CLA | CAA-CBA-CGA | -2.05 | 107.27 | 113.25 |
| 14 | A | 1128 | CLA | CHC-C1C-NC | 2.05 | 127.31 | 124.20 |
| 14 | q | 518 | CLA | O2A-CGA-O1A | -2.05 | 118.19 | 123.30 |
| 14 | G | 1116 | CLA | O2A-CGA-O1A | -2.05 | 118.42 | 123.59 |
| 14 | e | 1125 | CLA | CAA-CBA-CGA | -2.05 | 107.27 | 113.25 |
| 17 | q | 523 | BCR | C7-C8-C9 | -2.05 | 123.14 | 126.23 |
| 17 | H | 4004 | BCR | C29-C30-C25 | 2.05 | 113.63 | 110.48 |
| 14 | b | 517 | CLA | O2A-CGA-O1A | -2.05 | 118.19 | 123.30 |
| 14 | e | 1116 | CLA | O2A-CGA-O1A | -2.05 | 118.42 | 123.59 |
| 14 | t | 508 | CLA | CMC-C2C-C1C | -2.05 | 121.92 | 125.04 |
| 14 | 2 | 508 | CLA | O1A-CGA-CBA | 2.05 | 129.66 | 123.08 |
| 18 | e | 5001 | LHG | C18-C17-C16 | -2.05 | 104.03 | 114.42 |
| 14 | e | 1132 | CLA | O2A-CGA-O1A | -2.05 | 118.43 | 123.59 |
| 14 | f | 1240 | CLA | O2A-CGA-O1A | -2.05 | 118.43 | 123.59 |
| 14 | 3 | 511 | CLA | C2A-C1A-CHA | 2.05 | 127.44 | 123.86 |
| 14 | 4 | 516 | CLA | CAA-C2A-C3A | -2.05 | 107.17 | 112.78 |
| 14 | 6 | 516 | CLA | CAA-C2A-C3A | -2.05 | 107.17 | 112.78 |
| 14 | v | 516 | CLA | CAA-C2A-C3A | -2.05 | 107.17 | 112.78 |
| 14 | d | 507 | CLA | O2A-CGA-O1A | -2.05 | 118.20 | 123.30 |
| 14 | H | 1217 | CLA | O2A-CGA-O1A | -2.05 | 118.43 | 123.59 |
| 14 | t | 502 | CLA | C2A-C1A-CHA | 2.05 | 127.44 | 123.86 |
| 20 | H | 5002 | LMG | C3-C4-C5 | -2.05 | 106.59 | 110.24 |
| 14 | A | 1132 | CLA | O2A-CGA-O1A | -2.05 | 118.43 | 123.59 |
| 14 | G | 1114 | CLA | CHD-C1D-ND | -2.05 | 122.57 | 124.45 |
| 14 | d | 508 | CLA | CHD-C1D-ND | -2.05 | 122.57 | 124.45 |
| 14 | v | 502 | CLA | C2A-C1A-CHA | 2.05 | 127.44 | 123.86 |
| 17 | q | 522 | BCR | C27-C26-C25 | -2.05 | 119.76 | 122.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | j | 1302 | CLA | O2A-CGA-O1A | -2.05 | 118.20 | 123.30 |
| 17 | e | 4011 | BCR | C36-C18-C17 | -2.05 | 120.06 | 122.92 |
| 14 | s | 516 | CLA | C2A-C1A-CHA | 2.05 | 127.44 | 123.86 |
| 14 | d | 516 | CLA | CAA-C2A-C3A | -2.04 | 107.18 | 112.78 |
| 14 | 4 | 508 | CLA | CMC-C2C-C1C | -2.04 | 121.92 | 125.04 |
| 21 | 2 | 822 | SQD | C45-O47-C7 | 2.04 | 122.83 | 117.79 |
| 14 | 1 | 509 | CLA | O2A-CGA-O1A | -2.04 | 118.20 | 123.30 |
| 14 | f | 1202 | CLA | O2D-CGD-CBD | 2.04 | 114.90 | 111.27 |
| 14 | 2 | 516 | CLA | CAA-C2A-C3A | -2.04 | 107.18 | 112.78 |
| 14 | v | 507 | CLA | O2A-CGA-O1A | -2.04 | 118.20 | 123.30 |
| 17 | S | 4018 | BCR | C31-C1-C6 | -2.04 | 106.98 | 110.30 |
| 14 | c | 518 | CLA | O2A-CGA-O1A | -2.04 | 118.20 | 123.30 |
| 17 | 6 | 522 | BCR | C30-C25-C26 | -2.04 | 119.73 | 122.61 |
| 17 | r | 523 | BCR | C34-C9-C8 | 2.04 | 121.30 | 118.08 |
| 17 | q | 521 | BCR | C29-C30-C25 | 2.04 | 113.63 | 110.48 |
| 14 | 3 | 516 | CLA | C2A-C1A-CHA | 2.04 | 127.43 | 123.86 |
| 14 | s | 511 | CLA | O2A-CGA-O1A | -2.04 | 118.21 | 123.30 |
| 18 | V | 5220 | LHG | O8-C23-O10 | -2.04 | 118.44 | 123.59 |
| 14 | v | 505 | CLA | C2A-C1A-CHA | 2.04 | 127.43 | 123.86 |
| 14 | Z | 504 | CLA | CAA-C2A-C3A | -2.04 | 107.18 | 112.78 |
| 14 | d | 508 | CLA | CAA-C2A-C3A | -2.04 | 107.18 | 112.78 |
| 21 | c | 822 | SQD | O47-C7-O49 | -2.04 | 118.90 | 122.96 |
| 14 | 2 | 511 | CLA | O2A-CGA-O1A | -2.04 | 118.21 | 123.30 |
| 14 | 6 | 507 | CLA | O2A-CGA-O1A | -2.04 | 118.21 | 123.30 |
| 17 | A | 4011 | BCR | C36-C18-C17 | -2.04 | 120.06 | 122.92 |
| 17 | H | 4004 | BCR | C34-C9-C8 | 2.04 | 121.30 | 118.08 |
| 14 | H | 1202 | CLA | O2D-CGD-CBD | 2.04 | 114.90 | 111.27 |
| 14 | 2 | 505 | CLA | C2D-C1D-ND | -2.04 | 108.60 | 110.10 |
| 14 | u | 518 | CLA | C2D-C1D-ND | -2.04 | 108.60 | 110.10 |
| 14 | r | 511 | CLA | O2A-CGA-O1A | -2.04 | 118.21 | 123.30 |
| 17 | v | 523 | BCR | C8-C7-C6 | -2.04 | 121.47 | 127.20 |
| 17 | U | 4104 | BCR | C35-C13-C12 | 2.04 | 121.29 | 118.08 |
| 20 | B | 5002 | LMG | C23-C22-C21 | -2.04 | 104.06 | 114.42 |
| 14 | B | 1202 | CLA | O2D-CGD-CBD | 2.04 | 114.90 | 111.27 |
| 17 | e | 4003 | BCR | C15-C16-C17 | -2.04 | 119.29 | 123.47 |
| 18 | A | 5001 | LHG | C18-C17-C16 | -2.04 | 104.06 | 114.42 |
| 20 | H | 5002 | LMG | C23-C22-C21 | -2.04 | 104.06 | 114.42 |
| 14 | 4 | 502 | CLA | C2A-C1A-CHA | 2.04 | 127.43 | 123.86 |
| 17 | M | 4021 | BCR | C19-C18-C17 | -2.04 | 115.81 | 118.94 |
| 14 | u | 503 | CLA | CAA-C2A-C3A | -2.04 | 107.19 | 112.78 |
| 14 | q | 512 | CLA | CHB-C4A-NA | 2.04 | 127.33 | 124.51 |
| 18 | V | 5218 | LHG | C5-O7-C7 | -2.04 | 112.77 | 117.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 504 | CLA | O2D-CGD-CBD | 2.04 | 114.89 | 111.27 |
| 21 | u | 822 | SQD | O47-C7-O49 | -2.04 | 118.91 | 122.96 |
| 17 | l | 523 | BCR | C7-C8-C9 | -2.04 | 123.15 | 126.23 |
| 18 | e | 5006 | LHG | C5-O7-C7 | -2.04 | 112.77 | 117.79 |
| 14 | 5 | 503 | CLA | CAA-C2A-C3A | -2.04 | 107.19 | 112.78 |
| 14 | 3 | 504 | CLA | O2D-CGD-CBD | 2.04 | 114.89 | 111.27 |
| 14 | e | 1022 | CLA | O1D-CGD-CBD | 2.04 | 128.66 | 124.48 |
| 21 | r | 822 | SQD | C45-O47-C7 | 2.04 | 122.81 | 117.79 |
| 14 | 6 | 519 | CLA | O2A-CGA-O1A | -2.04 | 118.22 | 123.30 |
| 17 | f | 4009 | BCR | C4-C5-C6 | -2.04 | 119.77 | 122.73 |
| 14 | u | 509 | CLA | O2A-CGA-O1A | -2.04 | 118.44 | 123.59 |
| 14 | d | 519 | CLA | O2A-CGA-O1A | -2.04 | 118.22 | 123.30 |
| 14 | B | 1238 | CLA | CAC-C3C-C4C | 2.04 | 127.46 | 124.81 |
| 14 | H | 1238 | CLA | CAC-C3C-C4C | 2.04 | 127.46 | 124.81 |
| 14 | H | 1238 | CLA | CHD-C1D-ND | -2.04 | 122.58 | 124.45 |
| 14 | H | 1204 | CLA | O2A-CGA-O1A | -2.04 | 118.45 | 123.59 |
| 14 | t | 517 | CLA | O2A-CGA-O1A | -2.04 | 118.22 | 123.30 |
| 14 | d | 505 | CLA | C2A-C1A-CHA | 2.04 | 127.42 | 123.86 |
| 14 | Z | 516 | CLA | CAA-C2A-C3A | -2.04 | 107.20 | 112.78 |
| 14 | 4 | 517 | CLA | O2A-CGA-O1A | -2.04 | 118.22 | 123.30 |
| 14 | 6 | 508 | CLA | CAA-C2A-C3A | -2.04 | 107.20 | 112.78 |
| 14 | r | 518 | CLA | O2A-CGA-O1A | -2.04 | 118.45 | 123.59 |
| 20 | f | 5002 | LMG | C23-C22-C21 | -2.04 | 104.08 | 114.42 |
| 14 | b | 502 | CLA | C2A-C1A-CHA | 2.04 | 127.42 | 123.86 |
| 14 | 3 | 519 | CLA | O2A-CGA-O1A | -2.04 | 118.22 | 123.30 |
| 17 | 5 | 523 | BCR | C37-C22-C23 | 2.04 | 121.29 | 118.08 |
| 17 | v | 523 | BCR | C15-C16-C17 | -2.04 | 119.30 | 123.47 |
| 14 | q | 509 | CLA | O1D-CGD-CBD | 2.04 | 128.65 | 124.48 |
| 14 | 2 | 504 | CLA | C2A-C1A-CHA | 2.04 | 127.42 | 123.86 |
| 17 | W | 4021 | BCR | C19-C18-C17 | -2.04 | 115.82 | 118.94 |
| 18 | A | 5006 | LHG | C5-O7-C7 | -2.04 | 112.78 | 117.79 |
| 17 | A | 4008 | BCR | C8-C7-C6 | -2.04 | 121.48 | 127.20 |
| 21 | Z | 822 | SQD | C45-O47-C7 | 2.04 | 122.80 | 117.79 |
| 14 | e | 1131 | CLA | CAA-CBA-CGA | -2.04 | 107.30 | 113.25 |
| 14 | c | 503 | CLA | CAA-C2A-C3A | -2.04 | 107.20 | 112.78 |
| 17 | r | 524 | BCR | C38-C26-C25 | -2.04 | 122.24 | 124.53 |
| 17 | A | 4003 | BCR | C15-C16-C17 | -2.04 | 119.30 | 123.47 |
| 14 | v | 505 | CLA | C2D-C1D-ND | -2.04 | 108.60 | 110.10 |
| 14 | s | 502 | CLA | O2A-CGA-O1A | -2.04 | 118.23 | 123.30 |
| 14 | 4 | 511 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 17 | e | 4008 | BCR | C8-C7-C6 | -2.03 | 121.49 | 127.20 |
| 14 | u | 510 | CLA | CHD-C1D-ND | -2.03 | 122.58 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 18 | G | 5001 | LHG | C18-C17-C16 | -2.03 | 104.09 | 114.42 |
| 14 | B | 1204 | CLA | O2A-CGA-O1A | -2.03 | 118.46 | 123.59 |
| 17 | B | 4005 | BCR | C3-C4-C5 | -2.03 | 110.44 | 114.08 |
| 17 | H | 4005 | BCR | C3-C4-C5 | -2.03 | 110.44 | 114.08 |
| 17 | B | 4009 | BCR | C19-C18-C17 | -2.03 | 115.82 | 118.94 |
| 17 | o | 4021 | BCR | C19-C18-C17 | -2.03 | 115.82 | 118.94 |
| 14 | A | 1131 | CLA | CAA-CBA-CGA | -2.03 | 107.31 | 113.25 |
| 14 | a | 501 | CLA | O2D-CGD-CBD | 2.03 | 114.88 | 111.27 |
| 18 | G | 5007 | LHG | C11-C10-C9 | -2.03 | 104.10 | 114.42 |
| 14 | Y | 509 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 14 | Y | 511 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 17 | k | 4018 | BCR | C33-C5-C6 | -2.03 | 122.24 | 124.53 |
| 14 | U | 1103 | CLA | CAC-C3C-C4C | 2.03 | 127.45 | 124.81 |
| 14 | s | 519 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 14 | r | 516 | CLA | CAA-C2A-C3A | -2.03 | 107.21 | 112.78 |
| 14 | c | 509 | CLA | O2A-CGA-O1A | -2.03 | 118.46 | 123.59 |
| 17 | H | 4009 | BCR | C4-C5-C6 | -2.03 | 119.78 | 122.73 |
| 14 | G | 1135 | CLA | CHA-C1A-NA | -2.03 | 121.74 | 126.40 |
| 14 | l | 518 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 14 | d | 502 | CLA | C2A-C1A-CHA | 2.03 | 127.41 | 123.86 |
| 17 | Z | 523 | BCR | C23-C24-C25 | -2.03 | 121.49 | 127.20 |
| 17 | 4 | 521 | BCR | C38-C26-C25 | -2.03 | 122.25 | 124.53 |
| 14 | c | 506 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 14 | 6 | 502 | CLA | C2A-C1A-CHA | 2.03 | 127.41 | 123.86 |
| 17 | 6 | 522 | BCR | C27-C26-C25 | -2.03 | 119.78 | 122.73 |
| 14 | Y | 518 | CLA | O2A-CGA-O1A | -2.03 | 118.23 | 123.30 |
| 17 | K | 4104 | BCR | C35-C13-C12 | 2.03 | 121.28 | 118.08 |
| 14 | A | 1130 | CLA | CHD-C1D-ND | -2.03 | 122.59 | 124.45 |
| 14 | B | 1220 | CLA | CHD-C1D-ND | -2.03 | 122.59 | 124.45 |
| 14 | F | 1302 | CLA | O2A-CGA-O1A | -2.03 | 118.24 | 123.30 |
| 14 | s | 501 | CLA | CAA-C2A-C3A | -2.03 | 107.22 | 112.78 |
| 17 | T | 4013 | BCR | C35-C13-C12 | 2.03 | 121.28 | 118.08 |
| 14 | B | 1205 | CLA | C3A-C2A-C1A | 2.03 | 104.38 | 101.34 |
| 17 | 3 | 523 | BCR | C1-C6-C5 | -2.03 | 119.75 | 122.61 |
| 18 | n | 5218 | LHG | C5-O7-C7 | -2.03 | 112.79 | 117.79 |
| 17 | l | 4013 | BCR | C39-C30-C25 | -2.03 | 107.00 | 110.30 |
| 14 | H | 1239 | CLA | C2A-C1A-CHA | 2.03 | 127.41 | 123.86 |
| 21 | 5 | 822 | SQD | O47-C7-O49 | -2.03 | 118.93 | 122.96 |
| 18 | A | 5007 | LHG | C11-C10-C9 | -2.03 | 104.12 | 114.42 |
| 14 | e | 1135 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 14 | G | 1131 | CLA | CAA-CBA-CGA | -2.03 | 107.32 | 113.25 |
| 14 | G | 1132 | CLA | O2A-CGA-O1A | -2.03 | 118.47 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | a | 508 | CLA | O1A-CGA-CBA | 2.03 | 129.60 | 123.08 |
| 14 | v | 516 | CLA | O2A-CGA-O1A | -2.03 | 118.24 | 123.30 |
| 17 | B | 4010 | BCR | C10-C11-C12 | -2.03 | 116.88 | 123.22 |
| 14 | A | 1120 | CLA | CHD-C1D-ND | -2.03 | 122.59 | 124.45 |
| 17 | H | 4017 | BCR | C16-C15-C14 | -2.03 | 119.32 | 123.47 |
| 14 | a | 519 | CLA | O2A-CGA-O1A | -2.03 | 118.24 | 123.30 |
| 14 | a | 501 | CLA | CAA-C2A-C3A | -2.03 | 107.22 | 112.78 |
| 14 | e | 1134 | CLA | O2A-CGA-O1A | -2.03 | 118.47 | 123.59 |
| 17 | B | 4004 | BCR | C29-C30-C25 | 2.03 | 113.60 | 110.48 |
| 14 | s | 507 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 14 | 3 | 511 | CLA | O2A-CGA-O1A | -2.03 | 118.24 | 123.30 |
| 14 | 6 | 504 | CLA | C2A-C1A-CHA | 2.03 | 127.41 | 123.86 |
| 14 | Z | 504 | CLA | C2A-C1A-CHA | 2.03 | 127.41 | 123.86 |
| 14 | e | 1107 | CLA | C2A-C1A-CHA | 2.03 | 127.41 | 123.86 |
| 14 | A | 1128 | CLA | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 14 | r | 519 | CLA | CHD-C1D-ND | -2.03 | 122.59 | 124.45 |
| 14 | s | 501 | CLA | CHD-C1D-ND | -2.03 | 122.59 | 124.45 |
| 14 | Z | 511 | CLA | O2A-CGA-O1A | -2.03 | 118.25 | 123.30 |
| 14 | a | 516 | CLA | C2A-C1A-CHA | 2.03 | 127.40 | 123.86 |
| 17 | f | 4004 | BCR | C29-C30-C25 | 2.03 | 113.60 | 110.48 |
| 17 | G | 4008 | BCR | C8-C7-C6 | -2.03 | 121.51 | 127.20 |
| 17 | J | 4013 | BCR | C39-C30-C25 | -2.03 | 107.01 | 110.30 |
| 14 | d | 504 | CLA | C2A-C1A-CHA | 2.03 | 127.40 | 123.86 |
| 14 | G | 1022 | CLA | O2A-CGA-O1A | -2.03 | 118.48 | 123.59 |
| 17 | T | 4013 | BCR | C39-C30-C25 | -2.03 | 107.01 | 110.30 |
| 17 | B | 4009 | BCR | C4-C5-C6 | -2.03 | 119.79 | 122.73 |
| 14 | 3 | 501 | CLA | CAA-C2A-C3A | -2.03 | 107.23 | 112.78 |
| 14 | R | 1302 | CLA | O2A-CGA-O1A | -2.03 | 118.25 | 123.30 |
| 14 | c | 510 | CLA | O2A-CGA-O1A | -2.03 | 118.25 | 123.30 |
| 18 | G | 5006 | LHG | C5-O7-C7 | -2.03 | 112.81 | 117.79 |
| 14 | 2 | 501 | CLA | C2A-C1A-CHA | 2.03 | 127.40 | 123.86 |
| 14 | G | 1123 | CLA | O2D-CGD-CBD | 2.02 | 114.87 | 111.27 |
| 14 | 3 | 508 | CLA | O1A-CGA-CBA | 2.02 | 129.59 | 123.08 |
| 14 | A | 1127 | CLA | O2A-CGA-O1A | -2.02 | 118.48 | 123.59 |
| 14 | v | 504 | CLA | C2A-C1A-CHA | 2.02 | 127.40 | 123.86 |
| 14 | e | 1128 | CLA | CHB-C4A-NA | 2.02 | 127.31 | 124.51 |
| 14 | A | 1114 | CLA | CHD-C1D-ND | -2.02 | 122.59 | 124.45 |
| 14 | H | 1220 | CLA | CHD-C1D-ND | -2.02 | 122.59 | 124.45 |
| 14 | 6 | 505 | CLA | C2A-C1A-CHA | 2.02 | 127.40 | 123.86 |
| 17 | G | 4003 | BCR | C33-C5-C4 | 2.02 | 117.50 | 113.62 |
| 17 | 5 | 522 | BCR | C30-C25-C26 | -2.02 | 119.76 | 122.61 |
| 14 | A | 1022 | CLA | O1D-CGD-CBD | 2.02 | 128.62 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 2 | 523 | BCR | C23-C24-C25 | -2.02 | 121.52 | 127.20 |
| 18 | e | 5007 | LHG | C11-C10-C9 | -2.02 | 104.15 | 114.42 |
| 14 | A | 1107 | CLA | C2A-C1A-CHA | 2.02 | 127.40 | 123.86 |
| 14 | q | 508 | CLA | C2D-C1D-ND | -2.02 | 108.61 | 110.10 |
| 14 | H | 1205 | CLA | C3A-C2A-C1A | 2.02 | 104.37 | 101.34 |
| 17 | f | 4009 | BCR | C19-C18-C17 | -2.02 | 115.84 | 118.94 |
| 14 | f | 1231 | CLA | C1-C2-C3 | -2.02 | 122.55 | 126.04 |
| 17 | S | 4018 | BCR | C33-C5-C6 | -2.02 | 122.26 | 124.53 |
| 14 | G | 1128 | CLA | CHC-C1C-NC | 2.02 | 127.27 | 124.20 |
| 14 | A | 1111 | CLA | C2A-C1A-CHA | 2.02 | 127.39 | 123.86 |
| 14 | e | 1139 | CLA | CHB-C4A-NA | 2.02 | 127.31 | 124.51 |
| 14 | r | 503 | CLA | C2D-C1D-ND | -2.02 | 108.61 | 110.10 |
| 14 | r | 518 | CLA | CHD-C1D-ND | -2.02 | 122.60 | 124.45 |
| 14 | q | 509 | CLA | C2A-C1A-CHA | 2.02 | 127.39 | 123.86 |
| 14 | 4 | 519 | CLA | O2A-CGA-O1A | -2.02 | 118.26 | 123.30 |
| 14 | 6 | 517 | CLA | O2A-CGA-O1A | -2.02 | 118.26 | 123.30 |
| 14 | e | 1123 | CLA | O2D-CGD-CBD | 2.02 | 114.86 | 111.27 |
| 14 | f | 1238 | CLA | CAC-C3C-C4C | 2.02 | 127.43 | 124.81 |
| 17 | J | 4013 | BCR | C35-C13-C12 | 2.02 | 121.26 | 118.08 |
| 17 | l | 4013 | BCR | C35-C13-C12 | 2.02 | 121.26 | 118.08 |
| 14 | l | 509 | CLA | C2A-C1A-CHA | 2.02 | 127.39 | 123.86 |
| 14 | v | 517 | CLA | O2A-CGA-O1A | -2.02 | 118.26 | 123.30 |
| 14 | A | 1139 | CLA | CHB-C4A-NA | 2.02 | 127.31 | 124.51 |
| 17 | f | 4005 | BCR | C3-C4-C5 | -2.02 | 110.47 | 114.08 |
| 17 | H | 4010 | BCR | C10-C11-C12 | -2.02 | 116.92 | 123.22 |
| 14 | s | 504 | CLA | C2A-C1A-CHA | 2.02 | 127.39 | 123.86 |
| 14 | f | 1201 | CLA | C11-C10-C8 | -2.02 | 109.39 | 115.92 |
| 14 | B | 1231 | CLA | C1-C2-C3 | -2.02 | 122.55 | 126.04 |
| 18 | S | 5001 | LHG | C27-C26-C25 | -2.02 | 104.18 | 114.42 |
| 14 | s | 508 | CLA | O1A-CGA-CBA | 2.02 | 129.57 | 123.08 |
| 14 | f | 1239 | CLA | CHD-C1D-ND | -2.02 | 122.60 | 124.45 |
| 14 | b | 511 | CLA | O2A-CGA-O1A | -2.02 | 118.27 | 123.30 |
| 14 | B | 1214 | CLA | C1-C2-C3 | 2.02 | 129.53 | 126.04 |
| 18 | I | 5001 | LHG | C27-C26-C25 | -2.02 | 104.18 | 114.42 |
| 18 | k | 5001 | LHG | C27-C26-C25 | -2.02 | 104.18 | 114.42 |
| 17 | r | 523 | BCR | C33-C5-C4 | 2.02 | 117.49 | 113.62 |
| 17 | c | 523 | BCR | C23-C24-C25 | -2.02 | 121.53 | 127.20 |
| 17 | f | 4017 | BCR | C16-C15-C14 | -2.02 | 119.34 | 123.47 |
| 14 | b | 519 | CLA | O2A-CGA-O1A | -2.02 | 118.27 | 123.30 |
| 17 | A | 4003 | BCR | C33-C5-C4 | 2.02 | 117.49 | 113.62 |
| 14 | r | 510 | CLA | CHD-C1D-ND | -2.02 | 122.60 | 124.45 |
| 17 | r | 523 | BCR | C23-C24-C25 | -2.02 | 121.54 | 127.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | 4 | 522 | BCR | C21-C20-C19 | -2.02 | 116.92 | 123.22 |
| 14 | 6 | 508 | CLA | O1A-CGA-CBA | 2.02 | 129.56 | 123.08 |
| 21 | 3 | 822 | SQD | O6-C1-C2 | 2.02 | 111.45 | 108.30 |
| 14 | A | 1123 | CLA | O2D-CGD-CBD | 2.02 | 114.85 | 111.27 |
| 14 | A | 1134 | CLA | O2A-CGA-O1A | -2.02 | 118.50 | 123.59 |
| 14 | A | 1103 | CLA | CHD-C1D-ND | -2.02 | 122.60 | 124.45 |
| 14 | A | 1139 | CLA | C11-C10-C8 | -2.02 | 109.40 | 115.92 |
| 17 | H | 4009 | BCR | C29-C28-C27 | -2.02 | 106.87 | 111.38 |
| 14 | B | 1201 | CLA | C11-C10-C8 | -2.02 | 109.40 | 115.92 |
| 17 | B | 4017 | BCR | C16-C15-C14 | -2.02 | 119.35 | 123.47 |
| 14 | A | 1135 | CLA | CHA-C1A-NA | -2.02 | 121.78 | 126.40 |
| 14 | e | 1128 | CLA | CHC-C1C-NC | 2.01 | 127.26 | 124.20 |
| 14 | G | 1128 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.51 |
| 14 | A | 1022 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 14 | 5 | 510 | CLA | CHD-C1D-ND | -2.01 | 122.60 | 124.45 |
| 14 | Y | 519 | CLA | O2A-CGA-O1A | -2.01 | 118.28 | 123.30 |
| 14 | t | 511 | CLA | O2A-CGA-O1A | -2.01 | 118.28 | 123.30 |
| 17 | l | 522 | BCR | C27-C26-C25 | -2.01 | 119.81 | 122.73 |
| 17 | r | 523 | BCR | C3-C4-C5 | -2.01 | 110.48 | 114.08 |
| 17 | G | 4007 | BCR | C36-C18-C19 | 2.01 | 121.25 | 118.08 |
| 17 | m | 4104 | BCR | C35-C13-C12 | 2.01 | 121.25 | 118.08 |
| 14 | 3 | 507 | CLA | CHA-C1A-NA | -2.01 | 121.79 | 126.40 |
| 14 | u | 511 | CLA | C2A-C1A-CHA | 2.01 | 127.38 | 123.86 |
| 14 | f | 1205 | CLA | C3A-C2A-C1A | 2.01 | 104.36 | 101.34 |
| 14 | H | 1225 | CLA | O2D-CGD-CBD | 2.01 | 114.85 | 111.27 |
| 14 | e | 1139 | CLA | C11-C10-C8 | -2.01 | 109.41 | 115.92 |
| 14 | H | 1226 | CLA | C3C-C4C-NC | -2.01 | 108.31 | 110.57 |
| 14 | d | 517 | CLA | O2A-CGA-O1A | -2.01 | 118.28 | 123.30 |
| 17 | q | 524 | BCR | C15-C16-C17 | -2.01 | 119.35 | 123.47 |
| 14 | Z | 503 | CLA | CHD-C1D-ND | -2.01 | 122.60 | 124.45 |
| 14 | q | 504 | CLA | CHD-C1D-ND | -2.01 | 122.60 | 124.45 |
| 14 | Y | 509 | CLA | O1D-CGD-CBD | 2.01 | 128.60 | 124.48 |
| 17 | f | 4010 | BCR | C10-C11-C12 | -2.01 | 116.94 | 123.22 |
| 18 | H | 1855 | LHG | C27-C26-C25 | -2.01 | 104.21 | 114.42 |
| 14 | H | 1214 | CLA | C1-C2-C3 | 2.01 | 129.52 | 126.04 |
| 14 | l | 509 | CLA | O1D-CGD-CBD | 2.01 | 128.60 | 124.48 |
| 14 | u | 506 | CLA | O2A-CGA-O1A | -2.01 | 118.28 | 123.30 |
| 14 | G | 1127 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 14 | 5 | 518 | CLA | C2D-C1D-ND | -2.01 | 108.62 | 110.10 |
| 14 | Z | 505 | CLA | C2D-C1D-ND | -2.01 | 108.62 | 110.10 |
| 14 | t | 509 | CLA | O1A-CGA-CBA | 2.01 | 129.54 | 123.08 |
| 18 | e | 5008 | LHG | O8-C23-C24 | 2.01 | 118.22 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | q | 519 | CLA | O2A-CGA-O1A | -2.01 | 118.28 | 123.30 |
| 17 | H | 4009 | BCR | C35-C13-C12 | 2.01 | 121.25 | 118.08 |
| 18 | A | 5009 | LHG | O8-C23-O10 | -2.01 | 118.52 | 123.59 |
| 14 | e | 1124 | CLA | CHB-C4A-NA | 2.01 | 127.29 | 124.51 |
| 14 | m | 1103 | CLA | CAC-C3C-C4C | 2.01 | 127.42 | 124.81 |
| 14 | d | 508 | CLA | O1A-CGA-CBA | 2.01 | 129.54 | 123.08 |
| 17 | Z | 523 | BCR | C33-C5-C4 | 2.01 | 117.48 | 113.62 |
| 17 | u | 522 | BCR | C30-C25-C26 | -2.01 | 119.78 | 122.61 |
| 18 | f | 1855 | LHG | C27-C26-C25 | -2.01 | 104.22 | 114.42 |
| 14 | v | 508 | CLA | O1A-CGA-CBA | 2.01 | 129.54 | 123.08 |
| 14 | G | 1103 | CLA | CHD-C1D-ND | -2.01 | 122.61 | 124.45 |
| 17 | Y | 524 | BCR | C15-C16-C17 | -2.01 | 119.36 | 123.47 |
| 14 | e | 1022 | CLA | O2A-CGA-O1A | -2.01 | 118.52 | 123.59 |
| 14 | Y | 509 | CLA | C2A-C1A-CHA | 2.01 | 127.37 | 123.86 |
| 17 | Z | 523 | BCR | C3-C4-C5 | -2.01 | 110.49 | 114.08 |
| 17 | I | 4018 | BCR | C35-C13-C12 | 2.01 | 121.24 | 118.08 |
| 14 | H | 1231 | CLA | C1-C2-C3 | -2.01 | 122.57 | 126.04 |
| 14 | G | 1139 | CLA | C11-C10-C8 | -2.01 | 109.42 | 115.92 |
| 14 | 3 | 504 | CLA | C2A-C1A-CHA | 2.01 | 127.37 | 123.86 |
| 14 | G | 1130 | CLA | CHD-C1D-ND | -2.01 | 122.61 | 124.45 |
| 14 | 5 | 506 | CLA | O2A-CGA-O1A | -2.01 | 118.29 | 123.30 |
| 14 | b | 502 | CLA | O2A-CGA-O1A | -2.01 | 118.29 | 123.30 |
| 18 | B | 1855 | LHG | C27-C26-C25 | -2.01 | 104.23 | 114.42 |
| 14 | 4 | 509 | CLA | O1A-CGA-CBA | 2.01 | 129.53 | 123.08 |
| 17 | 3 | 522 | BCR | C36-C18-C19 | 2.01 | 121.24 | 118.08 |
| 17 | 2 | 523 | BCR | C3-C4-C5 | -2.01 | 110.49 | 114.08 |
| 14 | K | 1103 | CLA | CAC-C3C-C4C | 2.01 | 127.42 | 124.81 |
| 14 | t | 519 | CLA | O2A-CGA-O1A | -2.01 | 118.30 | 123.30 |
| 14 | f | 1214 | CLA | C1-C2-C3 | 2.01 | 129.51 | 126.04 |
| 14 | f | 1225 | CLA | O2D-CGD-CBD | 2.01 | 114.83 | 111.27 |
| 17 | V | 4020 | BCR | C29-C30-C25 | 2.01 | 113.57 | 110.48 |
| 14 | B | 1213 | CLA | O2A-C1-C2 | -2.01 | 103.36 | 108.64 |
| 14 | H | 1213 | CLA | O2A-C1-C2 | -2.01 | 103.36 | 108.64 |
| 17 | b | 522 | BCR | C21-C20-C19 | -2.01 | 116.95 | 123.22 |
| 17 | 2 | 523 | BCR | C33-C5-C4 | 2.01 | 117.47 | 113.62 |
| 14 | H | 1201 | CLA | C11-C10-C8 | -2.01 | 109.43 | 115.92 |
| 14 | e | 1127 | CLA | O2A-CGA-O1A | -2.01 | 118.53 | 123.59 |
| 14 | Y | 516 | CLA | O2A-CGA-O1A | -2.01 | 118.30 | 123.30 |
| 14 | a | 507 | CLA | CHA-C1A-NA | -2.01 | 121.80 | 126.40 |
| 17 | d | 522 | BCR | C27-C26-C25 | -2.01 | 119.82 | 122.73 |
| 17 | T | 4012 | BCR | C38-C26-C25 | -2.01 | 122.28 | 124.53 |
| 14 | a | 504 | CLA | C2A-C1A-CHA | 2.01 | 127.37 | 123.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | f | 1204 | CLA | O2A-CGA-O1A | -2.01 | 118.53 | 123.59 |
| 17 | e | 4003 | BCR | C33-C5-C4 | 2.01 | 117.47 | 113.62 |
| 17 | u | 522 | BCR | C36-C18-C19 | 2.01 | 121.24 | 118.08 |
| 17 | t | 522 | BCR | C21-C20-C19 | -2.01 | 116.96 | 123.22 |
| 17 | l | 524 | BCR | C15-C16-C17 | -2.00 | 119.37 | 123.47 |
| 17 | 5 | 524 | BCR | C10-C11-C12 | -2.00 | 116.96 | 123.22 |
| 17 | a | 523 | BCR | C1-C6-C5 | -2.00 | 119.79 | 122.61 |
| 14 | e | 1111 | CLA | C2A-C1A-CHA | 2.00 | 127.36 | 123.86 |
| 14 | B | 1239 | CLA | CHD-C1D-ND | -2.00 | 122.61 | 124.45 |
| 14 | c | 518 | CLA | C2D-C1D-ND | -2.00 | 108.63 | 110.10 |
| 18 | A | 5008 | LHG | O8-C23-C24 | 2.00 | 118.20 | 111.91 |
| 17 | c | 524 | BCR | C10-C11-C12 | -2.00 | 116.96 | 123.22 |
| 14 | B | 1239 | CLA | C2A-C1A-CHA | 2.00 | 127.36 | 123.86 |
| 17 | u | 523 | BCR | C23-C24-C25 | -2.00 | 121.57 | 127.20 |
| 14 | 6 | 516 | CLA | O2A-CGA-O1A | -2.00 | 118.31 | 123.30 |
| 17 | R | 4016 | BCR | C15-C16-C17 | -2.00 | 119.37 | 123.47 |
| 14 | e | 1114 | CLA | CHD-C1D-ND | -2.00 | 122.61 | 124.45 |
| 17 | s | 522 | BCR | C36-C18-C19 | 2.00 | 121.23 | 118.08 |
| 14 | G | 1134 | CLA | O2A-CGA-O1A | -2.00 | 118.54 | 123.59 |
| 14 | e | 1801 | CLA | CAA-C2A-C3A | -2.00 | 107.29 | 112.78 |
| 14 | r | 511 | CLA | C2D-C1D-ND | -2.00 | 108.63 | 110.10 |
| 17 | 5 | 523 | BCR | C23-C24-C25 | -2.00 | 121.58 | 127.20 |
| 17 | Y | 522 | BCR | C27-C26-C25 | -2.00 | 119.82 | 122.73 |
| 14 | H | 1214 | CLA | CHD-C1D-ND | -2.00 | 122.61 | 124.45 |
| 14 | H | 1229 | CLA | O2A-CGA-O1A | -2.00 | 118.54 | 123.59 |
| 17 | A | 4007 | BCR | C36-C18-C19 | 2.00 | 121.23 | 118.08 |
| 14 | q | 516 | CLA | O2A-CGA-O1A | -2.00 | 118.31 | 123.30 |
| 14 | Y | 508 | CLA | C2D-C1D-ND | -2.00 | 108.63 | 110.10 |
| 14 | q | 511 | CLA | C2D-C1D-ND | -2.00 | 108.63 | 110.10 |
| 17 | v | 523 | BCR | C34-C9-C8 | 2.00 | 121.23 | 118.08 |
| 14 | Y | 504 | CLA | CED-O2D-CGD | 2.00 | 120.46 | 115.94 |
| 14 | q | 504 | CLA | CED-O2D-CGD | 2.00 | 120.46 | 115.94 |
| 14 | c | 511 | CLA | C2A-C1A-CHA | 2.00 | 127.36 | 123.86 |
| 17 | Y | 523 | BCR | C11-C10-C9 | -2.00 | 124.45 | 127.31 |
| 14 | A | 1801 | CLA | CAA-C2A-C3A | -2.00 | 107.30 | 112.78 |
| 17 | L | 4020 | BCR | C29-C30-C25 | 2.00 | 113.56 | 110.48 |

All (588) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | A | 1011 | CLA | ND |
| 14 | A | 1013 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | A | 1102 | CLA | ND |
| 14 | A | 1103 | CLA | ND |
| 14 | A | 1104 | CLA | ND |
| 14 | A | 1105 | CLA | ND |
| 14 | A | 1106 | CLA | ND |
| 14 | A | 1107 | CLA | ND |
| 14 | A | 1108 | CLA | ND |
| 14 | A | 1109 | CLA | ND |
| 14 | A | 1110 | CLA | ND |
| 14 | A | 1111 | CLA | ND |
| 14 | A | 1112 | CLA | ND |
| 14 | A | 1113 | CLA | ND |
| 14 | A | 1114 | CLA | ND |
| 14 | A | 1115 | CLA | ND |
| 14 | A | 1116 | CLA | ND |
| 14 | A | 1117 | CLA | ND |
| 14 | A | 1118 | CLA | ND |
| 14 | A | 1119 | CLA | ND |
| 14 | A | 1120 | CLA | ND |
| 14 | A | 1121 | CLA | ND |
| 14 | A | 1122 | CLA | ND |
| 14 | A | 1123 | CLA | ND |
| 14 | A | 1124 | CLA | ND |
| 14 | A | 1125 | CLA | ND |
| 14 | A | 1126 | CLA | ND |
| 14 | A | 1127 | CLA | ND |
| 14 | A | 1128 | CLA | ND |
| 14 | A | 1129 | CLA | ND |
| 14 | A | 1131 | CLA | ND |
| 14 | A | 1132 | CLA | ND |
| 14 | A | 1133 | CLA | ND |
| 14 | A | 1134 | CLA | ND |
| 14 | A | 1135 | CLA | ND |
| 14 | A | 1136 | CLA | ND |
| 14 | A | 1137 | CLA | ND |
| 14 | A | 1138 | CLA | ND |
| 14 | A | 1139 | CLA | ND |
| 14 | A | 1140 | CLA | ND |
| 14 | A | 1237 | CLA | ND |
| 14 | A | 1801 | CLA | ND |
| 14 | A | 1022 | CLA | ND |
| 14 | A | 1130 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | A | 1101 | CLA | ND |
| 14 | B | 1012 | CLA | ND |
| 14 | B | 1021 | CLA | ND |
| 14 | B | 1023 | CLA | ND |
| 14 | B | 1201 | CLA | ND |
| 14 | B | 1202 | CLA | ND |
| 14 | B | 1203 | CLA | ND |
| 14 | B | 1204 | CLA | ND |
| 14 | B | 1205 | CLA | ND |
| 14 | B | 1206 | CLA | ND |
| 14 | B | 1208 | CLA | ND |
| 14 | B | 1209 | CLA | ND |
| 14 | B | 1210 | CLA | ND |
| 14 | B | 1211 | CLA | ND |
| 14 | B | 1212 | CLA | ND |
| 14 | B | 1213 | CLA | ND |
| 14 | B | 1214 | CLA | ND |
| 14 | B | 1215 | CLA | ND |
| 14 | B | 1216 | CLA | ND |
| 14 | B | 1217 | CLA | ND |
| 14 | B | 1218 | CLA | ND |
| 14 | B | 1219 | CLA | ND |
| 14 | B | 1220 | CLA | ND |
| 14 | B | 1221 | CLA | ND |
| 14 | B | 1222 | CLA | ND |
| 14 | B | 1223 | CLA | ND |
| 14 | B | 1224 | CLA | ND |
| 14 | B | 1225 | CLA | ND |
| 14 | B | 1226 | CLA | ND |
| 14 | B | 1227 | CLA | ND |
| 14 | B | 1228 | CLA | ND |
| 14 | B | 1229 | CLA | ND |
| 14 | B | 1231 | CLA | ND |
| 14 | B | 1232 | CLA | ND |
| 14 | B | 1234 | CLA | ND |
| 14 | B | 1235 | CLA | ND |
| 14 | B | 1236 | CLA | ND |
| 14 | B | 1238 | CLA | ND |
| 14 | B | 1239 | CLA | ND |
| 14 | B | 1240 | CLA | ND |
| 14 | B | 1207 | CLA | ND |
| 14 | B | 1230 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | F | 1301 | CLA | ND |
| 14 | F | 1302 | CLA | ND |
| 14 | J | 1302 | CLA | ND |
| 14 | J | 1303 | CLA | ND |
| 14 | K | 1401 | CLA | ND |
| 14 | K | 1103 | CLA | ND |
| 14 | K | 1105 | CLA | ND |
| 14 | L | 1501 | CLA | ND |
| 14 | L | 1502 | CLA | ND |
| 14 | L | 1503 | CLA | ND |
| 14 | 1 | 501 | CLA | ND |
| 14 | 1 | 502 | CLA | ND |
| 14 | 1 | 503 | CLA | ND |
| 14 | 1 | 504 | CLA | ND |
| 14 | 1 | 505 | CLA | ND |
| 14 | 1 | 506 | CLA | ND |
| 14 | 1 | 507 | CLA | ND |
| 14 | 1 | 508 | CLA | ND |
| 14 | 1 | 509 | CLA | ND |
| 14 | 1 | 510 | CLA | ND |
| 14 | 1 | 511 | CLA | ND |
| 14 | 1 | 512 | CLA | ND |
| 14 | 1 | 513 | CLA | ND |
| 14 | 1 | 516 | CLA | ND |
| 14 | 1 | 517 | CLA | ND |
| 14 | 1 | 518 | CLA | ND |
| 14 | 1 | 519 | CLA | ND |
| 14 | 2 | 501 | CLA | ND |
| 14 | 2 | 502 | CLA | ND |
| 14 | 2 | 503 | CLA | ND |
| 14 | 2 | 504 | CLA | ND |
| 14 | 2 | 505 | CLA | ND |
| 14 | 2 | 506 | CLA | ND |
| 14 | 2 | 507 | CLA | ND |
| 14 | 2 | 508 | CLA | ND |
| 14 | 2 | 509 | CLA | ND |
| 14 | 2 | 510 | CLA | ND |
| 14 | 2 | 511 | CLA | ND |
| 14 | 2 | 512 | CLA | ND |
| 14 | 2 | 513 | CLA | ND |
| 14 | 2 | 518 | CLA | ND |
| 14 | 2 | 519 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | 3 | 501 | CLA | ND |
| 14 | 3 | 502 | CLA | ND |
| 14 | 3 | 503 | CLA | ND |
| 14 | 3 | 504 | CLA | ND |
| 14 | 3 | 505 | CLA | ND |
| 14 | 3 | 506 | CLA | ND |
| 14 | 3 | 507 | CLA | ND |
| 14 | 3 | 508 | CLA | ND |
| 14 | 3 | 509 | CLA | ND |
| 14 | 3 | 510 | CLA | ND |
| 14 | 3 | 511 | CLA | ND |
| 14 | 3 | 512 | CLA | ND |
| 14 | 3 | 513 | CLA | ND |
| 14 | 3 | 516 | CLA | ND |
| 14 | 3 | 517 | CLA | ND |
| 14 | 3 | 518 | CLA | ND |
| 14 | 3 | 519 | CLA | ND |
| 14 | 4 | 501 | CLA | ND |
| 14 | 4 | 502 | CLA | ND |
| 14 | 4 | 503 | CLA | ND |
| 14 | 4 | 504 | CLA | ND |
| 14 | 4 | 505 | CLA | ND |
| 14 | 4 | 506 | CLA | ND |
| 14 | 4 | 507 | CLA | ND |
| 14 | 4 | 508 | CLA | ND |
| 14 | 4 | 509 | CLA | ND |
| 14 | 4 | 510 | CLA | ND |
| 14 | 4 | 511 | CLA | ND |
| 14 | 4 | 512 | CLA | ND |
| 14 | 4 | 513 | CLA | ND |
| 14 | 4 | 516 | CLA | ND |
| 14 | 4 | 517 | CLA | ND |
| 14 | 4 | 518 | CLA | ND |
| 14 | 4 | 519 | CLA | ND |
| 14 | 5 | 501 | CLA | ND |
| 14 | 5 | 502 | CLA | ND |
| 14 | 5 | 503 | CLA | ND |
| 14 | 5 | 504 | CLA | ND |
| 14 | 5 | 505 | CLA | ND |
| 14 | 5 | 506 | CLA | ND |
| 14 | 5 | 507 | CLA | ND |
| 14 | 5 | 508 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | 5 | 509 | CLA | ND |
| 14 | 5 | 510 | CLA | ND |
| 14 | 5 | 511 | CLA | ND |
| 14 | 5 | 512 | CLA | ND |
| 14 | 5 | 513 | CLA | ND |
| 14 | 5 | 516 | CLA | ND |
| 14 | 5 | 517 | CLA | ND |
| 14 | 5 | 518 | CLA | ND |
| 14 | 5 | 519 | CLA | ND |
| 14 | 6 | 501 | CLA | ND |
| 14 | 6 | 502 | CLA | ND |
| 14 | 6 | 503 | CLA | ND |
| 14 | 6 | 504 | CLA | ND |
| 14 | 6 | 505 | CLA | ND |
| 14 | 6 | 506 | CLA | ND |
| 14 | 6 | 507 | CLA | ND |
| 14 | 6 | 508 | CLA | ND |
| 14 | 6 | 509 | CLA | ND |
| 14 | 6 | 510 | CLA | ND |
| 14 | 6 | 511 | CLA | ND |
| 14 | 6 | 512 | CLA | ND |
| 14 | 6 | 513 | CLA | ND |
| 14 | 6 | 516 | CLA | ND |
| 14 | 6 | 517 | CLA | ND |
| 14 | 6 | 518 | CLA | ND |
| 14 | 6 | 519 | CLA | ND |
| 14 | G | 1011 | CLA | ND |
| 14 | G | 1013 | CLA | ND |
| 14 | G | 1102 | CLA | ND |
| 14 | G | 1103 | CLA | ND |
| 14 | G | 1104 | CLA | ND |
| 14 | G | 1105 | CLA | ND |
| 14 | G | 1106 | CLA | ND |
| 14 | G | 1107 | CLA | ND |
| 14 | G | 1108 | CLA | ND |
| 14 | G | 1109 | CLA | ND |
| 14 | G | 1110 | CLA | ND |
| 14 | G | 1111 | CLA | ND |
| 14 | G | 1112 | CLA | ND |
| 14 | G | 1113 | CLA | ND |
| 14 | G | 1114 | CLA | ND |
| 14 | G | 1115 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | G | 1116 | CLA | ND |
| 14 | G | 1117 | CLA | ND |
| 14 | G | 1118 | CLA | ND |
| 14 | G | 1119 | CLA | ND |
| 14 | G | 1120 | CLA | ND |
| 14 | G | 1121 | CLA | ND |
| 14 | G | 1122 | CLA | ND |
| 14 | G | 1123 | CLA | ND |
| 14 | G | 1124 | CLA | ND |
| 14 | G | 1125 | CLA | ND |
| 14 | G | 1126 | CLA | ND |
| 14 | G | 1127 | CLA | ND |
| 14 | G | 1128 | CLA | ND |
| 14 | G | 1129 | CLA | ND |
| 14 | G | 1131 | CLA | ND |
| 14 | G | 1132 | CLA | ND |
| 14 | G | 1133 | CLA | ND |
| 14 | G | 1134 | CLA | ND |
| 14 | G | 1135 | CLA | ND |
| 14 | G | 1136 | CLA | ND |
| 14 | G | 1137 | CLA | ND |
| 14 | G | 1138 | CLA | ND |
| 14 | G | 1139 | CLA | ND |
| 14 | G | 1140 | CLA | ND |
| 14 | G | 1237 | CLA | ND |
| 14 | G | 1801 | CLA | ND |
| 14 | G | 1022 | CLA | ND |
| 14 | G | 1130 | CLA | ND |
| 14 | G | 1101 | CLA | ND |
| 14 | H | 1012 | CLA | ND |
| 14 | H | 1021 | CLA | ND |
| 14 | H | 1023 | CLA | ND |
| 14 | H | 1201 | CLA | ND |
| 14 | H | 1202 | CLA | ND |
| 14 | H | 1203 | CLA | ND |
| 14 | H | 1204 | CLA | ND |
| 14 | H | 1205 | CLA | ND |
| 14 | H | 1206 | CLA | ND |
| 14 | H | 1208 | CLA | ND |
| 14 | H | 1209 | CLA | ND |
| 14 | H | 1210 | CLA | ND |
| 14 | H | 1211 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | H | 1212 | CLA | ND |
| 14 | H | 1213 | CLA | ND |
| 14 | H | 1214 | CLA | ND |
| 14 | H | 1215 | CLA | ND |
| 14 | H | 1216 | CLA | ND |
| 14 | H | 1217 | CLA | ND |
| 14 | H | 1218 | CLA | ND |
| 14 | H | 1219 | CLA | ND |
| 14 | H | 1220 | CLA | ND |
| 14 | H | 1221 | CLA | ND |
| 14 | H | 1222 | CLA | ND |
| 14 | H | 1223 | CLA | ND |
| 14 | H | 1224 | CLA | ND |
| 14 | H | 1225 | CLA | ND |
| 14 | H | 1226 | CLA | ND |
| 14 | H | 1227 | CLA | ND |
| 14 | H | 1228 | CLA | ND |
| 14 | H | 1229 | CLA | ND |
| 14 | H | 1231 | CLA | ND |
| 14 | H | 1232 | CLA | ND |
| 14 | H | 1234 | CLA | ND |
| 14 | H | 1235 | CLA | ND |
| 14 | H | 1236 | CLA | ND |
| 14 | H | 1238 | CLA | ND |
| 14 | H | 1239 | CLA | ND |
| 14 | H | 1240 | CLA | ND |
| 14 | H | 1207 | CLA | ND |
| 14 | H | 1230 | CLA | ND |
| 14 | R | 1301 | CLA | ND |
| 14 | R | 1302 | CLA | ND |
| 14 | T | 1302 | CLA | ND |
| 14 | T | 1303 | CLA | ND |
| 14 | U | 1401 | CLA | ND |
| 14 | U | 1103 | CLA | ND |
| 14 | U | 1105 | CLA | ND |
| 14 | V | 1501 | CLA | ND |
| 14 | V | 1502 | CLA | ND |
| 14 | V | 1503 | CLA | ND |
| 14 | Y | 501 | CLA | ND |
| 14 | Y | 502 | CLA | ND |
| 14 | Y | 503 | CLA | ND |
| 14 | Y | 504 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | Y | 505 | CLA | ND |
| 14 | Y | 506 | CLA | ND |
| 14 | Y | 507 | CLA | ND |
| 14 | Y | 508 | CLA | ND |
| 14 | Y | 509 | CLA | ND |
| 14 | Y | 510 | CLA | ND |
| 14 | Y | 511 | CLA | ND |
| 14 | Y | 512 | CLA | ND |
| 14 | Y | 513 | CLA | ND |
| 14 | Y | 516 | CLA | ND |
| 14 | Y | 517 | CLA | ND |
| 14 | Y | 518 | CLA | ND |
| 14 | Y | 519 | CLA | ND |
| 14 | Z | 501 | CLA | ND |
| 14 | Z | 502 | CLA | ND |
| 14 | Z | 503 | CLA | ND |
| 14 | Z | 504 | CLA | ND |
| 14 | Z | 505 | CLA | ND |
| 14 | Z | 506 | CLA | ND |
| 14 | Z | 507 | CLA | ND |
| 14 | Z | 508 | CLA | ND |
| 14 | Z | 509 | CLA | ND |
| 14 | Z | 510 | CLA | ND |
| 14 | Z | 511 | CLA | ND |
| 14 | Z | 512 | CLA | ND |
| 14 | Z | 513 | CLA | ND |
| 14 | Z | 518 | CLA | ND |
| 14 | Z | 519 | CLA | ND |
| 14 | a | 501 | CLA | ND |
| 14 | a | 502 | CLA | ND |
| 14 | a | 503 | CLA | ND |
| 14 | a | 504 | CLA | ND |
| 14 | a | 505 | CLA | ND |
| 14 | a | 506 | CLA | ND |
| 14 | a | 507 | CLA | ND |
| 14 | a | 508 | CLA | ND |
| 14 | a | 509 | CLA | ND |
| 14 | a | 510 | CLA | ND |
| 14 | a | 511 | CLA | ND |
| 14 | a | 512 | CLA | ND |
| 14 | a | 513 | CLA | ND |
| 14 | a | 516 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | a | 517 | CLA | ND |
| 14 | a | 518 | CLA | ND |
| 14 | a | 519 | CLA | ND |
| 14 | b | 501 | CLA | ND |
| 14 | b | 502 | CLA | ND |
| 14 | b | 503 | CLA | ND |
| 14 | b | 504 | CLA | ND |
| 14 | b | 505 | CLA | ND |
| 14 | b | 506 | CLA | ND |
| 14 | b | 507 | CLA | ND |
| 14 | b | 508 | CLA | ND |
| 14 | b | 509 | CLA | ND |
| 14 | b | 510 | CLA | ND |
| 14 | b | 511 | CLA | ND |
| 14 | b | 512 | CLA | ND |
| 14 | b | 513 | CLA | ND |
| 14 | b | 516 | CLA | ND |
| 14 | b | 517 | CLA | ND |
| 14 | b | 518 | CLA | ND |
| 14 | b | 519 | CLA | ND |
| 14 | c | 501 | CLA | ND |
| 14 | c | 502 | CLA | ND |
| 14 | c | 503 | CLA | ND |
| 14 | c | 504 | CLA | ND |
| 14 | c | 505 | CLA | ND |
| 14 | c | 506 | CLA | ND |
| 14 | c | 507 | CLA | ND |
| 14 | c | 508 | CLA | ND |
| 14 | c | 509 | CLA | ND |
| 14 | c | 510 | CLA | ND |
| 14 | c | 511 | CLA | ND |
| 14 | c | 512 | CLA | ND |
| 14 | c | 513 | CLA | ND |
| 14 | c | 516 | CLA | ND |
| 14 | c | 517 | CLA | ND |
| 14 | c | 518 | CLA | ND |
| 14 | c | 519 | CLA | ND |
| 14 | d | 501 | CLA | ND |
| 14 | d | 502 | CLA | ND |
| 14 | d | 503 | CLA | ND |
| 14 | d | 504 | CLA | ND |
| 14 | d | 505 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | d | 506 | CLA | ND |
| 14 | d | 507 | CLA | ND |
| 14 | d | 508 | CLA | ND |
| 14 | d | 509 | CLA | ND |
| 14 | d | 510 | CLA | ND |
| 14 | d | 511 | CLA | ND |
| 14 | d | 512 | CLA | ND |
| 14 | d | 513 | CLA | ND |
| 14 | d | 516 | CLA | ND |
| 14 | d | 517 | CLA | ND |
| 14 | d | 518 | CLA | ND |
| 14 | d | 519 | CLA | ND |
| 14 | e | 1011 | CLA | ND |
| 14 | e | 1013 | CLA | ND |
| 14 | e | 1102 | CLA | ND |
| 14 | e | 1103 | CLA | ND |
| 14 | e | 1104 | CLA | ND |
| 14 | e | 1105 | CLA | ND |
| 14 | e | 1106 | CLA | ND |
| 14 | e | 1107 | CLA | ND |
| 14 | e | 1108 | CLA | ND |
| 14 | e | 1109 | CLA | ND |
| 14 | e | 1110 | CLA | ND |
| 14 | e | 1111 | CLA | ND |
| 14 | e | 1112 | CLA | ND |
| 14 | e | 1113 | CLA | ND |
| 14 | e | 1114 | CLA | ND |
| 14 | e | 1115 | CLA | ND |
| 14 | e | 1116 | CLA | ND |
| 14 | e | 1117 | CLA | ND |
| 14 | e | 1118 | CLA | ND |
| 14 | e | 1119 | CLA | ND |
| 14 | e | 1120 | CLA | ND |
| 14 | e | 1121 | CLA | ND |
| 14 | e | 1122 | CLA | ND |
| 14 | e | 1123 | CLA | ND |
| 14 | e | 1124 | CLA | ND |
| 14 | e | 1125 | CLA | ND |
| 14 | e | 1126 | CLA | ND |
| 14 | e | 1127 | CLA | ND |
| 14 | e | 1128 | CLA | ND |
| 14 | e | 1129 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | e | 1131 | CLA | ND |
| 14 | e | 1132 | CLA | ND |
| 14 | e | 1133 | CLA | ND |
| 14 | e | 1134 | CLA | ND |
| 14 | e | 1135 | CLA | ND |
| 14 | e | 1136 | CLA | ND |
| 14 | e | 1137 | CLA | ND |
| 14 | e | 1138 | CLA | ND |
| 14 | e | 1139 | CLA | ND |
| 14 | e | 1140 | CLA | ND |
| 14 | e | 1237 | CLA | ND |
| 14 | e | 1801 | CLA | ND |
| 14 | e | 1022 | CLA | ND |
| 14 | e | 1130 | CLA | ND |
| 14 | e | 1101 | CLA | ND |
| 14 | f | 1012 | CLA | ND |
| 14 | f | 1021 | CLA | ND |
| 14 | f | 1023 | CLA | ND |
| 14 | f | 1201 | CLA | ND |
| 14 | f | 1202 | CLA | ND |
| 14 | f | 1203 | CLA | ND |
| 14 | f | 1204 | CLA | ND |
| 14 | f | 1205 | CLA | ND |
| 14 | f | 1206 | CLA | ND |
| 14 | f | 1208 | CLA | ND |
| 14 | f | 1209 | CLA | ND |
| 14 | f | 1210 | CLA | ND |
| 14 | f | 1211 | CLA | ND |
| 14 | f | 1212 | CLA | ND |
| 14 | f | 1213 | CLA | ND |
| 14 | f | 1214 | CLA | ND |
| 14 | f | 1215 | CLA | ND |
| 14 | f | 1216 | CLA | ND |
| 14 | f | 1217 | CLA | ND |
| 14 | f | 1218 | CLA | ND |
| 14 | f | 1219 | CLA | ND |
| 14 | f | 1220 | CLA | ND |
| 14 | f | 1221 | CLA | ND |
| 14 | f | 1222 | CLA | ND |
| 14 | f | 1223 | CLA | ND |
| 14 | f | 1224 | CLA | ND |
| 14 | f | 1225 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | f | 1226 | CLA | ND |
| 14 | f | 1227 | CLA | ND |
| 14 | f | 1228 | CLA | ND |
| 14 | f | 1229 | CLA | ND |
| 14 | f | 1231 | CLA | ND |
| 14 | f | 1232 | CLA | ND |
| 14 | f | 1234 | CLA | ND |
| 14 | f | 1235 | CLA | ND |
| 14 | f | 1236 | CLA | ND |
| 14 | f | 1238 | CLA | ND |
| 14 | f | 1239 | CLA | ND |
| 14 | f | 1240 | CLA | ND |
| 14 | f | 1207 | CLA | ND |
| 14 | f | 1230 | CLA | ND |
| 14 | j | 1301 | CLA | ND |
| 14 | j | 1302 | CLA | ND |
| 14 | l | 1302 | CLA | ND |
| 14 | l | 1303 | CLA | ND |
| 14 | m | 1401 | CLA | ND |
| 14 | m | 1103 | CLA | ND |
| 14 | m | 1105 | CLA | ND |
| 14 | n | 1501 | CLA | ND |
| 14 | n | 1502 | CLA | ND |
| 14 | n | 1503 | CLA | ND |
| 14 | q | 501 | CLA | ND |
| 14 | q | 502 | CLA | ND |
| 14 | q | 503 | CLA | ND |
| 14 | q | 504 | CLA | ND |
| 14 | q | 505 | CLA | ND |
| 14 | q | 506 | CLA | ND |
| 14 | q | 507 | CLA | ND |
| 14 | q | 508 | CLA | ND |
| 14 | q | 509 | CLA | ND |
| 14 | q | 510 | CLA | ND |
| 14 | q | 511 | CLA | ND |
| 14 | q | 512 | CLA | ND |
| 14 | q | 513 | CLA | ND |
| 14 | q | 516 | CLA | ND |
| 14 | q | 517 | CLA | ND |
| 14 | q | 518 | CLA | ND |
| 14 | q | 519 | CLA | ND |
| 14 | r | 501 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | r | 502 | CLA | ND |
| 14 | r | 503 | CLA | ND |
| 14 | r | 504 | CLA | ND |
| 14 | r | 505 | CLA | ND |
| 14 | r | 506 | CLA | ND |
| 14 | r | 507 | CLA | ND |
| 14 | r | 508 | CLA | ND |
| 14 | r | 509 | CLA | ND |
| 14 | r | 510 | CLA | ND |
| 14 | r | 511 | CLA | ND |
| 14 | r | 512 | CLA | ND |
| 14 | r | 513 | CLA | ND |
| 14 | r | 518 | CLA | ND |
| 14 | r | 519 | CLA | ND |
| 14 | s | 501 | CLA | ND |
| 14 | s | 502 | CLA | ND |
| 14 | s | 503 | CLA | ND |
| 14 | s | 504 | CLA | ND |
| 14 | s | 505 | CLA | ND |
| 14 | s | 506 | CLA | ND |
| 14 | s | 507 | CLA | ND |
| 14 | s | 508 | CLA | ND |
| 14 | s | 509 | CLA | ND |
| 14 | s | 510 | CLA | ND |
| 14 | s | 511 | CLA | ND |
| 14 | s | 512 | CLA | ND |
| 14 | s | 513 | CLA | ND |
| 14 | s | 516 | CLA | ND |
| 14 | s | 517 | CLA | ND |
| 14 | s | 518 | CLA | ND |
| 14 | s | 519 | CLA | ND |
| 14 | t | 501 | CLA | ND |
| 14 | t | 502 | CLA | ND |
| 14 | t | 503 | CLA | ND |
| 14 | t | 504 | CLA | ND |
| 14 | t | 505 | CLA | ND |
| 14 | t | 506 | CLA | ND |
| 14 | t | 507 | CLA | ND |
| 14 | t | 508 | CLA | ND |
| 14 | t | 509 | CLA | ND |
| 14 | t | 510 | CLA | ND |
| 14 | t | 511 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14 | t | 512 | CLA | ND |
| 14 | t | 513 | CLA | ND |
| 14 | t | 516 | CLA | ND |
| 14 | t | 517 | CLA | ND |
| 14 | t | 518 | CLA | ND |
| 14 | t | 519 | CLA | ND |
| 14 | u | 501 | CLA | ND |
| 14 | u | 502 | CLA | ND |
| 14 | u | 503 | CLA | ND |
| 14 | u | 504 | CLA | ND |
| 14 | u | 505 | CLA | ND |
| 14 | u | 506 | CLA | ND |
| 14 | u | 507 | CLA | ND |
| 14 | u | 508 | CLA | ND |
| 14 | u | 509 | CLA | ND |
| 14 | u | 510 | CLA | ND |
| 14 | u | 511 | CLA | ND |
| 14 | u | 512 | CLA | ND |
| 14 | u | 513 | CLA | ND |
| 14 | u | 516 | CLA | ND |
| 14 | u | 517 | CLA | ND |
| 14 | u | 518 | CLA | ND |
| 14 | u | 519 | CLA | ND |
| 14 | v | 501 | CLA | ND |
| 14 | v | 502 | CLA | ND |
| 14 | v | 503 | CLA | ND |
| 14 | v | 504 | CLA | ND |
| 14 | v | 505 | CLA | ND |
| 14 | v | 506 | CLA | ND |
| 14 | v | 507 | CLA | ND |
| 14 | v | 508 | CLA | ND |
| 14 | v | 509 | CLA | ND |
| 14 | v | 510 | CLA | ND |
| 14 | v | 511 | CLA | ND |
| 14 | v | 512 | CLA | ND |
| 14 | v | 513 | CLA | ND |
| 14 | v | 516 | CLA | ND |
| 14 | v | 517 | CLA | ND |
| 14 | v | 518 | CLA | ND |
| 14 | v | 519 | CLA | ND |

All (7071) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1011 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1102 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1103 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1103 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1103 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1103 | CLA | CAD-CBD-CGD-O1D |
| 14 | A | 1104 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1104 | CLA | C4-C3-C5-C6 |
| 14 | A | 1106 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1108 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1108 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1110 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1113 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1113 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1116 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1117 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1117 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1119 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1119 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1119 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1120 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1122 | CLA | C2-C3-C5-C6 |
| 14 | A | 1122 | CLA | C4-C3-C5-C6 |
| 14 | A | 1126 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1126 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1132 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1132 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1134 | CLA | C2-C3-C5-C6 |
| 14 | A | 1134 | CLA | C4-C3-C5-C6 |
| 14 | A | 1134 | CLA | C11-C10-C8-C7 |
| 14 | A | 1137 | CLA | C4-C3-C5-C6 |
| 14 | A | 1138 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1139 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1139 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1139 | CLA | C2-C3-C5-C6 |
| 14 | A | 1139 | CLA | C4-C3-C5-C6 |
| 14 | A | 1139 | CLA | C6-C7-C8-C9 |
| 14 | A | 1140 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1140 | CLA | C2-C3-C5-C6 |
| 14 | A | 1140 | CLA | C4-C3-C5-C6 |
| 14 | A | 1237 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1237 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1237 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1801 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1801 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1101 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1101 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1012 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1012 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1012 | CLA | C2-C3-C5-C6 |
| 14 | B | 1012 | CLA | C4-C3-C5-C6 |
| 14 | B | 1021 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1021 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1202 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1202 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1202 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1202 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1202 | CLA | CAD-CBD-CGD-O1D |
| 14 | B | 1205 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1205 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1206 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1209 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1209 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1209 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1210 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1211 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1211 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1212 | CLA | C2-C3-C5-C6 |
| 14 | B | 1212 | CLA | C4-C3-C5-C6 |
| 14 | B | 1214 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1214 | CLA | O2A-C1-C2-C3 |
| 14 | B | 1215 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1215 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1216 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1216 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1217 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1217 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1217 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1219 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1219 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1220 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1220 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1224 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1224 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1227 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1234 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1240 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1240 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1240 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1230 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1230 | CLA | C3A-C2A-CAA-CBA |
| 14 | J | 1302 | CLA | CHA-CBD-CGD-O1D |
| 14 | J | 1302 | CLA | CHA-CBD-CGD-O2D |
| 14 | J | 1302 | CLA | CAD-CBD-CGD-O1D |
| 14 | J | 1302 | CLA | CAD-CBD-CGD-O2D |
| 14 | J | 1302 | CLA | CBD-CGD-O2D-CED |
| 14 | K | 1401 | CLA | C1A-C2A-CAA-CBA |
| 14 | K | 1401 | CLA | CHA-CBD-CGD-O1D |
| 14 | K | 1401 | CLA | CHA-CBD-CGD-O2D |
| 14 | K | 1105 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 501 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | 1 | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | 1 | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | 1 | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | 1 | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | 1 | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | 1 | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 501 | CLA | C2-C3-C5-C6 |
| 14 | 2 | 501 | CLA | C4-C3-C5-C6 |
| 14 | 2 | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | 2 | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | 2 | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | 2 | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | 2 | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | 2 | 518 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | 2 | 518 | CLA | C2-C3-C5-C6 |
| 14 | 2 | 518 | CLA | C4-C3-C5-C6 |
| 14 | 3 | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 507 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | 3 | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | 4 | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 519 | CLA | CHA-CBD-CGD-O2D |
| 14 | 4 | 519 | CLA | CAD-CBD-CGD-O1D |
| 14 | 4 | 519 | CLA | CAD-CBD-CGD-O2D |
| 14 | 4 | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 502 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | 5 | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | 6 | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 508 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 6 | 508 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | 6 | 510 | CLA | CAD-CBD-CGD-O2D |
| 14 | 6 | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | 6 | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 518 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1011 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1102 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1103 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1103 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1103 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1103 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1104 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1104 | CLA | C4-C3-C5-C6 |
| 14 | G | 1106 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1108 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1108 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1110 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1113 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1113 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1116 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1117 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1117 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1119 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1119 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1119 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1120 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1122 | CLA | C2-C3-C5-C6 |
| 14 | G | 1122 | CLA | C4-C3-C5-C6 |
| 14 | G | 1126 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1126 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1132 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1132 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1134 | CLA | C2-C3-C5-C6 |
| 14 | G | 1134 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1134 | CLA | C11-C10-C8-C7 |
| 14 | G | 1137 | CLA | C4-C3-C5-C6 |
| 14 | G | 1138 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1139 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1139 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1139 | CLA | C2-C3-C5-C6 |
| 14 | G | 1139 | CLA | C4-C3-C5-C6 |
| 14 | G | 1139 | CLA | C6-C7-C8-C9 |
| 14 | G | 1140 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1140 | CLA | C2-C3-C5-C6 |
| 14 | G | 1140 | CLA | C4-C3-C5-C6 |
| 14 | G | 1237 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1237 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1237 | CLA | C4-C3-C5-C6 |
| 14 | G | 1801 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1801 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1101 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1101 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1012 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1012 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1012 | CLA | C2-C3-C5-C6 |
| 14 | H | 1012 | CLA | C4-C3-C5-C6 |
| 14 | H | 1021 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1021 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1202 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1202 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1202 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1202 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1202 | CLA | CAD-CBD-CGD-O1D |
| 14 | H | 1205 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1205 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1206 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1209 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1209 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1209 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1210 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1211 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1211 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1212 | CLA | C2-C3-C5-C6 |
| 14 | H | 1212 | CLA | C4-C3-C5-C6 |
| 14 | H | 1214 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1214 | CLA | O2A-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1215 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1215 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1216 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1216 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1217 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1217 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1217 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1219 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1219 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1220 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1220 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1224 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1224 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1227 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1234 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1239 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1240 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1240 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1240 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1230 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1230 | CLA | C3A-C2A-CAA-CBA |
| 14 | T | 1302 | CLA | CHA-CBD-CGD-O1D |
| 14 | T | 1302 | CLA | CHA-CBD-CGD-O2D |
| 14 | T | 1302 | CLA | CAD-CBD-CGD-O1D |
| 14 | T | 1302 | CLA | CAD-CBD-CGD-O2D |
| 14 | T | 1302 | CLA | CBD-CGD-O2D-CED |
| 14 | U | 1401 | CLA | C1A-C2A-CAA-CBA |
| 14 | U | 1401 | CLA | CHA-CBD-CGD-O1D |
| 14 | U | 1401 | CLA | CHA-CBD-CGD-O2D |
| 14 | U | 1105 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 501 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | Y | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | Y | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | Y | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | Y | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 516 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | Y | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | Y | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 501 | CLA | C2-C3-C5-C6 |
| 14 | Z | 501 | CLA | C4-C3-C5-C6 |
| 14 | Z | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | Z | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | Z | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | Z | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | Z | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | Z | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 518 | CLA | C2-C3-C5-C6 |
| 14 | Z | 518 | CLA | C4-C3-C5-C6 |
| 14 | a | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 507 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | a | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | b | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 519 | CLA | CHA-CBD-CGD-O2D |
| 14 | b | 519 | CLA | CAD-CBD-CGD-O1D |
| 14 | b | 519 | CLA | CAD-CBD-CGD-O2D |
| 14 | b | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 502 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 507 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | c | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | c | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 508 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 508 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 510 | CLA | CAD-CBD-CGD-O2D |
| 14 | d | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 518 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1011 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1102 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1103 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1103 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1103 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1103 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1104 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1104 | CLA | C4-C3-C5-C6 |
| 14 | e | 1106 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1108 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1108 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1110 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1113 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1113 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1116 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1117 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1117 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1119 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1119 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1119 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1120 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1122 | CLA | C2-C3-C5-C6 |
| 14 | e | 1122 | CLA | C4-C3-C5-C6 |
| 14 | e | 1126 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1126 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1132 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1132 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1134 | CLA | C2-C3-C5-C6 |
| 14 | e | 1134 | CLA | C4-C3-C5-C6 |
| 14 | e | 1134 | CLA | C11-C10-C8-C7 |
| 14 | e | 1137 | CLA | C4-C3-C5-C6 |
| 14 | e | 1138 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1139 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1139 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1139 | CLA | C2-C3-C5-C6 |
| 14 | e | 1139 | CLA | C4-C3-C5-C6 |
| 14 | e | 1139 | CLA | C6-C7-C8-C9 |
| 14 | e | 1140 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1140 | CLA | C2-C3-C5-C6 |
| 14 | e | 1140 | CLA | C4-C3-C5-C6 |
| 14 | e | 1237 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1237 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1237 | CLA | C4-C3-C5-C6 |
| 14 | e | 1801 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1801 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1101 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1101 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1012 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1012 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1012 | CLA | C2-C3-C5-C6 |
| 14 | f | 1012 | CLA | C4-C3-C5-C6 |
| 14 | f | 1021 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1021 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1202 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1202 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1202 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | f | 1202 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1202 | CLA | CAD-CBD-CGD-O1D |
| 14 | f | 1205 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1205 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1206 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1209 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1209 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1209 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1210 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1211 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1211 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1212 | CLA | C2-C3-C5-C6 |
| 14 | f | 1212 | CLA | C4-C3-C5-C6 |
| 14 | f | 1214 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1214 | CLA | O2A-C1-C2-C3 |
| 14 | f | 1215 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1215 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1216 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1216 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1217 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1217 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1217 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1219 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1219 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1220 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1220 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1224 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1224 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1227 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1234 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1240 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1240 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1240 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1230 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1230 | CLA | C3A-C2A-CAA-CBA |
| 14 | l | 1302 | CLA | CHA-CBD-CGD-O1D |
| 14 | l | 1302 | CLA | CHA-CBD-CGD-O2D |
| 14 | l | 1302 | CLA | CAD-CBD-CGD-O1D |
| 14 | l | 1302 | CLA | CAD-CBD-CGD-O2D |
| 14 | l | 1302 | CLA | CBD-CGD-O2D-CED |
| 14 | m | 1401 | CLA | C1A-C2A-CAA-CBA |
| 14 | m | 1401 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | m | 1401 | CLA | CHA-CBD-CGD-O2D |
| 14 | m | 1105 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 501 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | q | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | q | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | q | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | q | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | q | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | q | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 501 | CLA | C2-C3-C5-C6 |
| 14 | r | 501 | CLA | C4-C3-C5-C6 |
| 14 | r | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | r | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | r | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | r | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | r | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 518 | CLA | C2-C3-C5-C6 |
| 14 | r | 518 | CLA | C4-C3-C5-C6 |
| 14 | s | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 507 | CLA | CAD-CBD-CGD-O1D |
| 14 | s | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | s | 517 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 14 | s | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | t | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 519 | CLA | CHA-CBD-CGD-O2D |
| 14 | t | 519 | CLA | CAD-CBD-CGD-O1D |
| 14 | t | 519 | CLA | CAD-CBD-CGD-O2D |
| 14 | t | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 502 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | u | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | v | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 508 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 508 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | v | 510 | CLA | CAD-CBD-CGD-O2D |
| 14 | v | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | v | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 518 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | A | 4001 | BCR | C11-C12-C13-C14 |
| 17 | A | 4001 | BCR | C37-C22-C23-C24 |
| 17 | A | 4008 | BCR | C21-C22-C23-C24 |
| 17 | A | 4008 | BCR | C37-C22-C23-C24 |
| 17 | A | 4008 | BCR | C23-C24-C25-C26 |
| 17 | A | 4011 | BCR | C36-C18-C19-C20 |
| 17 | B | 4004 | BCR | C7-C8-C9-C10 |
| 17 | B | 4004 | BCR | C7-C8-C9-C34 |
| 17 | B | 4004 | BCR | C21-C22-C23-C24 |
| 17 | B | 4004 | BCR | C37-C22-C23-C24 |
| 17 | B | 4004 | BCR | C23-C24-C25-C30 |
| 17 | B | 4005 | BCR | C7-C8-C9-C10 |
| 17 | B | 4005 | BCR | C7-C8-C9-C34 |
| 17 | B | 4005 | BCR | C21-C22-C23-C24 |
| 17 | B | 4005 | BCR | C37-C22-C23-C24 |
| 17 | B | 4005 | BCR | C23-C24-C25-C30 |
| 17 | B | 4010 | BCR | C23-C24-C25-C26 |
| 17 | B | 4017 | BCR | C1-C6-C7-C8 |
| 17 | B | 4014 | BCR | C17-C18-C19-C20 |
| 17 | B | 4014 | BCR | C36-C18-C19-C20 |
| 17 | J | 4013 | BCR | C17-C18-C19-C20 |
| 17 | J | 4013 | BCR | C36-C18-C19-C20 |
| 17 | J | 4015 | BCR | C23-C24-C25-C30 |
| 17 | J | 4012 | BCR | C5-C6-C7-C8 |
| 17 | J | 4012 | BCR | C11-C12-C13-C14 |
| 17 | J | 4012 | BCR | C11-C12-C13-C35 |
| 17 | K | 4104 | BCR | C21-C22-C23-C24 |
| 17 | K | 4104 | BCR | C37-C22-C23-C24 |
| 17 | L | 4019 | BCR | C7-C8-C9-C10 |
| 17 | L | 4019 | BCR | C7-C8-C9-C34 |
| 17 | L | 4219 | BCR | C7-C8-C9-C10 |
| 17 | M | 4021 | BCR | C5-C6-C7-C8 |
| 17 | M | 4021 | BCR | C11-C12-C13-C35 |
| 17 | M | 4021 | BCR | C17-C18-C19-C20 |
| 17 | M | 4021 | BCR | C36-C18-C19-C20 |
| 17 | 1 | 521 | BCR | C7-C8-C9-C10 |
| 17 | 1 | 521 | BCR | C7-C8-C9-C34 |
| 17 | 1 | 522 | BCR | C1-C6-C7-C8 |
| 17 | 1 | 522 | BCR | C5-C6-C7-C8 |
| 17 | 1 | 522 | BCR | C7-C8-C9-C10 |
| 17 | 1 | 522 | BCR | C7-C8-C9-C34 |
| 17 | 1 | 523 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | 1 | 523 | BCR | C37-C22-C23-C24 |
| 17 | 2 | 521 | BCR | C7-C8-C9-C10 |
| 17 | 2 | 521 | BCR | C7-C8-C9-C34 |
| 17 | 2 | 522 | BCR | C5-C6-C7-C8 |
| 17 | 2 | 522 | BCR | C7-C8-C9-C10 |
| 17 | 2 | 522 | BCR | C7-C8-C9-C34 |
| 17 | 2 | 523 | BCR | C21-C22-C23-C24 |
| 17 | 2 | 523 | BCR | C37-C22-C23-C24 |
| 17 | 3 | 521 | BCR | C7-C8-C9-C34 |
| 17 | 3 | 522 | BCR | C7-C8-C9-C10 |
| 17 | 3 | 522 | BCR | C7-C8-C9-C34 |
| 17 | 3 | 523 | BCR | C37-C22-C23-C24 |
| 17 | 4 | 521 | BCR | C7-C8-C9-C10 |
| 17 | 4 | 521 | BCR | C7-C8-C9-C34 |
| 17 | 4 | 523 | BCR | C37-C22-C23-C24 |
| 17 | 5 | 521 | BCR | C7-C8-C9-C10 |
| 17 | 5 | 521 | BCR | C7-C8-C9-C34 |
| 17 | 5 | 521 | BCR | C17-C18-C19-C20 |
| 17 | 5 | 521 | BCR | C36-C18-C19-C20 |
| 17 | 5 | 522 | BCR | C5-C6-C7-C8 |
| 17 | 5 | 522 | BCR | C7-C8-C9-C10 |
| 17 | 5 | 522 | BCR | C7-C8-C9-C34 |
| 17 | 5 | 523 | BCR | C21-C22-C23-C24 |
| 17 | 5 | 523 | BCR | C37-C22-C23-C24 |
| 17 | 6 | 522 | BCR | C5-C6-C7-C8 |
| 17 | 6 | 523 | BCR | C21-C22-C23-C24 |
| 17 | 6 | 523 | BCR | C37-C22-C23-C24 |
| 17 | 6 | 524 | BCR | C7-C8-C9-C10 |
| 17 | 6 | 524 | BCR | C7-C8-C9-C34 |
| 17 | G | 4001 | BCR | C11-C12-C13-C14 |
| 17 | G | 4001 | BCR | C37-C22-C23-C24 |
| 17 | G | 4008 | BCR | C21-C22-C23-C24 |
| 17 | G | 4008 | BCR | C37-C22-C23-C24 |
| 17 | G | 4008 | BCR | C23-C24-C25-C26 |
| 17 | G | 4011 | BCR | C36-C18-C19-C20 |
| 17 | H | 4004 | BCR | C7-C8-C9-C10 |
| 17 | H | 4004 | BCR | C7-C8-C9-C34 |
| 17 | H | 4004 | BCR | C21-C22-C23-C24 |
| 17 | H | 4004 | BCR | C37-C22-C23-C24 |
| 17 | H | 4004 | BCR | C23-C24-C25-C30 |
| 17 | H | 4005 | BCR | C7-C8-C9-C10 |
| 17 | H | 4005 | BCR | C7-C8-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | H | 4005 | BCR | C21-C22-C23-C24 |
| 17 | H | 4005 | BCR | C37-C22-C23-C24 |
| 17 | H | 4005 | BCR | C23-C24-C25-C30 |
| 17 | H | 4010 | BCR | C23-C24-C25-C26 |
| 17 | H | 4017 | BCR | C1-C6-C7-C8 |
| 17 | H | 4014 | BCR | C17-C18-C19-C20 |
| 17 | H | 4014 | BCR | C36-C18-C19-C20 |
| 17 | T | 4013 | BCR | C17-C18-C19-C20 |
| 17 | T | 4013 | BCR | C36-C18-C19-C20 |
| 17 | T | 4015 | BCR | C23-C24-C25-C30 |
| 17 | T | 4012 | BCR | C5-C6-C7-C8 |
| 17 | T | 4012 | BCR | C11-C12-C13-C14 |
| 17 | T | 4012 | BCR | C11-C12-C13-C35 |
| 17 | U | 4104 | BCR | C21-C22-C23-C24 |
| 17 | U | 4104 | BCR | C37-C22-C23-C24 |
| 17 | V | 4019 | BCR | C7-C8-C9-C10 |
| 17 | V | 4019 | BCR | C7-C8-C9-C34 |
| 17 | V | 4219 | BCR | C7-C8-C9-C10 |
| 17 | W | 4021 | BCR | C5-C6-C7-C8 |
| 17 | W | 4021 | BCR | C11-C12-C13-C35 |
| 17 | W | 4021 | BCR | C17-C18-C19-C20 |
| 17 | W | 4021 | BCR | C36-C18-C19-C20 |
| 17 | Y | 521 | BCR | C7-C8-C9-C10 |
| 17 | Y | 521 | BCR | C7-C8-C9-C34 |
| 17 | Y | 522 | BCR | C1-C6-C7-C8 |
| 17 | Y | 522 | BCR | C5-C6-C7-C8 |
| 17 | Y | 522 | BCR | C7-C8-C9-C10 |
| 17 | Y | 522 | BCR | C7-C8-C9-C34 |
| 17 | Y | 523 | BCR | C21-C22-C23-C24 |
| 17 | Y | 523 | BCR | C37-C22-C23-C24 |
| 17 | Z | 521 | BCR | C7-C8-C9-C10 |
| 17 | Z | 521 | BCR | C7-C8-C9-C34 |
| 17 | Z | 522 | BCR | C5-C6-C7-C8 |
| 17 | Z | 522 | BCR | C7-C8-C9-C10 |
| 17 | Z | 522 | BCR | C7-C8-C9-C34 |
| 17 | Z | 523 | BCR | C21-C22-C23-C24 |
| 17 | Z | 523 | BCR | C37-C22-C23-C24 |
| 17 | a | 521 | BCR | C7-C8-C9-C34 |
| 17 | a | 522 | BCR | C7-C8-C9-C10 |
| 17 | a | 522 | BCR | C7-C8-C9-C34 |
| 17 | a | 523 | BCR | C37-C22-C23-C24 |
| 17 | b | 521 | BCR | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | b | 521 | BCR | C7-C8-C9-C34 |
| 17 | b | 523 | BCR | C37-C22-C23-C24 |
| 17 | c | 521 | BCR | C7-C8-C9-C10 |
| 17 | c | 521 | BCR | C7-C8-C9-C34 |
| 17 | c | 521 | BCR | C17-C18-C19-C20 |
| 17 | c | 521 | BCR | C36-C18-C19-C20 |
| 17 | c | 522 | BCR | C5-C6-C7-C8 |
| 17 | c | 522 | BCR | C7-C8-C9-C10 |
| 17 | c | 522 | BCR | C7-C8-C9-C34 |
| 17 | c | 523 | BCR | C21-C22-C23-C24 |
| 17 | c | 523 | BCR | C37-C22-C23-C24 |
| 17 | d | 522 | BCR | C5-C6-C7-C8 |
| 17 | d | 523 | BCR | C21-C22-C23-C24 |
| 17 | d | 523 | BCR | C37-C22-C23-C24 |
| 17 | d | 524 | BCR | C7-C8-C9-C10 |
| 17 | d | 524 | BCR | C7-C8-C9-C34 |
| 17 | e | 4001 | BCR | C11-C12-C13-C14 |
| 17 | e | 4001 | BCR | C37-C22-C23-C24 |
| 17 | e | 4008 | BCR | C21-C22-C23-C24 |
| 17 | e | 4008 | BCR | C37-C22-C23-C24 |
| 17 | e | 4008 | BCR | C23-C24-C25-C26 |
| 17 | e | 4011 | BCR | C36-C18-C19-C20 |
| 17 | f | 4004 | BCR | C7-C8-C9-C10 |
| 17 | f | 4004 | BCR | C7-C8-C9-C34 |
| 17 | f | 4004 | BCR | C21-C22-C23-C24 |
| 17 | f | 4004 | BCR | C37-C22-C23-C24 |
| 17 | f | 4004 | BCR | C23-C24-C25-C30 |
| 17 | f | 4005 | BCR | C7-C8-C9-C10 |
| 17 | f | 4005 | BCR | C7-C8-C9-C34 |
| 17 | f | 4005 | BCR | C21-C22-C23-C24 |
| 17 | f | 4005 | BCR | C37-C22-C23-C24 |
| 17 | f | 4005 | BCR | C23-C24-C25-C30 |
| 17 | f | 4010 | BCR | C23-C24-C25-C26 |
| 17 | f | 4017 | BCR | C1-C6-C7-C8 |
| 17 | f | 4014 | BCR | C17-C18-C19-C20 |
| 17 | f | 4014 | BCR | C36-C18-C19-C20 |
| 17 | l | 4013 | BCR | C17-C18-C19-C20 |
| 17 | l | 4013 | BCR | C36-C18-C19-C20 |
| 17 | l | 4015 | BCR | C23-C24-C25-C30 |
| 17 | l | 4012 | BCR | C5-C6-C7-C8 |
| 17 | l | 4012 | BCR | C11-C12-C13-C14 |
| 17 | l | 4012 | BCR | C11-C12-C13-C35 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | m | 4104 | BCR | C21-C22-C23-C24 |
| 17 | m | 4104 | BCR | C37-C22-C23-C24 |
| 17 | n | 4019 | BCR | C7-C8-C9-C10 |
| 17 | n | 4019 | BCR | C7-C8-C9-C34 |
| 17 | n | 4219 | BCR | C7-C8-C9-C10 |
| 17 | o | 4021 | BCR | C5-C6-C7-C8 |
| 17 | o | 4021 | BCR | C11-C12-C13-C35 |
| 17 | o | 4021 | BCR | C17-C18-C19-C20 |
| 17 | o | 4021 | BCR | C36-C18-C19-C20 |
| 17 | q | 521 | BCR | C7-C8-C9-C10 |
| 17 | q | 521 | BCR | C7-C8-C9-C34 |
| 17 | q | 522 | BCR | C1-C6-C7-C8 |
| 17 | q | 522 | BCR | C5-C6-C7-C8 |
| 17 | q | 522 | BCR | C7-C8-C9-C10 |
| 17 | q | 522 | BCR | C7-C8-C9-C34 |
| 17 | q | 523 | BCR | C21-C22-C23-C24 |
| 17 | q | 523 | BCR | C37-C22-C23-C24 |
| 17 | r | 521 | BCR | C7-C8-C9-C10 |
| 17 | r | 521 | BCR | C7-C8-C9-C34 |
| 17 | r | 522 | BCR | C5-C6-C7-C8 |
| 17 | r | 522 | BCR | C7-C8-C9-C10 |
| 17 | r | 522 | BCR | C7-C8-C9-C34 |
| 17 | r | 523 | BCR | C21-C22-C23-C24 |
| 17 | r | 523 | BCR | C37-C22-C23-C24 |
| 17 | s | 521 | BCR | C7-C8-C9-C34 |
| 17 | s | 522 | BCR | C7-C8-C9-C10 |
| 17 | s | 522 | BCR | C7-C8-C9-C34 |
| 17 | s | 523 | BCR | C37-C22-C23-C24 |
| 17 | t | 521 | BCR | C7-C8-C9-C10 |
| 17 | t | 521 | BCR | C7-C8-C9-C34 |
| 17 | t | 523 | BCR | C37-C22-C23-C24 |
| 17 | u | 521 | BCR | C7-C8-C9-C10 |
| 17 | u | 521 | BCR | C7-C8-C9-C34 |
| 17 | u | 521 | BCR | C17-C18-C19-C20 |
| 17 | u | 521 | BCR | C36-C18-C19-C20 |
| 17 | u | 522 | BCR | C5-C6-C7-C8 |
| 17 | u | 522 | BCR | C7-C8-C9-C10 |
| 17 | u | 522 | BCR | C7-C8-C9-C34 |
| 17 | u | 523 | BCR | C21-C22-C23-C24 |
| 17 | u | 523 | BCR | C37-C22-C23-C24 |
| 17 | v | 522 | BCR | C5-C6-C7-C8 |
| 17 | v | 523 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | v | 523 | BCR | C37-C22-C23-C24 |
| 17 | v | 524 | BCR | C7-C8-C9-C10 |
| 17 | v | 524 | BCR | C7-C8-C9-C34 |
| 18 | A | 5002 | LHG | O2-C2-C3-O3 |
| 18 | A | 5002 | LHG | O9-C7-O7-C5 |
| 18 | A | 5002 | LHG | C8-C7-O7-C5 |
| 18 | A | 5004 | LHG | O1-C1-C2-C3 |
| 18 | A | 5004 | LHG | C3-O3-P-O4 |
| 18 | A | 5004 | LHG | C3-O3-P-O6 |
| 18 | A | 5004 | LHG | C8-C7-O7-C5 |
| 18 | A | 5005 | LHG | C3-O3-P-O4 |
| 18 | A | 5006 | LHG | C4-O6-P-O4 |
| 18 | A | 5008 | LHG | C4-O6-P-O3 |
| 18 | A | 5008 | LHG | O7-C5-C6-O8 |
| 18 | A | 5008 | LHG | C8-C7-O7-C5 |
| 18 | A | 5009 | LHG | C3-O3-P-O4 |
| 18 | A | 5009 | LHG | C3-O3-P-O5 |
| 18 | A | 5009 | LHG | C3-O3-P-O6 |
| 18 | A | 5009 | LHG | C4-O6-P-O4 |
| 18 | A | 5009 | LHG | O9-C7-O7-C5 |
| 18 | B | 1842 | LHG | C3-O3-P-O5 |
| 18 | B | 1842 | LHG | O9-C7-O7-C5 |
| 18 | B | 1842 | LHG | C8-C7-O7-C5 |
| 18 | B | 1855 | LHG | C3-O3-P-O4 |
| 18 | B | 1855 | LHG | C4-O6-P-O5 |
| 18 | I | 5001 | LHG | O1-C1-C2-C3 |
| 18 | I | 5001 | LHG | C3-O3-P-O4 |
| 18 | I | 5001 | LHG | O9-C7-O7-C5 |
| 18 | I | 5001 | LHG | C8-C7-O7-C5 |
| 18 | I | 5001 | LHG | C24-C23-O8-C6 |
| 18 | L | 5218 | LHG | C3-O3-P-O4 |
| 18 | L | 5218 | LHG | C3-O3-P-O5 |
| 18 | L | 5218 | LHG | O7-C5-C6-O8 |
| 18 | L | 5218 | LHG | C8-C7-O7-C5 |
| 18 | L | 5220 | LHG | C4-O6-P-O5 |
| 18 | L | 5220 | LHG | C8-C7-O7-C5 |
| 18 | L | 5221 | LHG | O1-C1-C2-C3 |
| 18 | L | 5221 | LHG | C3-O3-P-O5 |
| 18 | L | 5221 | LHG | C4-O6-P-O3 |
| 18 | L | 5221 | LHG | C4-O6-P-O5 |
| 18 | G | 5002 | LHG | O2-C2-C3-O3 |
| 18 | G | 5002 | LHG | O9-C7-O7-C5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 18 | G | 5002 | LHG | C8-C7-O7-C5 |
| 18 | G | 5004 | LHG | O1-C1-C2-C3 |
| 18 | G | 5004 | LHG | C3-O3-P-O4 |
| 18 | G | 5004 | LHG | C3-O3-P-O6 |
| 18 | G | 5004 | LHG | C8-C7-O7-C5 |
| 18 | G | 5005 | LHG | C3-O3-P-O4 |
| 18 | G | 5006 | LHG | C4-O6-P-O4 |
| 18 | G | 5008 | LHG | C4-O6-P-O3 |
| 18 | G | 5008 | LHG | O7-C5-C6-O8 |
| 18 | G | 5008 | LHG | C8-C7-O7-C5 |
| 18 | G | 5009 | LHG | C3-O3-P-O4 |
| 18 | G | 5009 | LHG | C3-O3-P-O5 |
| 18 | G | 5009 | LHG | C3-O3-P-O6 |
| 18 | G | 5009 | LHG | C4-O6-P-O4 |
| 18 | G | 5009 | LHG | O9-C7-O7-C5 |
| 18 | H | 1842 | LHG | C3-O3-P-O5 |
| 18 | H | 1842 | LHG | O9-C7-O7-C5 |
| 18 | H | 1842 | LHG | C8-C7-O7-C5 |
| 18 | H | 1855 | LHG | C3-O3-P-O4 |
| 18 | H | 1855 | LHG | C4-O6-P-O5 |
| 18 | S | 5001 | LHG | O1-C1-C2-C3 |
| 18 | S | 5001 | LHG | C3-O3-P-O4 |
| 18 | S | 5001 | LHG | O9-C7-O7-C5 |
| 18 | S | 5001 | LHG | C8-C7-O7-C5 |
| 18 | S | 5001 | LHG | C24-C23-O8-C6 |
| 18 | V | 5218 | LHG | C3-O3-P-O4 |
| 18 | V | 5218 | LHG | C3-O3-P-O5 |
| 18 | V | 5218 | LHG | O7-C5-C6-O8 |
| 18 | V | 5218 | LHG | C8-C7-O7-C5 |
| 18 | V | 5220 | LHG | C4-O6-P-O5 |
| 18 | V | 5220 | LHG | C8-C7-O7-C5 |
| 18 | V | 5221 | LHG | O1-C1-C2-C3 |
| 18 | V | 5221 | LHG | C3-O3-P-O5 |
| 18 | V | 5221 | LHG | C4-O6-P-O3 |
| 18 | V | 5221 | LHG | C4-O6-P-O5 |
| 18 | e | 5002 | LHG | O2-C2-C3-O3 |
| 18 | e | 5002 | LHG | O9-C7-O7-C5 |
| 18 | e | 5002 | LHG | C8-C7-O7-C5 |
| 18 | e | 5004 | LHG | O1-C1-C2-C3 |
| 18 | e | 5004 | LHG | C3-O3-P-O4 |
| 18 | e | 5004 | LHG | C3-O3-P-O6 |
| 18 | e | 5004 | LHG | C8-C7-O7-C5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 18 | e | 5005 | LHG | C3-O3-P-O4 |
| 18 | e | 5006 | LHG | C4-O6-P-O4 |
| 18 | e | 5008 | LHG | C4-O6-P-O3 |
| 18 | e | 5008 | LHG | O7-C5-C6-O8 |
| 18 | e | 5008 | LHG | C8-C7-O7-C5 |
| 18 | e | 5009 | LHG | C3-O3-P-O4 |
| 18 | e | 5009 | LHG | C3-O3-P-O5 |
| 18 | e | 5009 | LHG | C3-O3-P-O6 |
| 18 | e | 5009 | LHG | C4-O6-P-O4 |
| 18 | e | 5009 | LHG | O9-C7-O7-C5 |
| 18 | f | 1842 | LHG | C3-O3-P-O5 |
| 18 | f | 1842 | LHG | O9-C7-O7-C5 |
| 18 | f | 1842 | LHG | C8-C7-O7-C5 |
| 18 | f | 1855 | LHG | C3-O3-P-O4 |
| 18 | f | 1855 | LHG | C4-O6-P-O5 |
| 18 | k | 5001 | LHG | O1-C1-C2-C3 |
| 18 | k | 5001 | LHG | C3-O3-P-O4 |
| 18 | k | 5001 | LHG | O9-C7-O7-C5 |
| 18 | k | 5001 | LHG | C8-C7-O7-C5 |
| 18 | k | 5001 | LHG | C24-C23-O8-C6 |
| 18 | n | 5218 | LHG | C3-O3-P-O4 |
| 18 | n | 5218 | LHG | C3-O3-P-O5 |
| 18 | n | 5218 | LHG | O7-C5-C6-O8 |
| 18 | n | 5218 | LHG | C8-C7-O7-C5 |
| 18 | n | 5220 | LHG | C4-O6-P-O5 |
| 18 | n | 5220 | LHG | C8-C7-O7-C5 |
| 18 | n | 5221 | LHG | O1-C1-C2-C3 |
| 18 | n | 5221 | LHG | C3-O3-P-O5 |
| 18 | n | 5221 | LHG | C4-O6-P-O3 |
| 18 | n | 5221 | LHG | C4-O6-P-O5 |
| 19 | B | 1843 | LMU | C2'-C1'-O1'-C1 |
| 19 | B | 1843 | LMU | O5'-C1'-O1'-C1 |
| 19 | J | 5105 | LMU | C2'-C1'-O1'-C1 |
| 19 | J | 5105 | LMU | O5'-C1'-O1'-C1 |
| 19 | H | 1843 | LMU | C2'-C1'-O1'-C1 |
| 19 | H | 1843 | LMU | O5'-C1'-O1'-C1 |
| 19 | T | 5105 | LMU | C2'-C1'-O1'-C1 |
| 19 | T | 5105 | LMU | O5'-C1'-O1'-C1 |
| 19 | f | 1843 | LMU | C2'-C1'-O1'-C1 |
| 19 | f | 1843 | LMU | O5'-C1'-O1'-C1 |
| 19 | l | 5105 | LMU | C2'-C1'-O1'-C1 |
| 19 | l | 5105 | LMU | O5'-C1'-O1'-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | L | 5216 | SQD | C5-C6-S-O7 |
| 21 | L | 5216 | SQD | C5-C6-S-O8 |
| 21 | L | 5216 | SQD | C5-C6-S-O9 |
| 21 | 1 | 822 | SQD | O47-C45-C46-O48 |
| 21 | 1 | 822 | SQD | O49-C7-O47-C45 |
| 21 | 1 | 822 | SQD | C8-C7-O47-C45 |
| 21 | 2 | 822 | SQD | O49-C7-O47-C45 |
| 21 | 2 | 822 | SQD | C8-C7-O47-C45 |
| 21 | 3 | 822 | SQD | O47-C45-C46-O48 |
| 21 | 3 | 822 | SQD | O49-C7-O47-C45 |
| 21 | 3 | 822 | SQD | C8-C7-O47-C45 |
| 21 | 4 | 822 | SQD | C8-C7-O47-C45 |
| 21 | 6 | 822 | SQD | C46-C45-O47-C7 |
| 21 | V | 5216 | SQD | C5-C6-S-O7 |
| 21 | V | 5216 | SQD | C5-C6-S-O8 |
| 21 | V | 5216 | SQD | C5-C6-S-O9 |
| 21 | Y | 822 | SQD | O47-C45-C46-O48 |
| 21 | Y | 822 | SQD | O49-C7-O47-C45 |
| 21 | Y | 822 | SQD | C8-C7-O47-C45 |
| 21 | Z | 822 | SQD | O49-C7-O47-C45 |
| 21 | Z | 822 | SQD | C8-C7-O47-C45 |
| 21 | a | 822 | SQD | O47-C45-C46-O48 |
| 21 | a | 822 | SQD | O49-C7-O47-C45 |
| 21 | a | 822 | SQD | C8-C7-O47-C45 |
| 21 | b | 822 | SQD | C8-C7-O47-C45 |
| 21 | d | 822 | SQD | C46-C45-O47-C7 |
| 21 | n | 5216 | SQD | C5-C6-S-O7 |
| 21 | n | 5216 | SQD | C5-C6-S-O8 |
| 21 | n | 5216 | SQD | C5-C6-S-O9 |
| 21 | q | 822 | SQD | O47-C45-C46-O48 |
| 21 | q | 822 | SQD | O49-C7-O47-C45 |
| 21 | q | 822 | SQD | C8-C7-O47-C45 |
| 21 | r | 822 | SQD | O49-C7-O47-C45 |
| 21 | r | 822 | SQD | C8-C7-O47-C45 |
| 21 | s | 822 | SQD | O47-C45-C46-O48 |
| 21 | s | 822 | SQD | O49-C7-O47-C45 |
| 21 | s | 822 | SQD | C8-C7-O47-C45 |
| 21 | t | 822 | SQD | C8-C7-O47-C45 |
| 21 | v | 822 | SQD | C46-C45-O47-C7 |
| 21 | 4 | 822 | SQD | O49-C7-O47-C45 |
| 21 | 5 | 822 | SQD | O49-C7-O47-C45 |
| 21 | 5 | 822 | SQD | C8-C7-O47-C45 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | 6 | 822 | SQD | C8-C7-O47-C45 |
| 21 | b | 822 | SQD | O49-C7-O47-C45 |
| 21 | c | 822 | SQD | O49-C7-O47-C45 |
| 21 | c | 822 | SQD | C8-C7-O47-C45 |
| 21 | d | 822 | SQD | C8-C7-O47-C45 |
| 21 | t | 822 | SQD | O49-C7-O47-C45 |
| 21 | u | 822 | SQD | O49-C7-O47-C45 |
| 21 | u | 822 | SQD | C8-C7-O47-C45 |
| 21 | v | 822 | SQD | C8-C7-O47-C45 |
| 14 | A | 1139 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1023 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1139 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1023 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1139 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1023 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 518 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | 6 | 822 | SQD | O49-C7-O47-C45 |
| 21 | d | 822 | SQD | O49-C7-O47-C45 |
| 21 | v | 822 | SQD | O49-C7-O47-C45 |
| 14 | B | 1219 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1219 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1219 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 506 | CLA | O1D-CGD-O2D-CED |
| 21 | 4 | 822 | SQD | C24-C23-O48-C46 |
| 21 | b | 822 | SQD | C24-C23-O48-C46 |
| 21 | t | 822 | SQD | C24-C23-O48-C46 |
| 14 | A | 1108 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1123 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1132 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1139 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1801 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1021 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1023 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1203 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1216 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1219 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1239 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1207 | CLA | CBD-CGD-O2D-CED |
| 14 | F | 1301 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 508 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 1 | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1108 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1123 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1132 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1139 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1801 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1021 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1023 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1203 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1216 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1219 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1207 | CLA | CBD-CGD-O2D-CED |
| 14 | R | 1301 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 516 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | Z | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1108 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1123 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1132 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1139 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1801 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1021 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1023 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1203 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1216 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1219 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1239 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1207 | CLA | CBD-CGD-O2D-CED |
| 14 | j | 1301 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 516 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 506 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | s | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 501 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 503 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 506 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1109 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1209 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1227 | CLA | O1A-CGA-O2A-C1 |
| 14 | 3 | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | 6 | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1109 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1209 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1227 | CLA | O1A-CGA-O2A-C1 |
| 14 | a | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | d | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1109 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1209 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1227 | CLA | O1A-CGA-O2A-C1 |
| 14 | s | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | v | 505 | CLA | O1A-CGA-O2A-C1 |
| 18 | I | 5001 | LHG | O10-C23-O8-C6 |
| 18 | L | 5221 | LHG | O10-C23-O8-C6 |
| 18 | S | 5001 | LHG | O10-C23-O8-C6 |
| 18 | V | 5221 | LHG | O10-C23-O8-C6 |
| 18 | k | 5001 | LHG | O10-C23-O8-C6 |
| 18 | n | 5221 | LHG | O10-C23-O8-C6 |
| 14 | A | 1108 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 506 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 4 | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1108 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1108 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | K | 1105 | CLA | C4C-C3C-CAC-CBC |
| 14 | U | 1105 | CLA | C4C-C3C-CAC-CBC |
| 14 | m | 1105 | CLA | C4C-C3C-CAC-CBC |
| 14 | B | 1021 | CLA | O1D-CGD-O2D-CED |
| 14 | K | 1105 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 502 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1021 | CLA | O1D-CGD-O2D-CED |
| 14 | U | 1105 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 516 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 502 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 516 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | f | 1021 | CLA | O1D-CGD-O2D-CED |
| 14 | m | 1105 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 502 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1109 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1206 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1209 | CLA | CBA-CGA-O2A-C1 |
| 14 | 6 | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1109 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1206 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1209 | CLA | CBA-CGA-O2A-C1 |
| 14 | d | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1109 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1206 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1209 | CLA | CBA-CGA-O2A-C1 |
| 14 | v | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1106 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1111 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1115 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1126 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1131 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1022 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1204 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1209 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1229 | CLA | CBD-CGD-O2D-CED |
| 14 | K | 1103 | CLA | CBD-CGD-O2D-CED |
| 14 | L | 1503 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1106 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1111 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1115 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1126 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1131 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1022 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1204 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1209 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1229 | CLA | CBD-CGD-O2D-CED |
| 14 | U | 1103 | CLA | CBD-CGD-O2D-CED |
| 14 | V | 1503 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1106 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1111 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1115 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1126 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1131 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1022 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1204 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1209 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1229 | CLA | CBD-CGD-O2D-CED |
| 14 | m | 1103 | CLA | CBD-CGD-O2D-CED |
| 14 | n | 1503 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 513 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1110 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1119 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1140 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1206 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1217 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1240 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1207 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 2 | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1110 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1119 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1140 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1206 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1217 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1240 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1207 | CLA | O1A-CGA-O2A-C1 |
| 14 | Z | 505 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1110 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1119 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1140 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1206 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1217 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1240 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1207 | CLA | O1A-CGA-O2A-C1 |
| 14 | r | 505 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5006 | LHG | O10-C23-O8-C6 |
| 18 | A | 5009 | LHG | O10-C23-O8-C6 |
| 18 | L | 5220 | LHG | O10-C23-O8-C6 |
| 18 | G | 5006 | LHG | O10-C23-O8-C6 |
| 18 | G | 5009 | LHG | O10-C23-O8-C6 |
| 18 | V | 5220 | LHG | O10-C23-O8-C6 |
| 18 | e | 5006 | LHG | O10-C23-O8-C6 |
| 18 | e | 5009 | LHG | O10-C23-O8-C6 |
| 18 | n | 5220 | LHG | O10-C23-O8-C6 |
| 21 | 1 | 822 | SQD | O10-C23-O48-C46 |
| 21 | Y | 822 | SQD | O10-C23-O48-C46 |
| 21 | q | 822 | SQD | O10-C23-O48-C46 |
| 14 | A | 1119 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1138 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1119 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1138 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1119 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1138 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | J | 1302 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 518 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 5 | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | T | 1302 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | l | 1302 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 503 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 506 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1013 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1121 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1237 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1201 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1231 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1234 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 505 | CLA | CBD-CGD-O2D-CED |
| 14 | 4 | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1013 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1121 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1237 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1201 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1231 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1234 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 505 | CLA | CBD-CGD-O2D-CED |
| 14 | b | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1013 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1121 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1237 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1201 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1231 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1234 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 507 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 505 | CLA | CBD-CGD-O2D-CED |
| 14 | t | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1206 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1239 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1206 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1239 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1206 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1239 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 519 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5004 | LHG | O9-C7-O7-C5 |
| 18 | A | 5007 | LHG | O9-C7-O7-C5 |
| 18 | A | 5008 | LHG | O9-C7-O7-C5 |
| 18 | B | 1855 | LHG | O9-C7-O7-C5 |
| 18 | L | 5218 | LHG | O9-C7-O7-C5 |
| 18 | L | 5220 | LHG | O9-C7-O7-C5 |
| 18 | G | 5004 | LHG | O9-C7-O7-C5 |
| 18 | G | 5007 | LHG | O9-C7-O7-C5 |
| 18 | G | 5008 | LHG | O9-C7-O7-C5 |
| 18 | H | 1855 | LHG | O9-C7-O7-C5 |
| 18 | V | 5218 | LHG | O9-C7-O7-C5 |
| 18 | V | 5220 | LHG | O9-C7-O7-C5 |
| 18 | e | 5004 | LHG | O9-C7-O7-C5 |
| 18 | e | 5007 | LHG | O9-C7-O7-C5 |
| 18 | e | 5008 | LHG | O9-C7-O7-C5 |
| 18 | f | 1855 | LHG | O9-C7-O7-C5 |
| 18 | n | 5218 | LHG | O9-C7-O7-C5 |
| 18 | n | 5220 | LHG | O9-C7-O7-C5 |
| 18 | L | 5218 | LHG | O10-C23-O8-C6 |
| 18 | V | 5218 | LHG | O10-C23-O8-C6 |
| 18 | n | 5218 | LHG | O10-C23-O8-C6 |
| 14 | K | 1105 | CLA | C2C-C3C-CAC-CBC |
| 14 | U | 1105 | CLA | C2C-C3C-CAC-CBC |
| 14 | m | 1105 | CLA | C2C-C3C-CAC-CBC |
| 14 | A | 1116 | CLA | C3-C5-C6-C7 |
| 14 | A | 1118 | CLA | C3-C5-C6-C7 |
| 14 | A | 1119 | CLA | C3-C5-C6-C7 |
| 14 | A | 1121 | CLA | C3-C5-C6-C7 |
| 14 | A | 1122 | CLA | C3-C5-C6-C7 |
| 14 | A | 1133 | CLA | C3-C5-C6-C7 |
| 14 | A | 1136 | CLA | C3-C5-C6-C7 |
| 14 | A | 1139 | CLA | C3-C5-C6-C7 |
| 14 | B | 1211 | CLA | C3-C5-C6-C7 |
| 14 | B | 1231 | CLA | C3-C5-C6-C7 |
| 14 | B | 1239 | CLA | C3-C5-C6-C7 |
| 14 | L | 1503 | CLA | C3-C5-C6-C7 |
| 14 | 2 | 501 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 14 | 2 | 505 | CLA | C3-C5-C6-C7 |
| 14 | 2 | 518 | CLA | C3-C5-C6-C7 |
| 14 | 6 | 505 | CLA | C3-C5-C6-C7 |
| 14 | G | 1116 | CLA | C3-C5-C6-C7 |
| 14 | G | 1118 | CLA | C3-C5-C6-C7 |
| 14 | G | 1119 | CLA | C3-C5-C6-C7 |
| 14 | G | 1121 | CLA | C3-C5-C6-C7 |
| 14 | G | 1122 | CLA | C3-C5-C6-C7 |
| 14 | G | 1133 | CLA | C3-C5-C6-C7 |
| 14 | G | 1136 | CLA | C3-C5-C6-C7 |
| 14 | G | 1139 | CLA | C3-C5-C6-C7 |
| 14 | H | 1211 | CLA | C3-C5-C6-C7 |
| 14 | H | 1231 | CLA | C3-C5-C6-C7 |
| 14 | H | 1239 | CLA | C3-C5-C6-C7 |
| 14 | V | 1503 | CLA | C3-C5-C6-C7 |
| 14 | Z | 501 | CLA | C3-C5-C6-C7 |
| 14 | Z | 505 | CLA | C3-C5-C6-C7 |
| 14 | Z | 518 | CLA | C3-C5-C6-C7 |
| 14 | d | 505 | CLA | C3-C5-C6-C7 |
| 14 | e | 1116 | CLA | C3-C5-C6-C7 |
| 14 | e | 1118 | CLA | C3-C5-C6-C7 |
| 14 | e | 1119 | CLA | C3-C5-C6-C7 |
| 14 | e | 1121 | CLA | C3-C5-C6-C7 |
| 14 | e | 1122 | CLA | C3-C5-C6-C7 |
| 14 | e | 1133 | CLA | C3-C5-C6-C7 |
| 14 | e | 1136 | CLA | C3-C5-C6-C7 |
| 14 | e | 1139 | CLA | C3-C5-C6-C7 |
| 14 | f | 1211 | CLA | C3-C5-C6-C7 |
| 14 | f | 1231 | CLA | C3-C5-C6-C7 |
| 14 | f | 1239 | CLA | C3-C5-C6-C7 |
| 14 | n | 1503 | CLA | C3-C5-C6-C7 |
| 14 | r | 501 | CLA | C3-C5-C6-C7 |
| 14 | r | 505 | CLA | C3-C5-C6-C7 |
| 14 | r | 518 | CLA | C3-C5-C6-C7 |
| 14 | v | 505 | CLA | C3-C5-C6-C7 |
| 14 | A | 1110 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1217 | CLA | CBA-CGA-O2A-C1 |
| 14 | 2 | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | 3 | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1110 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1217 | CLA | CBA-CGA-O2A-C1 |
| 14 | Z | 505 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | a | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1110 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1217 | CLA | CBA-CGA-O2A-C1 |
| 14 | r | 505 | CLA | CBA-CGA-O2A-C1 |
| 14 | s | 505 | CLA | CBA-CGA-O2A-C1 |
| 18 | A | 5006 | LHG | C24-C23-O8-C6 |
| 18 | L | 5218 | LHG | C24-C23-O8-C6 |
| 18 | L | 5220 | LHG | C24-C23-O8-C6 |
| 18 | G | 5006 | LHG | C24-C23-O8-C6 |
| 18 | V | 5218 | LHG | C24-C23-O8-C6 |
| 18 | V | 5220 | LHG | C24-C23-O8-C6 |
| 18 | e | 5006 | LHG | C24-C23-O8-C6 |
| 18 | n | 5218 | LHG | C24-C23-O8-C6 |
| 18 | n | 5220 | LHG | C24-C23-O8-C6 |
| 21 | 4 | 822 | SQD | O10-C23-O48-C46 |
| 21 | b | 822 | SQD | O10-C23-O48-C46 |
| 21 | t | 822 | SQD | O10-C23-O48-C46 |
| 18 | A | 5009 | LHG | C8-C7-O7-C5 |
| 18 | G | 5009 | LHG | C8-C7-O7-C5 |
| 18 | e | 5009 | LHG | C8-C7-O7-C5 |
| 14 | 3 | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1011 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1011 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1011 | CLA | CBD-CGD-O2D-CED |
| 14 | 3 | 516 | CLA | C2C-C3C-CAC-CBC |
| 14 | a | 516 | CLA | C2C-C3C-CAC-CBC |
| 14 | s | 516 | CLA | C2C-C3C-CAC-CBC |
| 19 | J | 5105 | LMU | O5'-C5'-C6'-O6' |
| 19 | T | 5105 | LMU | O5'-C5'-C6'-O6' |
| 19 | l | 5105 | LMU | O5'-C5'-C6'-O6' |
| 14 | A | 1133 | CLA | C4-C3-C5-C6 |
| 14 | A | 1130 | CLA | C4-C3-C5-C6 |
| 14 | L | 1503 | CLA | C4-C3-C5-C6 |
| 14 | G | 1133 | CLA | C4-C3-C5-C6 |
| 14 | G | 1130 | CLA | C4-C3-C5-C6 |
| 14 | V | 1503 | CLA | C4-C3-C5-C6 |
| 14 | e | 1133 | CLA | C4-C3-C5-C6 |
| 14 | e | 1130 | CLA | C4-C3-C5-C6 |
| 14 | n | 1503 | CLA | C4-C3-C5-C6 |
| 14 | A | 1104 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1237 | CLA | C2-C3-C5-C6 |
| 14 | A | 1130 | CLA | C2-C3-C5-C6 |
| 14 | G | 1104 | CLA | C2-C3-C5-C6 |
| 14 | G | 1237 | CLA | C2-C3-C5-C6 |
| 14 | G | 1130 | CLA | C2-C3-C5-C6 |
| 14 | e | 1104 | CLA | C2-C3-C5-C6 |
| 14 | e | 1237 | CLA | C2-C3-C5-C6 |
| 14 | e | 1130 | CLA | C2-C3-C5-C6 |
| 14 | A | 1133 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1220 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1133 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1220 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1133 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1220 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 512 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1108 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1119 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1127 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1012 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1206 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1221 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1228 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1232 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1238 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | 2 | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | 2 | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | 5 | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | 6 | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | 6 | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1108 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1119 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1127 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1012 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1206 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1221 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1228 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1232 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1238 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | d | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | d | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1108 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1119 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1127 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1012 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1206 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1221 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1228 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1232 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1238 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 507 | CLA | C2A-CAA-CBA-CGA |
| 14 | v | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | v | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1801 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1216 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1801 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1216 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1801 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1216 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1102 | CLA | C3-C5-C6-C7 |
| 14 | B | 1206 | CLA | C3-C5-C6-C7 |
| 14 | B | 1232 | CLA | C3-C5-C6-C7 |
| 14 | G | 1102 | CLA | C3-C5-C6-C7 |
| 14 | H | 1206 | CLA | C3-C5-C6-C7 |
| 14 | H | 1232 | CLA | C3-C5-C6-C7 |
| 14 | e | 1102 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | f | 1206 | CLA | C3-C5-C6-C7 |
| 14 | f | 1232 | CLA | C3-C5-C6-C7 |
| 14 | A | 1119 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1122 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1140 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1240 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1207 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1230 | CLA | CBA-CGA-O2A-C1 |
| 14 | K | 1401 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1119 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1122 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1140 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1240 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1207 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1230 | CLA | CBA-CGA-O2A-C1 |
| 14 | U | 1401 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1119 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1122 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1140 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1240 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1207 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1230 | CLA | CBA-CGA-O2A-C1 |
| 14 | m | 1401 | CLA | CBA-CGA-O2A-C1 |
| 18 | A | 5009 | LHG | C24-C23-O8-C6 |
| 18 | G | 5009 | LHG | C24-C23-O8-C6 |
| 18 | e | 5009 | LHG | C24-C23-O8-C6 |
| 21 | 3 | 822 | SQD | C24-C23-O48-C46 |
| 21 | a | 822 | SQD | C24-C23-O48-C46 |
| 21 | s | 822 | SQD | C24-C23-O48-C46 |
| 21 | 2 | 822 | SQD | C24-C23-O48-C46 |
| 21 | Z | 822 | SQD | C24-C23-O48-C46 |
| 21 | r | 822 | SQD | C24-C23-O48-C46 |
| 14 | F | 1301 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | R | 1301 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | j | 1301 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 517 | CLA | O1D-CGD-O2D-CED |
| 15 | A | 2001 | PQN | C11-C12-C13-C14 |
| 15 | B | 2002 | PQN | C11-C12-C13-C14 |
| 15 | G | 2001 | PQN | C11-C12-C13-C14 |
| 15 | H | 2002 | PQN | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 15 | e | 2001 | PQN | C11-C12-C13-C14 |
| 15 | f | 2002 | PQN | C11-C12-C13-C14 |
| 14 | A | 1113 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1012 | CLA | CBD-CGD-O2D-CED |
| 14 | J | 1303 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1113 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1012 | CLA | CBD-CGD-O2D-CED |
| 14 | T | 1303 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1113 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1012 | CLA | CBD-CGD-O2D-CED |
| 14 | l | 1303 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1123 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1203 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1207 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1123 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1203 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1207 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1123 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1203 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1207 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 519 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 1852 | SQD | O49-C7-O47-C45 |
| 21 | H | 1852 | SQD | O49-C7-O47-C45 |
| 21 | f | 1852 | SQD | O49-C7-O47-C45 |
| 14 | A | 1130 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1230 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1130 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1230 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1130 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1230 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5001 | LHG | O10-C23-O8-C6 |
| 18 | G | 5001 | LHG | O10-C23-O8-C6 |
| 18 | e | 5001 | LHG | O10-C23-O8-C6 |
| 21 | 3 | 822 | SQD | O10-C23-O48-C46 |
| 21 | a | 822 | SQD | O10-C23-O48-C46 |
| 21 | s | 822 | SQD | O10-C23-O48-C46 |
| 21 | 2 | 822 | SQD | O10-C23-O48-C46 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | Z | 822 | SQD | O10-C23-O48-C46 |
| 21 | r | 822 | SQD | O10-C23-O48-C46 |
| 14 | 6 | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 501 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 501 | CLA | O1D-CGD-O2D-CED |
| 19 | A | 1848 | LMU | O5'-C5'-C6'-O6' |
| 19 | B | 1843 | LMU | O5B-C5B-C6B-O6B |
| 19 | G | 1848 | LMU | O5'-C5'-C6'-O6' |
| 19 | H | 1843 | LMU | O5B-C5B-C6B-O6B |
| 19 | e | 1848 | LMU | O5'-C5'-C6'-O6' |
| 19 | f | 1843 | LMU | O5B-C5B-C6B-O6B |
| 14 | A | 1120 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1122 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1221 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1235 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1230 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1120 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1122 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1221 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1235 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1230 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1120 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1122 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1221 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1235 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1230 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 517 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | 2 | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 517 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | r | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 517 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5005 | LHG | O2-C2-C3-O3 |
| 18 | L | 5220 | LHG | O2-C2-C3-O3 |
| 18 | G | 5005 | LHG | O2-C2-C3-O3 |
| 18 | V | 5220 | LHG | O2-C2-C3-O3 |
| 18 | e | 5005 | LHG | O2-C2-C3-O3 |
| 18 | n | 5220 | LHG | O2-C2-C3-O3 |
| 14 | A | 1107 | CLA | C3-C5-C6-C7 |
| 14 | A | 1108 | CLA | C3-C5-C6-C7 |
| 14 | A | 1129 | CLA | C3-C5-C6-C7 |
| 14 | B | 1205 | CLA | C3-C5-C6-C7 |
| 14 | G | 1107 | CLA | C3-C5-C6-C7 |
| 14 | G | 1108 | CLA | C3-C5-C6-C7 |
| 14 | G | 1129 | CLA | C3-C5-C6-C7 |
| 14 | H | 1205 | CLA | C3-C5-C6-C7 |
| 14 | e | 1107 | CLA | C3-C5-C6-C7 |
| 14 | e | 1108 | CLA | C3-C5-C6-C7 |
| 14 | e | 1129 | CLA | C3-C5-C6-C7 |
| 14 | f | 1205 | CLA | C3-C5-C6-C7 |
| 14 | A | 1108 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1129 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1130 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1234 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1108 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1129 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1130 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1234 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1108 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1129 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1130 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1234 | CLA | CBA-CGA-O2A-C1 |
| 18 | L | 5221 | LHG | C24-C23-O8-C6 |
| 18 | V | 5221 | LHG | C24-C23-O8-C6 |
| 18 | n | 5221 | LHG | C24-C23-O8-C6 |
| 21 | 1 | 822 | SQD | C24-C23-O48-C46 |
| 21 | Y | 822 | SQD | C24-C23-O48-C46 |
| 21 | q | 822 | SQD | C24-C23-O48-C46 |
| 19 | B | 1843 | LMU | O5'-C5'-C6'-O6' |
| 19 | H | 1843 | LMU | O5'-C5'-C6'-O6' |
| 19 | f | 1843 | LMU | O5'-C5'-C6'-O6' |
| 20 | J | 5104 | LMG | O6-C5-C6-O5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 20 | T | 5104 | LMG | O6-C5-C6-O5 |
| 20 | l | 5104 | LMG | O6-C5-C6-O5 |
| 19 | B | 1843 | LMU | C4'-C5'-C6'-O6' |
| 19 | H | 1843 | LMU | C4'-C5'-C6'-O6' |
| 19 | f | 1843 | LMU | C4'-C5'-C6'-O6' |
| 14 | A | 1132 | CLA | O1D-CGD-O2D-CED |
| 14 | l | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1132 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1132 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1103 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1103 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1103 | CLA | CBD-CGD-O2D-CED |
| 18 | B | 1855 | LHG | C5-C6-O8-C23 |
| 18 | H | 1855 | LHG | C5-C6-O8-C23 |
| 18 | f | 1855 | LHG | C5-C6-O8-C23 |
| 20 | B | 5002 | LMG | O6-C5-C6-O5 |
| 20 | H | 5002 | LMG | O6-C5-C6-O5 |
| 20 | f | 5002 | LMG | O6-C5-C6-O5 |
| 14 | A | 1013 | CLA | C3-C5-C6-C7 |
| 14 | B | 1215 | CLA | C3-C5-C6-C7 |
| 14 | G | 1013 | CLA | C3-C5-C6-C7 |
| 14 | H | 1215 | CLA | C3-C5-C6-C7 |
| 14 | e | 1013 | CLA | C3-C5-C6-C7 |
| 14 | f | 1215 | CLA | C3-C5-C6-C7 |
| 19 | B | 1843 | LMU | C4B-C5B-C6B-O6B |
| 19 | H | 1843 | LMU | C4B-C5B-C6B-O6B |
| 19 | f | 1843 | LMU | C4B-C5B-C6B-O6B |
| 14 | A | 1122 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1129 | CLA | O1A-CGA-O2A-C1 |
| 14 | K | 1401 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1108 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1122 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1129 | CLA | O1A-CGA-O2A-C1 |
| 14 | U | 1401 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1122 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1129 | CLA | O1A-CGA-O2A-C1 |
| 14 | m | 1401 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1115 | CLA | C4-C3-C5-C6 |
| 14 | G | 1115 | CLA | C4-C3-C5-C6 |
| 14 | e | 1115 | CLA | C4-C3-C5-C6 |
| 14 | A | 1115 | CLA | C2-C3-C5-C6 |
| 14 | A | 1137 | CLA | C2-C3-C5-C6 |
| 14 | G | 1115 | CLA | C2-C3-C5-C6 |
| 14 | G | 1137 | CLA | C2-C3-C5-C6 |
| 14 | e | 1115 | CLA | C2-C3-C5-C6 |
| 14 | e | 1137 | CLA | C2-C3-C5-C6 |
| 14 | A | 1134 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1218 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | 5 | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1134 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1218 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1134 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1218 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | 2 | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1108 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1108 | CLA | O1A-CGA-O2A-C1 |
| 19 | A | 1848 | LMU | O5'-C1'-O1'-C1 |
| 19 | G | 1848 | LMU | O5'-C1'-O1'-C1 |
| 19 | e | 1848 | LMU | O5'-C1'-O1'-C1 |
| 14 | A | 1133 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1135 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1237 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1211 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 3 | 518 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1133 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1135 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1237 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1211 | CLA | CBA-CGA-O2A-C1 |
| 14 | a | 518 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1133 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1135 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1237 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1211 | CLA | CBA-CGA-O2A-C1 |
| 14 | s | 518 | CLA | CBA-CGA-O2A-C1 |
| 18 | A | 5001 | LHG | C24-C23-O8-C6 |
| 18 | G | 5001 | LHG | C24-C23-O8-C6 |
| 14 | B | 1204 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1204 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1204 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1234 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1234 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1234 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1022 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1022 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1022 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5002 | LHG | C1-C2-C3-O3 |
| 18 | G | 5002 | LHG | C1-C2-C3-O3 |
| 18 | e | 5002 | LHG | C1-C2-C3-O3 |
| 20 | B | 5002 | LMG | C4-C5-C6-O5 |
| 20 | H | 5002 | LMG | C4-C5-C6-O5 |
| 20 | f | 5002 | LMG | C4-C5-C6-O5 |
| 14 | A | 1135 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1211 | CLA | O1A-CGA-O2A-C1 |
| 14 | 3 | 518 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1135 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1211 | CLA | O1A-CGA-O2A-C1 |
| 14 | a | 518 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1135 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1211 | CLA | O1A-CGA-O2A-C1 |
| 14 | s | 518 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1204 | CLA | C3-C5-C6-C7 |
| 14 | H | 1204 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | f | 1204 | CLA | C3-C5-C6-C7 |
| 14 | l | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1104 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1106 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1118 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1214 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1225 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1239 | CLA | CBA-CGA-O2A-C1 |
| 14 | J | 1302 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1104 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1106 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1118 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1214 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1225 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1239 | CLA | CBA-CGA-O2A-C1 |
| 14 | T | 1302 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1104 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1106 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1118 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1214 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1225 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1239 | CLA | CBA-CGA-O2A-C1 |
| 14 | l | 1302 | CLA | CBA-CGA-O2A-C1 |
| 18 | e | 5001 | LHG | C24-C23-O8-C6 |
| 19 | J | 5105 | LMU | C4'-C5'-C6'-O6' |
| 19 | T | 5105 | LMU | C4'-C5'-C6'-O6' |
| 19 | l | 5105 | LMU | C4'-C5'-C6'-O6' |
| 14 | A | 1115 | CLA | C10-C11-C12-C13 |
| 14 | G | 1115 | CLA | C10-C11-C12-C13 |
| 14 | B | 1211 | CLA | C5-C6-C7-C8 |
| 14 | B | 1215 | CLA | C10-C11-C12-C13 |
| 14 | B | 1220 | CLA | C5-C6-C7-C8 |
| 14 | B | 1223 | CLA | C8-C10-C11-C12 |
| 14 | B | 1225 | CLA | C15-C16-C17-C18 |
| 14 | L | 1503 | CLA | C5-C6-C7-C8 |
| 14 | L | 1503 | CLA | C8-C10-C11-C12 |
| 14 | H | 1211 | CLA | C5-C6-C7-C8 |
| 14 | H | 1215 | CLA | C10-C11-C12-C13 |
| 14 | H | 1220 | CLA | C5-C6-C7-C8 |
| 14 | H | 1223 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1225 | CLA | C15-C16-C17-C18 |
| 14 | V | 1503 | CLA | C5-C6-C7-C8 |
| 14 | V | 1503 | CLA | C8-C10-C11-C12 |
| 14 | e | 1115 | CLA | C10-C11-C12-C13 |
| 14 | f | 1211 | CLA | C5-C6-C7-C8 |
| 14 | f | 1215 | CLA | C10-C11-C12-C13 |
| 14 | f | 1220 | CLA | C5-C6-C7-C8 |
| 14 | f | 1223 | CLA | C8-C10-C11-C12 |
| 14 | f | 1225 | CLA | C15-C16-C17-C18 |
| 14 | n | 1503 | CLA | C5-C6-C7-C8 |
| 14 | n | 1503 | CLA | C8-C10-C11-C12 |
| 18 | A | 5003 | LHG | O2-C2-C3-O3 |
| 18 | G | 5003 | LHG | O2-C2-C3-O3 |
| 18 | e | 5003 | LHG | O2-C2-C3-O3 |
| 14 | K | 1103 | CLA | O2A-C1-C2-C3 |
| 14 | U | 1103 | CLA | O2A-C1-C2-C3 |
| 14 | m | 1103 | CLA | O2A-C1-C2-C3 |
| 21 | L | 5216 | SQD | O47-C45-C46-O48 |
| 21 | V | 5216 | SQD | O47-C45-C46-O48 |
| 21 | n | 5216 | SQD | O47-C45-C46-O48 |
| 14 | A | 1118 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1118 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1118 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1133 | CLA | C2-C3-C5-C6 |
| 14 | G | 1133 | CLA | C2-C3-C5-C6 |
| 14 | e | 1133 | CLA | C2-C3-C5-C6 |
| 14 | A | 1109 | CLA | C14-C13-C15-C16 |
| 14 | A | 1116 | CLA | C6-C7-C8-C9 |
| 14 | A | 1137 | CLA | C6-C7-C8-C9 |
| 14 | A | 1137 | CLA | C11-C10-C8-C9 |
| 14 | B | 1213 | CLA | C11-C12-C13-C14 |
| 14 | B | 1215 | CLA | C6-C7-C8-C9 |
| 14 | B | 1215 | CLA | C11-C12-C13-C14 |
| 14 | B | 1219 | CLA | C6-C7-C8-C9 |
| 14 | B | 1234 | CLA | C11-C12-C13-C14 |
| 14 | L | 1503 | CLA | C6-C7-C8-C9 |
| 14 | 6 | 505 | CLA | C6-C7-C8-C9 |
| 14 | G | 1109 | CLA | C14-C13-C15-C16 |
| 14 | G | 1116 | CLA | C6-C7-C8-C9 |
| 14 | G | 1137 | CLA | C6-C7-C8-C9 |
| 14 | G | 1137 | CLA | C11-C10-C8-C9 |
| 14 | H | 1213 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1215 | CLA | C6-C7-C8-C9 |
| 14 | H | 1215 | CLA | C11-C12-C13-C14 |
| 14 | H | 1219 | CLA | C6-C7-C8-C9 |
| 14 | H | 1234 | CLA | C11-C12-C13-C14 |
| 14 | V | 1503 | CLA | C6-C7-C8-C9 |
| 14 | d | 505 | CLA | C6-C7-C8-C9 |
| 14 | e | 1109 | CLA | C14-C13-C15-C16 |
| 14 | e | 1116 | CLA | C6-C7-C8-C9 |
| 14 | e | 1137 | CLA | C6-C7-C8-C9 |
| 14 | e | 1137 | CLA | C11-C10-C8-C9 |
| 14 | f | 1213 | CLA | C11-C12-C13-C14 |
| 14 | f | 1215 | CLA | C6-C7-C8-C9 |
| 14 | f | 1215 | CLA | C11-C12-C13-C14 |
| 14 | f | 1219 | CLA | C6-C7-C8-C9 |
| 14 | f | 1234 | CLA | C11-C12-C13-C14 |
| 14 | n | 1503 | CLA | C6-C7-C8-C9 |
| 14 | v | 505 | CLA | C6-C7-C8-C9 |
| 15 | A | 2001 | PQN | C21-C22-C23-C24 |
| 15 | G | 2001 | PQN | C21-C22-C23-C24 |
| 15 | e | 2001 | PQN | C21-C22-C23-C24 |
| 14 | A | 1111 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1209 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1229 | CLA | O1D-CGD-O2D-CED |
| 14 | K | 1103 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1111 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1209 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1229 | CLA | O1D-CGD-O2D-CED |
| 14 | U | 1103 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1111 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1115 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1209 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1229 | CLA | O1D-CGD-O2D-CED |
| 14 | m | 1103 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1106 | CLA | C8-C10-C11-C12 |
| 14 | A | 1133 | CLA | C8-C10-C11-C12 |
| 14 | A | 1101 | CLA | C10-C11-C12-C13 |
| 14 | G | 1106 | CLA | C8-C10-C11-C12 |
| 14 | G | 1133 | CLA | C8-C10-C11-C12 |
| 14 | G | 1101 | CLA | C10-C11-C12-C13 |
| 14 | e | 1106 | CLA | C8-C10-C11-C12 |
| 14 | e | 1133 | CLA | C8-C10-C11-C12 |
| 14 | e | 1101 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1207 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1207 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1207 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 502 | CLA | C2A-CAA-CBA-CGA |
| 17 | A | 4001 | BCR | C7-C8-C9-C34 |
| 17 | A | 4011 | BCR | C37-C22-C23-C24 |
| 17 | B | 4014 | BCR | C7-C8-C9-C34 |
| 17 | J | 4013 | BCR | C37-C22-C23-C24 |
| 17 | J | 4012 | BCR | C37-C22-C23-C24 |
| 17 | L | 4219 | BCR | C7-C8-C9-C34 |
| 17 | L | 4020 | BCR | C37-C22-C23-C24 |
| 17 | 3 | 524 | BCR | C7-C8-C9-C34 |
| 17 | 3 | 524 | BCR | C37-C22-C23-C24 |
| 17 | 4 | 521 | BCR | C36-C18-C19-C20 |
| 17 | 4 | 524 | BCR | C7-C8-C9-C34 |
| 17 | 6 | 522 | BCR | C7-C8-C9-C34 |
| 17 | G | 4001 | BCR | C7-C8-C9-C34 |
| 17 | G | 4011 | BCR | C37-C22-C23-C24 |
| 17 | H | 4014 | BCR | C7-C8-C9-C34 |
| 17 | T | 4013 | BCR | C37-C22-C23-C24 |
| 17 | T | 4012 | BCR | C37-C22-C23-C24 |
| 17 | V | 4219 | BCR | C7-C8-C9-C34 |
| 17 | V | 4020 | BCR | C37-C22-C23-C24 |
| 17 | a | 524 | BCR | C7-C8-C9-C34 |
| 17 | a | 524 | BCR | C37-C22-C23-C24 |
| 17 | b | 524 | BCR | C7-C8-C9-C34 |
| 17 | d | 522 | BCR | C7-C8-C9-C34 |
| 17 | e | 4001 | BCR | C7-C8-C9-C34 |
| 17 | e | 4011 | BCR | C37-C22-C23-C24 |
| 17 | f | 4014 | BCR | C7-C8-C9-C34 |
| 17 | l | 4013 | BCR | C37-C22-C23-C24 |
| 17 | l | 4012 | BCR | C37-C22-C23-C24 |
| 17 | n | 4219 | BCR | C7-C8-C9-C34 |
| 17 | n | 4020 | BCR | C37-C22-C23-C24 |
| 17 | s | 524 | BCR | C7-C8-C9-C34 |
| 17 | s | 524 | BCR | C37-C22-C23-C24 |
| 17 | t | 524 | BCR | C7-C8-C9-C34 |
| 17 | v | 522 | BCR | C7-C8-C9-C34 |
| 17 | A | 4011 | BCR | C21-C22-C23-C24 |
| 17 | J | 4013 | BCR | C21-C22-C23-C24 |
| 17 | J | 4012 | BCR | C21-C22-C23-C24 |
| 17 | L | 4022 | BCR | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | 3 | 521 | BCR | C7-C8-C9-C10 |
| 17 | G | 4011 | BCR | C21-C22-C23-C24 |
| 17 | T | 4013 | BCR | C21-C22-C23-C24 |
| 17 | T | 4012 | BCR | C21-C22-C23-C24 |
| 17 | V | 4022 | BCR | C7-C8-C9-C10 |
| 17 | a | 521 | BCR | C7-C8-C9-C10 |
| 17 | e | 4011 | BCR | C21-C22-C23-C24 |
| 17 | l | 4013 | BCR | C21-C22-C23-C24 |
| 17 | l | 4012 | BCR | C21-C22-C23-C24 |
| 17 | n | 4022 | BCR | C7-C8-C9-C10 |
| 17 | s | 521 | BCR | C7-C8-C9-C10 |
| 14 | A | 1115 | CLA | O1D-CGD-O2D-CED |
| 21 | B | 1852 | SQD | C8-C7-O47-C45 |
| 21 | H | 1852 | SQD | C8-C7-O47-C45 |
| 21 | f | 1852 | SQD | C8-C7-O47-C45 |
| 14 | B | 1023 | CLA | C2C-C3C-CAC-CBC |
| 14 | H | 1023 | CLA | C2C-C3C-CAC-CBC |
| 14 | f | 1023 | CLA | C2C-C3C-CAC-CBC |
| 20 | J | 5104 | LMG | C4-C5-C6-O5 |
| 20 | T | 5104 | LMG | C4-C5-C6-O5 |
| 20 | l | 5104 | LMG | C4-C5-C6-O5 |
| 14 | A | 1106 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1239 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1106 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1239 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1106 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1239 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1013 | CLA | C13-C15-C16-C17 |
| 14 | A | 1126 | CLA | C15-C16-C17-C18 |
| 14 | B | 1214 | CLA | C13-C15-C16-C17 |
| 14 | G | 1013 | CLA | C13-C15-C16-C17 |
| 14 | G | 1126 | CLA | C15-C16-C17-C18 |
| 14 | H | 1214 | CLA | C13-C15-C16-C17 |
| 14 | e | 1013 | CLA | C13-C15-C16-C17 |
| 14 | f | 1214 | CLA | C13-C15-C16-C17 |
| 14 | G | 1115 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1101 | CLA | C3-C5-C6-C7 |
| 14 | G | 1101 | CLA | C3-C5-C6-C7 |
| 14 | H | 1210 | CLA | C3-C5-C6-C7 |
| 14 | e | 1101 | CLA | C3-C5-C6-C7 |
| 14 | A | 1137 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1137 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1137 | CLA | CBA-CGA-O2A-C1 |
| 18 | B | 1842 | LHG | C24-C23-O8-C6 |
| 18 | H | 1842 | LHG | C24-C23-O8-C6 |
| 14 | A | 1115 | CLA | C5-C6-C7-C8 |
| 14 | A | 1125 | CLA | C5-C6-C7-C8 |
| 14 | A | 1137 | CLA | C10-C11-C12-C13 |
| 14 | B | 1203 | CLA | C8-C10-C11-C12 |
| 14 | B | 1240 | CLA | C10-C11-C12-C13 |
| 14 | G | 1115 | CLA | C5-C6-C7-C8 |
| 14 | G | 1125 | CLA | C5-C6-C7-C8 |
| 14 | G | 1137 | CLA | C10-C11-C12-C13 |
| 14 | H | 1203 | CLA | C8-C10-C11-C12 |
| 14 | H | 1240 | CLA | C10-C11-C12-C13 |
| 14 | e | 1115 | CLA | C5-C6-C7-C8 |
| 14 | e | 1125 | CLA | C5-C6-C7-C8 |
| 14 | e | 1126 | CLA | C15-C16-C17-C18 |
| 14 | e | 1137 | CLA | C10-C11-C12-C13 |
| 14 | f | 1203 | CLA | C8-C10-C11-C12 |
| 14 | f | 1240 | CLA | C10-C11-C12-C13 |
| 18 | L | 5220 | LHG | C23-C24-C25-C26 |
| 18 | V | 5220 | LHG | C23-C24-C25-C26 |
| 18 | n | 5220 | LHG | C23-C24-C25-C26 |
| 14 | 2 | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 518 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1106 | CLA | C5-C6-C7-C8 |
| 14 | A | 1116 | CLA | C5-C6-C7-C8 |
| 14 | B | 1012 | CLA | C5-C6-C7-C8 |
| 14 | B | 1204 | CLA | C5-C6-C7-C8 |
| 14 | B | 1213 | CLA | C5-C6-C7-C8 |
| 14 | B | 1219 | CLA | C5-C6-C7-C8 |
| 14 | B | 1223 | CLA | C13-C15-C16-C17 |
| 14 | B | 1239 | CLA | C15-C16-C17-C18 |
| 14 | L | 1503 | CLA | C10-C11-C12-C13 |
| 14 | G | 1106 | CLA | C5-C6-C7-C8 |
| 14 | G | 1116 | CLA | C5-C6-C7-C8 |
| 14 | H | 1012 | CLA | C5-C6-C7-C8 |
| 14 | H | 1204 | CLA | C5-C6-C7-C8 |
| 14 | H | 1213 | CLA | C5-C6-C7-C8 |
| 14 | H | 1219 | CLA | C5-C6-C7-C8 |
| 14 | H | 1223 | CLA | C13-C15-C16-C17 |
| 14 | H | 1239 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | V | 1503 | CLA | C10-C11-C12-C13 |
| 14 | e | 1106 | CLA | C5-C6-C7-C8 |
| 14 | e | 1116 | CLA | C5-C6-C7-C8 |
| 14 | f | 1012 | CLA | C5-C6-C7-C8 |
| 14 | f | 1204 | CLA | C5-C6-C7-C8 |
| 14 | f | 1213 | CLA | C5-C6-C7-C8 |
| 14 | f | 1219 | CLA | C5-C6-C7-C8 |
| 14 | f | 1223 | CLA | C13-C15-C16-C17 |
| 14 | f | 1239 | CLA | C15-C16-C17-C18 |
| 14 | n | 1503 | CLA | C10-C11-C12-C13 |
| 14 | A | 1013 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1126 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 509 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1013 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1126 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 509 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1013 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1126 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 509 | CLA | O1D-CGD-O2D-CED |
| 18 | L | 5218 | LHG | O1-C1-C2-O2 |
| 18 | V | 5218 | LHG | O1-C1-C2-O2 |
| 18 | n | 5218 | LHG | O1-C1-C2-O2 |
| 18 | A | 5002 | LHG | C7-C8-C9-C10 |
| 18 | A | 5008 | LHG | C23-C24-C25-C26 |
| 18 | A | 5009 | LHG | C23-C24-C25-C26 |
| 18 | A | 5001 | LHG | C23-C24-C25-C26 |
| 18 | I | 5001 | LHG | C23-C24-C25-C26 |
| 18 | L | 5220 | LHG | C7-C8-C9-C10 |
| 18 | G | 5002 | LHG | C7-C8-C9-C10 |
| 18 | G | 5008 | LHG | C23-C24-C25-C26 |
| 18 | G | 5009 | LHG | C23-C24-C25-C26 |
| 18 | G | 5001 | LHG | C23-C24-C25-C26 |
| 18 | S | 5001 | LHG | C23-C24-C25-C26 |
| 18 | V | 5220 | LHG | C7-C8-C9-C10 |
| 18 | e | 5002 | LHG | C7-C8-C9-C10 |
| 18 | e | 5008 | LHG | C23-C24-C25-C26 |
| 18 | e | 5009 | LHG | C23-C24-C25-C26 |
| 18 | e | 5001 | LHG | C23-C24-C25-C26 |
| 18 | k | 5001 | LHG | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | n | 5220 | LHG | C7-C8-C9-C10 |
| 14 | 2 | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | 6 | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | Z | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | d | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | r | 511 | CLA | CBD-CGD-O2D-CED |
| 14 | v | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1124 | CLA | C10-C11-C12-C13 |
| 14 | B | 1205 | CLA | C13-C15-C16-C17 |
| 14 | B | 1210 | CLA | C8-C10-C11-C12 |
| 14 | B | 1207 | CLA | C13-C15-C16-C17 |
| 14 | 2 | 505 | CLA | C8-C10-C11-C12 |
| 14 | 5 | 509 | CLA | C8-C10-C11-C12 |
| 14 | H | 1205 | CLA | C13-C15-C16-C17 |
| 14 | H | 1210 | CLA | C8-C10-C11-C12 |
| 14 | H | 1207 | CLA | C13-C15-C16-C17 |
| 14 | Z | 505 | CLA | C8-C10-C11-C12 |
| 14 | c | 509 | CLA | C8-C10-C11-C12 |
| 14 | e | 1124 | CLA | C10-C11-C12-C13 |
| 14 | f | 1205 | CLA | C13-C15-C16-C17 |
| 14 | f | 1210 | CLA | C8-C10-C11-C12 |
| 14 | f | 1207 | CLA | C13-C15-C16-C17 |
| 14 | r | 505 | CLA | C8-C10-C11-C12 |
| 14 | u | 509 | CLA | C8-C10-C11-C12 |
| 15 | A | 2001 | PQN | C15-C16-C17-C18 |
| 15 | G | 2001 | PQN | C15-C16-C17-C18 |
| 15 | e | 2001 | PQN | C15-C16-C17-C18 |
| 14 | A | 1125 | CLA | C3-C5-C6-C7 |
| 14 | B | 1210 | CLA | C3-C5-C6-C7 |
| 14 | G | 1125 | CLA | C3-C5-C6-C7 |
| 14 | e | 1125 | CLA | C3-C5-C6-C7 |
| 14 | f | 1210 | CLA | C3-C5-C6-C7 |
| 18 | f | 1842 | LHG | C24-C23-O8-C6 |
| 19 | A | 1849 | LMU | O1'-C1-C2-C3 |
| 19 | G | 1849 | LMU | O1'-C1-C2-C3 |
| 19 | e | 1849 | LMU | O1'-C1-C2-C3 |
| 21 | L | 5216 | SQD | C17-C18-C19-C20 |
| 21 | V | 5216 | SQD | C17-C18-C19-C20 |
| 21 | n | 5216 | SQD | C17-C18-C19-C20 |
| 14 | A | 1131 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1131 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 518 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1131 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1104 | CLA | C15-C16-C17-C18 |
| 14 | B | 1023 | CLA | C10-C11-C12-C13 |
| 14 | G | 1104 | CLA | C15-C16-C17-C18 |
| 14 | G | 1124 | CLA | C10-C11-C12-C13 |
| 14 | H | 1023 | CLA | C10-C11-C12-C13 |
| 14 | e | 1104 | CLA | C15-C16-C17-C18 |
| 14 | f | 1023 | CLA | C10-C11-C12-C13 |
| 14 | s | 518 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5005 | LHG | C23-C24-C25-C26 |
| 18 | A | 5006 | LHG | C23-C24-C25-C26 |
| 18 | A | 5008 | LHG | C7-C8-C9-C10 |
| 18 | G | 5005 | LHG | C23-C24-C25-C26 |
| 18 | G | 5006 | LHG | C23-C24-C25-C26 |
| 18 | G | 5008 | LHG | C7-C8-C9-C10 |
| 18 | e | 5005 | LHG | C23-C24-C25-C26 |
| 18 | e | 5006 | LHG | C23-C24-C25-C26 |
| 18 | e | 5008 | LHG | C7-C8-C9-C10 |
| 21 | B | 1852 | SQD | C23-C24-C25-C26 |
| 21 | 1 | 822 | SQD | C23-C24-C25-C26 |
| 21 | H | 1852 | SQD | C23-C24-C25-C26 |
| 21 | Y | 822 | SQD | C23-C24-C25-C26 |
| 21 | f | 1852 | SQD | C23-C24-C25-C26 |
| 21 | q | 822 | SQD | C23-C24-C25-C26 |
| 14 | A | 1109 | CLA | CBD-CGD-O2D-CED |
| 14 | 1 | 505 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1109 | CLA | CBD-CGD-O2D-CED |
| 14 | Y | 505 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1109 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 505 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1126 | CLA | C10-C11-C12-C13 |
| 14 | B | 1214 | CLA | C5-C6-C7-C8 |
| 14 | 6 | 505 | CLA | C8-C10-C11-C12 |
| 14 | G | 1126 | CLA | C10-C11-C12-C13 |
| 14 | H | 1214 | CLA | C5-C6-C7-C8 |
| 14 | d | 505 | CLA | C8-C10-C11-C12 |
| 14 | e | 1126 | CLA | C10-C11-C12-C13 |
| 14 | f | 1214 | CLA | C5-C6-C7-C8 |
| 14 | v | 505 | CLA | C8-C10-C11-C12 |
| 14 | A | 1237 | CLA | O1D-CGD-O2D-CED |
| 14 | L | 1503 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 505 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 3 | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | V | 1503 | CLA | O1D-CGD-O2D-CED |
| 14 | a | 505 | CLA | O1D-CGD-O2D-CED |
| 14 | n | 1503 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | s | 505 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1106 | CLA | C12-C13-C15-C16 |
| 14 | A | 1107 | CLA | C11-C10-C8-C7 |
| 14 | A | 1109 | CLA | C11-C12-C13-C15 |
| 14 | A | 1119 | CLA | C6-C7-C8-C10 |
| 14 | A | 1139 | CLA | C11-C10-C8-C7 |
| 14 | B | 1210 | CLA | C11-C12-C13-C15 |
| 14 | B | 1216 | CLA | C6-C7-C8-C10 |
| 14 | B | 1221 | CLA | C11-C10-C8-C7 |
| 14 | B | 1230 | CLA | C6-C7-C8-C10 |
| 14 | G | 1106 | CLA | C12-C13-C15-C16 |
| 14 | G | 1107 | CLA | C11-C10-C8-C7 |
| 14 | G | 1109 | CLA | C11-C12-C13-C15 |
| 14 | G | 1119 | CLA | C6-C7-C8-C10 |
| 14 | G | 1139 | CLA | C11-C10-C8-C7 |
| 14 | H | 1210 | CLA | C11-C12-C13-C15 |
| 14 | H | 1216 | CLA | C6-C7-C8-C10 |
| 14 | H | 1221 | CLA | C11-C10-C8-C7 |
| 14 | H | 1230 | CLA | C6-C7-C8-C10 |
| 14 | e | 1106 | CLA | C12-C13-C15-C16 |
| 14 | e | 1107 | CLA | C11-C10-C8-C7 |
| 14 | e | 1109 | CLA | C11-C12-C13-C15 |
| 14 | e | 1119 | CLA | C6-C7-C8-C10 |
| 14 | e | 1139 | CLA | C11-C10-C8-C7 |
| 14 | f | 1210 | CLA | C11-C12-C13-C15 |
| 14 | f | 1216 | CLA | C6-C7-C8-C10 |
| 14 | f | 1221 | CLA | C11-C10-C8-C7 |
| 14 | f | 1230 | CLA | C6-C7-C8-C10 |
| 15 | A | 2001 | PQN | C21-C22-C23-C25 |
| 15 | G | 2001 | PQN | C21-C22-C23-C25 |
| 15 | e | 2001 | PQN | C21-C22-C23-C25 |
| 14 | A | 1115 | CLA | C3-C5-C6-C7 |
| 14 | G | 1115 | CLA | C3-C5-C6-C7 |
| 14 | e | 1115 | CLA | C3-C5-C6-C7 |
| 14 | A | 1133 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1137 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1225 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1133 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1137 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1225 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1133 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1137 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1225 | CLA | O1A-CGA-O2A-C1 |
| 18 | B | 1855 | LHG | O10-C23-O8-C6 |
| 18 | H | 1855 | LHG | O10-C23-O8-C6 |
| 18 | f | 1855 | LHG | O10-C23-O8-C6 |
| 14 | 3 | 516 | CLA | C4C-C3C-CAC-CBC |
| 17 | 4 | 522 | BCR | C9-C10-C11-C12 |
| 17 | 6 | 522 | BCR | C9-C10-C11-C12 |
| 17 | b | 522 | BCR | C9-C10-C11-C12 |
| 17 | d | 522 | BCR | C9-C10-C11-C12 |
| 17 | t | 522 | BCR | C9-C10-C11-C12 |
| 17 | v | 522 | BCR | C9-C10-C11-C12 |
| 14 | A | 1107 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1201 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | 5 | 502 | CLA | C2A-CAA-CBA-CGA |
| 14 | 6 | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1107 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1201 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 502 | CLA | C2A-CAA-CBA-CGA |
| 14 | d | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1107 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1201 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | v | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | v | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1106 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1106 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1237 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 512 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | Z | 507 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | b | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1106 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1237 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | t | 513 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1126 | CLA | C8-C10-C11-C12 |
| 14 | B | 1216 | CLA | C5-C6-C7-C8 |
| 14 | 2 | 509 | CLA | C15-C16-C17-C18 |
| 14 | 6 | 505 | CLA | C5-C6-C7-C8 |
| 14 | G | 1126 | CLA | C8-C10-C11-C12 |
| 14 | H | 1216 | CLA | C5-C6-C7-C8 |
| 14 | Z | 509 | CLA | C15-C16-C17-C18 |
| 14 | d | 505 | CLA | C5-C6-C7-C8 |
| 14 | e | 1126 | CLA | C8-C10-C11-C12 |
| 14 | f | 1216 | CLA | C5-C6-C7-C8 |
| 14 | r | 509 | CLA | C15-C16-C17-C18 |
| 14 | v | 505 | CLA | C5-C6-C7-C8 |
| 15 | A | 2001 | PQN | C18-C20-C21-C22 |
| 15 | G | 2001 | PQN | C18-C20-C21-C22 |
| 15 | e | 2001 | PQN | C18-C20-C21-C22 |
| 14 | a | 516 | CLA | C4C-C3C-CAC-CBC |
| 14 | s | 516 | CLA | C4C-C3C-CAC-CBC |
| 14 | B | 1239 | CLA | C4C-C3C-CAC-CBC |
| 14 | H | 1239 | CLA | C4C-C3C-CAC-CBC |
| 14 | f | 1239 | CLA | C4C-C3C-CAC-CBC |
| 14 | A | 1104 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1237 | CLA | O1A-CGA-O2A-C1 |
| 14 | J | 1302 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1104 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1237 | CLA | O1A-CGA-O2A-C1 |
| 14 | T | 1302 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1104 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1237 | CLA | O1A-CGA-O2A-C1 |
| 14 | l | 1302 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1136 | CLA | C8-C10-C11-C12 |
| 14 | B | 1208 | CLA | C10-C11-C12-C13 |
| 14 | B | 1210 | CLA | C10-C11-C12-C13 |
| 14 | G | 1136 | CLA | C8-C10-C11-C12 |
| 14 | H | 1208 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1210 | CLA | C10-C11-C12-C13 |
| 14 | e | 1136 | CLA | C8-C10-C11-C12 |
| 14 | f | 1208 | CLA | C10-C11-C12-C13 |
| 14 | B | 1231 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1231 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1231 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1013 | CLA | C15-C16-C17-C18 |
| 14 | A | 1122 | CLA | C8-C10-C11-C12 |
| 14 | B | 1203 | CLA | C5-C6-C7-C8 |
| 14 | B | 1219 | CLA | C8-C10-C11-C12 |
| 14 | B | 1234 | CLA | C10-C11-C12-C13 |
| 14 | G | 1013 | CLA | C15-C16-C17-C18 |
| 14 | G | 1122 | CLA | C8-C10-C11-C12 |
| 14 | H | 1203 | CLA | C5-C6-C7-C8 |
| 14 | H | 1219 | CLA | C8-C10-C11-C12 |
| 14 | H | 1234 | CLA | C10-C11-C12-C13 |
| 14 | e | 1013 | CLA | C15-C16-C17-C18 |
| 14 | e | 1122 | CLA | C8-C10-C11-C12 |
| 14 | f | 1203 | CLA | C5-C6-C7-C8 |
| 14 | f | 1210 | CLA | C10-C11-C12-C13 |
| 14 | f | 1219 | CLA | C8-C10-C11-C12 |
| 14 | f | 1234 | CLA | C10-C11-C12-C13 |
| 14 | B | 1232 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1232 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1232 | CLA | CBA-CGA-O2A-C1 |
| 18 | A | 5002 | LHG | C28-C29-C30-C31 |
| 18 | G | 5002 | LHG | C28-C29-C30-C31 |
| 18 | e | 5002 | LHG | C28-C29-C30-C31 |
| 14 | B | 1214 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1214 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1214 | CLA | O1A-CGA-O2A-C1 |
| 19 | e | 1848 | LMU | C4'-C5'-C6'-O6' |
| 18 | A | 5005 | LHG | C28-C29-C30-C31 |
| 18 | G | 5005 | LHG | C28-C29-C30-C31 |
| 18 | e | 5005 | LHG | C28-C29-C30-C31 |
| 14 | B | 1221 | CLA | C8-C10-C11-C12 |
| 14 | B | 1225 | CLA | C13-C15-C16-C17 |
| 14 | H | 1217 | CLA | C8-C10-C11-C12 |
| 14 | H | 1221 | CLA | C8-C10-C11-C12 |
| 14 | H | 1225 | CLA | C13-C15-C16-C17 |
| 14 | f | 1221 | CLA | C8-C10-C11-C12 |
| 14 | f | 1225 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | r | 501 | CLA | C8-C10-C11-C12 |
| 14 | A | 1121 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1201 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1121 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1201 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1121 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1201 | CLA | O1D-CGD-O2D-CED |
| 19 | A | 1848 | LMU | C4'-C5'-C6'-O6' |
| 19 | G | 1848 | LMU | C4'-C5'-C6'-O6' |
| 14 | A | 1109 | CLA | C13-C15-C16-C17 |
| 14 | A | 1126 | CLA | C5-C6-C7-C8 |
| 14 | A | 1133 | CLA | C10-C11-C12-C13 |
| 14 | A | 1139 | CLA | C13-C15-C16-C17 |
| 14 | B | 1214 | CLA | C10-C11-C12-C13 |
| 14 | B | 1217 | CLA | C8-C10-C11-C12 |
| 14 | B | 1235 | CLA | C8-C10-C11-C12 |
| 14 | 2 | 501 | CLA | C8-C10-C11-C12 |
| 14 | G | 1109 | CLA | C13-C15-C16-C17 |
| 14 | G | 1126 | CLA | C5-C6-C7-C8 |
| 14 | G | 1133 | CLA | C10-C11-C12-C13 |
| 14 | G | 1139 | CLA | C13-C15-C16-C17 |
| 14 | H | 1214 | CLA | C10-C11-C12-C13 |
| 14 | H | 1235 | CLA | C8-C10-C11-C12 |
| 14 | Z | 501 | CLA | C8-C10-C11-C12 |
| 14 | e | 1109 | CLA | C13-C15-C16-C17 |
| 14 | e | 1126 | CLA | C5-C6-C7-C8 |
| 14 | e | 1133 | CLA | C10-C11-C12-C13 |
| 14 | e | 1139 | CLA | C13-C15-C16-C17 |
| 14 | f | 1214 | CLA | C10-C11-C12-C13 |
| 14 | f | 1217 | CLA | C8-C10-C11-C12 |
| 14 | f | 1235 | CLA | C8-C10-C11-C12 |
| 18 | A | 5005 | LHG | C3-O3-P-O6 |
| 18 | A | 5006 | LHG | C4-O6-P-O3 |
| 18 | A | 5009 | LHG | C4-O6-P-O3 |
| 18 | B | 1842 | LHG | C3-O3-P-O6 |
| 18 | B | 1855 | LHG | C3-O3-P-O6 |
| 18 | B | 1855 | LHG | C4-O6-P-O3 |
| 18 | L | 5218 | LHG | C3-O3-P-O6 |
| 18 | L | 5220 | LHG | C4-O6-P-O3 |
| 18 | L | 5221 | LHG | C3-O3-P-O6 |
| 18 | G | 5005 | LHG | C3-O3-P-O6 |
| 18 | G | 5006 | LHG | C4-O6-P-O3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | G | 5009 | LHG | C4-O6-P-O3 |
| 18 | H | 1842 | LHG | C3-O3-P-O6 |
| 18 | H | 1855 | LHG | C3-O3-P-O6 |
| 18 | H | 1855 | LHG | C4-O6-P-O3 |
| 18 | V | 5218 | LHG | C3-O3-P-O6 |
| 18 | V | 5220 | LHG | C4-O6-P-O3 |
| 18 | V | 5221 | LHG | C3-O3-P-O6 |
| 18 | e | 5005 | LHG | C3-O3-P-O6 |
| 18 | e | 5006 | LHG | C4-O6-P-O3 |
| 18 | e | 5009 | LHG | C4-O6-P-O3 |
| 18 | f | 1842 | LHG | C3-O3-P-O6 |
| 18 | f | 1855 | LHG | C3-O3-P-O6 |
| 18 | f | 1855 | LHG | C4-O6-P-O3 |
| 18 | n | 5218 | LHG | C3-O3-P-O6 |
| 18 | n | 5220 | LHG | C4-O6-P-O3 |
| 18 | n | 5221 | LHG | C3-O3-P-O6 |
| 18 | A | 5009 | LHG | C7-C8-C9-C10 |
| 18 | e | 5009 | LHG | C7-C8-C9-C10 |
| 21 | B | 1852 | SQD | C7-C8-C9-C10 |
| 21 | H | 1852 | SQD | C7-C8-C9-C10 |
| 21 | f | 1852 | SQD | C7-C8-C9-C10 |
| 14 | A | 1128 | CLA | C3-C5-C6-C7 |
| 14 | G | 1128 | CLA | C3-C5-C6-C7 |
| 14 | e | 1128 | CLA | C3-C5-C6-C7 |
| 14 | B | 1239 | CLA | C2C-C3C-CAC-CBC |
| 14 | f | 1239 | CLA | C2C-C3C-CAC-CBC |
| 14 | H | 1239 | CLA | C2C-C3C-CAC-CBC |
| 15 | B | 2002 | PQN | C15-C16-C17-C18 |
| 15 | H | 2002 | PQN | C15-C16-C17-C18 |
| 15 | f | 2002 | PQN | C15-C16-C17-C18 |
| 18 | G | 5009 | LHG | C7-C8-C9-C10 |
| 14 | B | 1234 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1234 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1234 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5003 | LHG | C1-C2-C3-O3 |
| 18 | G | 5003 | LHG | C1-C2-C3-O3 |
| 18 | e | 5003 | LHG | C1-C2-C3-O3 |
| 18 | A | 5001 | LHG | O9-C7-O7-C5 |
| 18 | G | 5001 | LHG | O9-C7-O7-C5 |
| 18 | e | 5001 | LHG | O9-C7-O7-C5 |
| 14 | A | 1132 | CLA | C4-C3-C5-C6 |
| 14 | G | 1132 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1132 | CLA | C4-C3-C5-C6 |
| 19 | J | 5105 | LMU | O1'-C1-C2-C3 |
| 14 | 5 | 509 | CLA | C15-C16-C17-C18 |
| 14 | c | 509 | CLA | C15-C16-C17-C18 |
| 14 | u | 509 | CLA | C15-C16-C17-C18 |
| 14 | 6 | 512 | CLA | O1D-CGD-O2D-CED |
| 19 | T | 5105 | LMU | O1'-C1-C2-C3 |
| 19 | l | 5105 | LMU | O1'-C1-C2-C3 |
| 14 | A | 1125 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1022 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1203 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1224 | CLA | C2A-CAA-CBA-CGA |
| 14 | K | 1103 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | 4 | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | 6 | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1125 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1022 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1203 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1224 | CLA | C2A-CAA-CBA-CGA |
| 14 | U | 1103 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | b | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | d | 516 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1125 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1022 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1203 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1224 | CLA | C2A-CAA-CBA-CGA |
| 14 | m | 1103 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | t | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1211 | CLA | C6-C7-C8-C9 |
| 14 | H | 1211 | CLA | C6-C7-C8-C9 |
| 14 | f | 1211 | CLA | C6-C7-C8-C9 |
| 15 | B | 2002 | PQN | C26-C27-C28-C30 |
| 15 | H | 2002 | PQN | C26-C27-C28-C30 |
| 15 | f | 2002 | PQN | C26-C27-C28-C30 |
| 14 | A | 1011 | CLA | C3-C5-C6-C7 |
| 14 | G | 1011 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1011 | CLA | C3-C5-C6-C7 |
| 14 | Z | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | r | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | L | 1502 | CLA | CBA-CGA-O2A-C1 |
| 14 | V | 1502 | CLA | CBA-CGA-O2A-C1 |
| 14 | n | 1502 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 5002 | LMG | C29-C28-O8-C9 |
| 20 | H | 5002 | LMG | C29-C28-O8-C9 |
| 20 | f | 5002 | LMG | C29-C28-O8-C9 |
| 14 | 2 | 504 | CLA | O1D-CGD-O2D-CED |
| 17 | 4 | 522 | BCR | C13-C14-C15-C16 |
| 17 | b | 522 | BCR | C13-C14-C15-C16 |
| 17 | t | 522 | BCR | C13-C14-C15-C16 |
| 18 | G | 5001 | LHG | C15-C16-C17-C18 |
| 18 | e | 5001 | LHG | C15-C16-C17-C18 |
| 14 | A | 1133 | CLA | O1D-CGD-O2D-CED |
| 18 | B | 1855 | LHG | C8-C7-O7-C5 |
| 18 | H | 1855 | LHG | C8-C7-O7-C5 |
| 18 | f | 1855 | LHG | C8-C7-O7-C5 |
| 14 | 5 | 509 | CLA | C13-C15-C16-C17 |
| 14 | c | 509 | CLA | C13-C15-C16-C17 |
| 14 | u | 509 | CLA | C13-C15-C16-C17 |
| 18 | A | 5005 | LHG | C12-C13-C14-C15 |
| 18 | A | 5005 | LHG | C24-C25-C26-C27 |
| 18 | A | 5007 | LHG | C31-C32-C33-C34 |
| 18 | A | 5009 | LHG | C9-C10-C11-C12 |
| 18 | A | 5001 | LHG | C15-C16-C17-C18 |
| 18 | A | 5001 | LHG | C25-C26-C27-C28 |
| 18 | A | 5003 | LHG | C11-C10-C9-C8 |
| 18 | A | 5003 | LHG | C10-C11-C12-C13 |
| 18 | L | 5221 | LHG | C30-C31-C32-C33 |
| 18 | G | 5005 | LHG | C12-C13-C14-C15 |
| 18 | G | 5005 | LHG | C24-C25-C26-C27 |
| 18 | G | 5007 | LHG | C31-C32-C33-C34 |
| 18 | G | 5009 | LHG | C9-C10-C11-C12 |
| 18 | G | 5001 | LHG | C25-C26-C27-C28 |
| 18 | G | 5003 | LHG | C11-C10-C9-C8 |
| 18 | G | 5003 | LHG | C10-C11-C12-C13 |
| 18 | V | 5221 | LHG | C30-C31-C32-C33 |
| 18 | e | 5005 | LHG | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | e | 5005 | LHG | C12-C13-C14-C15 |
| 18 | e | 5005 | LHG | C24-C25-C26-C27 |
| 18 | e | 5007 | LHG | C31-C32-C33-C34 |
| 18 | e | 5009 | LHG | C9-C10-C11-C12 |
| 18 | e | 5001 | LHG | C25-C26-C27-C28 |
| 18 | e | 5003 | LHG | C11-C10-C9-C8 |
| 18 | e | 5003 | LHG | C10-C11-C12-C13 |
| 18 | n | 5221 | LHG | C30-C31-C32-C33 |
| 20 | B | 5002 | LMG | C29-C30-C31-C32 |
| 20 | H | 5002 | LMG | C29-C30-C31-C32 |
| 20 | f | 5002 | LMG | C29-C30-C31-C32 |
| 14 | B | 1220 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1133 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1220 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1133 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1220 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 512 | CLA | O1D-CGD-O2D-CED |
| 14 | 3 | 505 | CLA | C6-C7-C8-C9 |
| 14 | a | 505 | CLA | C6-C7-C8-C9 |
| 14 | s | 505 | CLA | C6-C7-C8-C9 |
| 18 | A | 5005 | LHG | C10-C11-C12-C13 |
| 18 | A | 5005 | LHG | C14-C15-C16-C17 |
| 18 | B | 1855 | LHG | C12-C13-C14-C15 |
| 18 | G | 5005 | LHG | C10-C11-C12-C13 |
| 18 | G | 5005 | LHG | C14-C15-C16-C17 |
| 18 | H | 1855 | LHG | C12-C13-C14-C15 |
| 18 | V | 5221 | LHG | C31-C32-C33-C34 |
| 18 | e | 5005 | LHG | C14-C15-C16-C17 |
| 18 | f | 1855 | LHG | C12-C13-C14-C15 |
| 21 | 2 | 822 | SQD | C46-C45-O47-C7 |
| 21 | Z | 822 | SQD | C46-C45-O47-C7 |
| 21 | r | 822 | SQD | C46-C45-O47-C7 |
| 18 | L | 5221 | LHG | C31-C32-C33-C34 |
| 18 | n | 5221 | LHG | C31-C32-C33-C34 |
| 14 | J | 1303 | CLA | O1D-CGD-O2D-CED |
| 14 | T | 1303 | CLA | O1D-CGD-O2D-CED |
| 14 | l | 1303 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5004 | LHG | C27-C28-C29-C30 |
| 18 | L | 5220 | LHG | C27-C28-C29-C30 |
| 18 | G | 5004 | LHG | C27-C28-C29-C30 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | V | 5220 | LHG | C27-C28-C29-C30 |
| 18 | e | 5004 | LHG | C27-C28-C29-C30 |
| 18 | n | 5220 | LHG | C27-C28-C29-C30 |
| 21 | f | 1852 | SQD | C11-C10-C9-C8 |
| 14 | f | 1235 | CLA | O1D-CGD-O2D-CED |
| 18 | H | 1855 | LHG | C11-C12-C13-C14 |
| 21 | B | 1852 | SQD | C11-C10-C9-C8 |
| 21 | H | 1852 | SQD | C11-C10-C9-C8 |
| 20 | J | 5104 | LMG | C10-C11-C12-C13 |
| 20 | T | 5104 | LMG | C10-C11-C12-C13 |
| 20 | l | 5104 | LMG | C10-C11-C12-C13 |
| 14 | B | 1235 | CLA | O1D-CGD-O2D-CED |
| 19 | A | 1849 | LMU | C2'-C1'-O1'-C1 |
| 19 | G | 1849 | LMU | C2'-C1'-O1'-C1 |
| 19 | e | 1849 | LMU | C2'-C1'-O1'-C1 |
| 21 | B | 1852 | SQD | C2-C1-O6-C44 |
| 21 | H | 1852 | SQD | C2-C1-O6-C44 |
| 21 | f | 1852 | SQD | C2-C1-O6-C44 |
| 18 | A | 5005 | LHG | C11-C10-C9-C8 |
| 18 | A | 5003 | LHG | C12-C13-C14-C15 |
| 18 | B | 1855 | LHG | C11-C12-C13-C14 |
| 18 | G | 5005 | LHG | C11-C10-C9-C8 |
| 18 | G | 5003 | LHG | C12-C13-C14-C15 |
| 18 | e | 5005 | LHG | C11-C10-C9-C8 |
| 18 | e | 5003 | LHG | C12-C13-C14-C15 |
| 18 | f | 1855 | LHG | C11-C12-C13-C14 |
| 19 | A | 1849 | LMU | C4-C5-C6-C7 |
| 19 | B | 1843 | LMU | C5-C6-C7-C8 |
| 19 | G | 1849 | LMU | C4-C5-C6-C7 |
| 19 | H | 1843 | LMU | C5-C6-C7-C8 |
| 19 | e | 1849 | LMU | C4-C5-C6-C7 |
| 19 | f | 1843 | LMU | C5-C6-C7-C8 |
| 14 | A | 1103 | CLA | C10-C11-C12-C13 |
| 14 | A | 1103 | CLA | C15-C16-C17-C18 |
| 14 | B | 1218 | CLA | C8-C10-C11-C12 |
| 14 | G | 1103 | CLA | C10-C11-C12-C13 |
| 14 | G | 1103 | CLA | C15-C16-C17-C18 |
| 14 | H | 1218 | CLA | C8-C10-C11-C12 |
| 14 | e | 1103 | CLA | C10-C11-C12-C13 |
| 14 | e | 1103 | CLA | C15-C16-C17-C18 |
| 14 | f | 1218 | CLA | C8-C10-C11-C12 |
| 14 | A | 1121 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1140 | CLA | C16-C17-C18-C20 |
| 14 | B | 1217 | CLA | C11-C12-C13-C14 |
| 14 | B | 1207 | CLA | C16-C17-C18-C19 |
| 14 | 6 | 505 | CLA | C16-C17-C18-C20 |
| 14 | G | 1121 | CLA | C6-C7-C8-C9 |
| 14 | G | 1140 | CLA | C16-C17-C18-C20 |
| 14 | H | 1217 | CLA | C11-C12-C13-C14 |
| 14 | H | 1207 | CLA | C16-C17-C18-C19 |
| 14 | d | 505 | CLA | C16-C17-C18-C20 |
| 14 | e | 1121 | CLA | C6-C7-C8-C9 |
| 14 | e | 1140 | CLA | C16-C17-C18-C20 |
| 14 | f | 1217 | CLA | C11-C12-C13-C14 |
| 14 | f | 1207 | CLA | C16-C17-C18-C19 |
| 14 | v | 505 | CLA | C16-C17-C18-C20 |
| 14 | B | 1012 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1012 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1235 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1012 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1102 | CLA | C4-C3-C5-C6 |
| 14 | B | 1229 | CLA | C4-C3-C5-C6 |
| 14 | G | 1102 | CLA | C4-C3-C5-C6 |
| 14 | H | 1229 | CLA | C4-C3-C5-C6 |
| 14 | e | 1102 | CLA | C4-C3-C5-C6 |
| 14 | f | 1229 | CLA | C4-C3-C5-C6 |
| 18 | A | 5004 | LHG | C24-C25-C26-C27 |
| 18 | G | 5004 | LHG | C24-C25-C26-C27 |
| 18 | e | 5004 | LHG | C24-C25-C26-C27 |
| 18 | n | 5220 | LHG | C10-C11-C12-C13 |
| 19 | A | 1848 | LMU | C2-C3-C4-C5 |
| 19 | G | 1848 | LMU | C2-C3-C4-C5 |
| 19 | e | 1848 | LMU | C2-C3-C4-C5 |
| 14 | B | 1229 | CLA | C2-C3-C5-C6 |
| 14 | H | 1229 | CLA | C2-C3-C5-C6 |
| 14 | f | 1229 | CLA | C2-C3-C5-C6 |
| 14 | A | 1133 | CLA | C11-C12-C13-C14 |
| 14 | B | 1223 | CLA | C14-C13-C15-C16 |
| 14 | G | 1133 | CLA | C11-C12-C13-C14 |
| 14 | H | 1223 | CLA | C14-C13-C15-C16 |
| 14 | e | 1133 | CLA | C11-C12-C13-C14 |
| 14 | f | 1223 | CLA | C14-C13-C15-C16 |
| 14 | A | 1113 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1113 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1113 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5007 | LHG | C11-C10-C9-C8 |
| 18 | L | 5220 | LHG | C10-C11-C12-C13 |
| 18 | L | 5221 | LHG | C25-C26-C27-C28 |
| 18 | G | 5007 | LHG | C11-C10-C9-C8 |
| 18 | V | 5220 | LHG | C10-C11-C12-C13 |
| 18 | V | 5221 | LHG | C25-C26-C27-C28 |
| 18 | e | 5007 | LHG | C11-C10-C9-C8 |
| 20 | B | 5002 | LMG | C22-C23-C24-C25 |
| 20 | B | 5002 | LMG | C32-C33-C34-C35 |
| 20 | H | 5002 | LMG | C22-C23-C24-C25 |
| 20 | f | 5002 | LMG | C22-C23-C24-C25 |
| 20 | f | 5002 | LMG | C32-C33-C34-C35 |
| 14 | 5 | 509 | CLA | C10-C11-C12-C13 |
| 14 | c | 509 | CLA | C10-C11-C12-C13 |
| 14 | u | 509 | CLA | C10-C11-C12-C13 |
| 14 | A | 1116 | CLA | C2A-CAA-CBA-CGA |
| 14 | 4 | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | 5 | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1116 | CLA | C2A-CAA-CBA-CGA |
| 14 | b | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1116 | CLA | C2A-CAA-CBA-CGA |
| 14 | t | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 518 | CLA | C2A-CAA-CBA-CGA |
| 17 | A | 4001 | BCR | C11-C12-C13-C35 |
| 17 | L | 4019 | BCR | C37-C22-C23-C24 |
| 17 | L | 4022 | BCR | C7-C8-C9-C34 |
| 17 | G | 4001 | BCR | C11-C12-C13-C35 |
| 17 | V | 4019 | BCR | C37-C22-C23-C24 |
| 17 | V | 4022 | BCR | C7-C8-C9-C34 |
| 17 | b | 521 | BCR | C36-C18-C19-C20 |
| 17 | n | 4019 | BCR | C37-C22-C23-C24 |
| 17 | n | 4022 | BCR | C7-C8-C9-C34 |
| 17 | t | 521 | BCR | C36-C18-C19-C20 |
| 18 | n | 5221 | LHG | C25-C26-C27-C28 |
| 20 | H | 5002 | LMG | C32-C33-C34-C35 |
| 18 | A | 5008 | LHG | O1-C1-C2-C3 |
| 18 | L | 5218 | LHG | O1-C1-C2-C3 |
| 18 | L | 5220 | LHG | O1-C1-C2-C3 |
| 18 | G | 5008 | LHG | O1-C1-C2-C3 |
| 18 | V | 5218 | LHG | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | V | 5220 | LHG | O1-C1-C2-C3 |
| 18 | e | 5008 | LHG | O1-C1-C2-C3 |
| 18 | n | 5218 | LHG | O1-C1-C2-C3 |
| 18 | n | 5220 | LHG | O1-C1-C2-C3 |
| 17 | L | 4019 | BCR | C21-C22-C23-C24 |
| 17 | 4 | 523 | BCR | C21-C22-C23-C24 |
| 17 | V | 4019 | BCR | C21-C22-C23-C24 |
| 17 | b | 523 | BCR | C21-C22-C23-C24 |
| 17 | n | 4019 | BCR | C21-C22-C23-C24 |
| 17 | t | 523 | BCR | C21-C22-C23-C24 |
| 14 | B | 1203 | CLA | C3-C5-C6-C7 |
| 14 | B | 1218 | CLA | C3-C5-C6-C7 |
| 14 | H | 1203 | CLA | C3-C5-C6-C7 |
| 14 | H | 1218 | CLA | C3-C5-C6-C7 |
| 14 | f | 1203 | CLA | C3-C5-C6-C7 |
| 14 | f | 1218 | CLA | C3-C5-C6-C7 |
| 14 | B | 1208 | CLA | C8-C10-C11-C12 |
| 14 | H | 1208 | CLA | C8-C10-C11-C12 |
| 14 | f | 1208 | CLA | C8-C10-C11-C12 |
| 18 | A | 5005 | LHG | C8-C7-O7-C5 |
| 18 | A | 5007 | LHG | C8-C7-O7-C5 |
| 18 | G | 5005 | LHG | C8-C7-O7-C5 |
| 18 | G | 5007 | LHG | C8-C7-O7-C5 |
| 18 | e | 5005 | LHG | C8-C7-O7-C5 |
| 18 | e | 5007 | LHG | C8-C7-O7-C5 |
| 18 | A | 5006 | LHG | C24-C25-C26-C27 |
| 18 | I | 5001 | LHG | C10-C11-C12-C13 |
| 18 | G | 5006 | LHG | C24-C25-C26-C27 |
| 18 | S | 5001 | LHG | C10-C11-C12-C13 |
| 18 | e | 5006 | LHG | C24-C25-C26-C27 |
| 18 | k | 5001 | LHG | C10-C11-C12-C13 |
| 14 | B | 1230 | CLA | O1D-CGD-O2D-CED |
| 14 | l | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1230 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1230 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 511 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5006 | LHG | C30-C31-C32-C33 |
| 18 | A | 5008 | LHG | C10-C11-C12-C13 |
| 18 | A | 5001 | LHG | C27-C28-C29-C30 |
| 18 | L | 5220 | LHG | C9-C10-C11-C12 |
| 18 | L | 5220 | LHG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | L | 5221 | LHG | C11-C12-C13-C14 |
| 18 | G | 5006 | LHG | C30-C31-C32-C33 |
| 18 | G | 5008 | LHG | C10-C11-C12-C13 |
| 18 | G | 5001 | LHG | C27-C28-C29-C30 |
| 18 | V | 5220 | LHG | C9-C10-C11-C12 |
| 18 | V | 5220 | LHG | C13-C14-C15-C16 |
| 18 | V | 5221 | LHG | C11-C12-C13-C14 |
| 18 | e | 5006 | LHG | C30-C31-C32-C33 |
| 18 | e | 5001 | LHG | C27-C28-C29-C30 |
| 18 | n | 5220 | LHG | C9-C10-C11-C12 |
| 18 | n | 5220 | LHG | C13-C14-C15-C16 |
| 18 | n | 5221 | LHG | C11-C12-C13-C14 |
| 19 | B | 1843 | LMU | C4-C5-C6-C7 |
| 19 | H | 1843 | LMU | C4-C5-C6-C7 |
| 19 | f | 1843 | LMU | C4-C5-C6-C7 |
| 14 | A | 1105 | CLA | C6-C7-C8-C10 |
| 14 | A | 1126 | CLA | C16-C17-C18-C20 |
| 14 | A | 1101 | CLA | C16-C17-C18-C19 |
| 14 | A | 1101 | CLA | C16-C17-C18-C20 |
| 14 | B | 1218 | CLA | C11-C12-C13-C14 |
| 14 | B | 1238 | CLA | C16-C17-C18-C19 |
| 14 | 3 | 505 | CLA | C6-C7-C8-C10 |
| 14 | G | 1105 | CLA | C6-C7-C8-C10 |
| 14 | G | 1126 | CLA | C16-C17-C18-C20 |
| 14 | G | 1101 | CLA | C16-C17-C18-C19 |
| 14 | G | 1101 | CLA | C16-C17-C18-C20 |
| 14 | H | 1208 | CLA | C16-C17-C18-C19 |
| 14 | H | 1218 | CLA | C11-C12-C13-C14 |
| 14 | H | 1238 | CLA | C16-C17-C18-C19 |
| 14 | a | 505 | CLA | C6-C7-C8-C10 |
| 14 | e | 1105 | CLA | C6-C7-C8-C10 |
| 14 | e | 1126 | CLA | C16-C17-C18-C20 |
| 14 | e | 1101 | CLA | C16-C17-C18-C19 |
| 14 | e | 1101 | CLA | C16-C17-C18-C20 |
| 14 | f | 1208 | CLA | C16-C17-C18-C19 |
| 14 | f | 1218 | CLA | C11-C12-C13-C14 |
| 14 | f | 1238 | CLA | C16-C17-C18-C19 |
| 14 | s | 505 | CLA | C6-C7-C8-C10 |
| 15 | A | 2001 | PQN | C26-C27-C28-C29 |
| 15 | G | 2001 | PQN | C26-C27-C28-C29 |
| 15 | e | 2001 | PQN | C26-C27-C28-C29 |
| 21 | B | 1852 | SQD | O5-C1-O6-C44 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | H | 1852 | SQD | O5-C1-O6-C44 |
| 21 | f | 1852 | SQD | O5-C1-O6-C44 |
| 14 | A | 1127 | CLA | C15-C16-C17-C18 |
| 14 | B | 1229 | CLA | C15-C16-C17-C18 |
| 14 | G | 1127 | CLA | C15-C16-C17-C18 |
| 14 | e | 1127 | CLA | C15-C16-C17-C18 |
| 18 | A | 5002 | LHG | C11-C10-C9-C8 |
| 18 | B | 1855 | LHG | C26-C27-C28-C29 |
| 18 | I | 5001 | LHG | C29-C30-C31-C32 |
| 18 | G | 5002 | LHG | C11-C10-C9-C8 |
| 18 | H | 1855 | LHG | C26-C27-C28-C29 |
| 18 | S | 5001 | LHG | C29-C30-C31-C32 |
| 18 | e | 5002 | LHG | C11-C10-C9-C8 |
| 18 | e | 5008 | LHG | C10-C11-C12-C13 |
| 18 | f | 1855 | LHG | C26-C27-C28-C29 |
| 18 | k | 5001 | LHG | C29-C30-C31-C32 |
| 21 | B | 1852 | SQD | C27-C28-C29-C30 |
| 21 | H | 1852 | SQD | C27-C28-C29-C30 |
| 21 | f | 1852 | SQD | C27-C28-C29-C30 |
| 14 | B | 1221 | CLA | O1D-CGD-O2D-CED |
| 14 | 6 | 509 | CLA | O1D-CGD-O2D-CED |
| 14 | H | 1221 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1221 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 509 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5002 | LHG | C31-C32-C33-C34 |
| 18 | A | 5007 | LHG | C32-C33-C34-C35 |
| 18 | L | 5218 | LHG | C32-C33-C34-C35 |
| 18 | G | 5002 | LHG | C31-C32-C33-C34 |
| 18 | G | 5007 | LHG | C32-C33-C34-C35 |
| 18 | V | 5218 | LHG | C32-C33-C34-C35 |
| 18 | e | 5002 | LHG | C31-C32-C33-C34 |
| 18 | e | 5007 | LHG | C32-C33-C34-C35 |
| 18 | n | 5218 | LHG | C32-C33-C34-C35 |
| 14 | H | 1229 | CLA | C15-C16-C17-C18 |
| 14 | f | 1229 | CLA | C15-C16-C17-C18 |
| 18 | A | 5005 | LHG | C13-C14-C15-C16 |
| 18 | G | 5005 | LHG | C13-C14-C15-C16 |
| 18 | e | 5005 | LHG | C13-C14-C15-C16 |
| 21 | L | 5216 | SQD | C24-C23-O48-C46 |
| 21 | V | 5216 | SQD | C24-C23-O48-C46 |
| 21 | n | 5216 | SQD | C24-C23-O48-C46 |
| 18 | A | 5001 | LHG | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | G | 5001 | LHG | C32-C33-C34-C35 |
| 18 | e | 5001 | LHG | C32-C33-C34-C35 |
| 14 | 5 | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 509 | CLA | O1D-CGD-O2D-CED |
| 14 | u | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1103 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1110 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1125 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1134 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1135 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1139 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1140 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1022 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1101 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1210 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1219 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1221 | CLA | C3A-C2A-CAA-CBA |
| 14 | F | 1302 | CLA | C3A-C2A-CAA-CBA |
| 14 | K | 1105 | CLA | C3A-C2A-CAA-CBA |
| 14 | 5 | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | 6 | 512 | CLA | C3A-C2A-CAA-CBA |
| 14 | 6 | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1103 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1110 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1125 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1134 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1135 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1139 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1140 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1022 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1101 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1210 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1219 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1221 | CLA | C3A-C2A-CAA-CBA |
| 14 | R | 1302 | CLA | C3A-C2A-CAA-CBA |
| 14 | U | 1105 | CLA | C3A-C2A-CAA-CBA |
| 14 | c | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | d | 512 | CLA | C3A-C2A-CAA-CBA |
| 14 | d | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1103 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1110 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1125 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1134 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1135 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1139 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1140 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1022 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1101 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1210 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1219 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1221 | CLA | C3A-C2A-CAA-CBA |
| 14 | j | 1302 | CLA | C3A-C2A-CAA-CBA |
| 14 | m | 1105 | CLA | C3A-C2A-CAA-CBA |
| 14 | u | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | v | 512 | CLA | C3A-C2A-CAA-CBA |
| 14 | v | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1208 | CLA | C13-C15-C16-C17 |
| 14 | B | 1210 | CLA | C5-C6-C7-C8 |
| 14 | H | 1208 | CLA | C13-C15-C16-C17 |
| 14 | f | 1208 | CLA | C13-C15-C16-C17 |
| 19 | B | 1843 | LMU | C2-C1-O1'-C1' |
| 19 | J | 5105 | LMU | C2-C1-O1'-C1' |
| 19 | H | 1843 | LMU | C2-C1-O1'-C1' |
| 19 | T | 5105 | LMU | C2-C1-O1'-C1' |
| 19 | f | 1843 | LMU | C2-C1-O1'-C1' |
| 19 | l | 5105 | LMU | C2-C1-O1'-C1' |
| 18 | A | 5001 | LHG | C29-C30-C31-C32 |
| 18 | G | 5001 | LHG | C29-C30-C31-C32 |
| 18 | e | 5001 | LHG | C29-C30-C31-C32 |
| 14 | A | 1105 | CLA | C6-C7-C8-C9 |
| 14 | A | 1140 | CLA | C16-C17-C18-C19 |
| 14 | B | 1208 | CLA | C16-C17-C18-C19 |
| 14 | B | 1210 | CLA | C16-C17-C18-C19 |
| 14 | B | 1238 | CLA | C16-C17-C18-C20 |
| 14 | 6 | 505 | CLA | C16-C17-C18-C19 |
| 14 | G | 1105 | CLA | C6-C7-C8-C9 |
| 14 | G | 1140 | CLA | C16-C17-C18-C19 |
| 14 | H | 1210 | CLA | C16-C17-C18-C19 |
| 14 | H | 1238 | CLA | C16-C17-C18-C20 |
| 14 | d | 505 | CLA | C16-C17-C18-C19 |
| 14 | e | 1105 | CLA | C6-C7-C8-C9 |
| 14 | e | 1140 | CLA | C16-C17-C18-C19 |
| 14 | f | 1210 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | f | 1238 | CLA | C16-C17-C18-C20 |
| 14 | v | 505 | CLA | C16-C17-C18-C19 |
| 20 | B | 5002 | LMG | C21-C22-C23-C24 |
| 20 | H | 5002 | LMG | C21-C22-C23-C24 |
| 20 | f | 5002 | LMG | C21-C22-C23-C24 |
| 14 | H | 1210 | CLA | C5-C6-C7-C8 |
| 18 | A | 5001 | LHG | C4-C5-C6-O8 |
| 18 | G | 5001 | LHG | C4-C5-C6-O8 |
| 18 | e | 5001 | LHG | C4-C5-C6-O8 |
| 14 | A | 1110 | CLA | CBD-CGD-O2D-CED |
| 14 | l | 519 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1110 | CLA | CBD-CGD-O2D-CED |
| 14 | e | 1110 | CLA | CBD-CGD-O2D-CED |
| 14 | q | 519 | CLA | CBD-CGD-O2D-CED |
| 18 | I | 5001 | LHG | C33-C34-C35-C36 |
| 18 | S | 5001 | LHG | C33-C34-C35-C36 |
| 18 | k | 5001 | LHG | C33-C34-C35-C36 |
| 14 | q | 517 | CLA | O1D-CGD-O2D-CED |
| 18 | L | 5221 | LHG | C28-C29-C30-C31 |
| 18 | V | 5221 | LHG | C28-C29-C30-C31 |
| 18 | f | 1842 | LHG | C31-C32-C33-C34 |
| 18 | n | 5221 | LHG | C28-C29-C30-C31 |
| 14 | L | 1502 | CLA | O1A-CGA-O2A-C1 |
| 14 | V | 1502 | CLA | O1A-CGA-O2A-C1 |
| 14 | n | 1502 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1210 | CLA | C5-C6-C7-C8 |
| 14 | A | 1124 | CLA | C4-C3-C5-C6 |
| 14 | B | 1208 | CLA | C4-C3-C5-C6 |
| 14 | G | 1124 | CLA | C4-C3-C5-C6 |
| 14 | H | 1208 | CLA | C4-C3-C5-C6 |
| 14 | e | 1124 | CLA | C4-C3-C5-C6 |
| 14 | f | 1208 | CLA | C4-C3-C5-C6 |
| 15 | B | 2002 | PQN | C14-C13-C15-C16 |
| 15 | H | 2002 | PQN | C14-C13-C15-C16 |
| 15 | f | 2002 | PQN | C14-C13-C15-C16 |
| 14 | A | 1120 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1120 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1120 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1102 | CLA | C2-C3-C5-C6 |
| 14 | A | 1124 | CLA | C2-C3-C5-C6 |
| 14 | B | 1227 | CLA | C2-C3-C5-C6 |
| 14 | L | 1503 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1102 | CLA | C2-C3-C5-C6 |
| 14 | G | 1124 | CLA | C2-C3-C5-C6 |
| 14 | H | 1227 | CLA | C2-C3-C5-C6 |
| 14 | V | 1503 | CLA | C2-C3-C5-C6 |
| 14 | e | 1102 | CLA | C2-C3-C5-C6 |
| 14 | e | 1124 | CLA | C2-C3-C5-C6 |
| 14 | f | 1227 | CLA | C2-C3-C5-C6 |
| 14 | n | 1503 | CLA | C2-C3-C5-C6 |
| 14 | A | 1011 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1122 | CLA | O1D-CGD-O2D-CED |
| 14 | l | 517 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1011 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1122 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1011 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1122 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 519 | CLA | CBD-CGD-O2D-CED |
| 18 | A | 5009 | LHG | C24-C25-C26-C27 |
| 18 | B | 1842 | LHG | C31-C32-C33-C34 |
| 18 | G | 5009 | LHG | C24-C25-C26-C27 |
| 18 | H | 1842 | LHG | C31-C32-C33-C34 |
| 18 | e | 5009 | LHG | C24-C25-C26-C27 |
| 14 | Y | 517 | CLA | O1D-CGD-O2D-CED |
| 18 | I | 5001 | LHG | O1-C1-C2-O2 |
| 18 | L | 5221 | LHG | O1-C1-C2-O2 |
| 18 | S | 5001 | LHG | O1-C1-C2-O2 |
| 18 | V | 5221 | LHG | O1-C1-C2-O2 |
| 18 | k | 5001 | LHG | O1-C1-C2-O2 |
| 18 | n | 5221 | LHG | O1-C1-C2-O2 |
| 14 | A | 1121 | CLA | C6-C7-C8-C10 |
| 14 | B | 1207 | CLA | C16-C17-C18-C20 |
| 14 | G | 1121 | CLA | C6-C7-C8-C10 |
| 14 | H | 1207 | CLA | C16-C17-C18-C20 |
| 14 | e | 1121 | CLA | C6-C7-C8-C10 |
| 14 | f | 1207 | CLA | C16-C17-C18-C20 |
| 18 | A | 5008 | LHG | C13-C14-C15-C16 |
| 18 | G | 5008 | LHG | C13-C14-C15-C16 |
| 18 | e | 5008 | LHG | C13-C14-C15-C16 |
| 14 | A | 1127 | CLA | C8-C10-C11-C12 |
| 14 | B | 1235 | CLA | C5-C6-C7-C8 |
| 14 | 2 | 503 | CLA | C8-C10-C11-C12 |
| 14 | G | 1127 | CLA | C8-C10-C11-C12 |
| 14 | H | 1235 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | Z | 503 | CLA | C8-C10-C11-C12 |
| 14 | e | 1127 | CLA | C8-C10-C11-C12 |
| 14 | f | 1235 | CLA | C5-C6-C7-C8 |
| 14 | r | 503 | CLA | C8-C10-C11-C12 |
| 18 | A | 5006 | LHG | C26-C27-C28-C29 |
| 18 | G | 5006 | LHG | C26-C27-C28-C29 |
| 18 | e | 5006 | LHG | C26-C27-C28-C29 |
| 14 | B | 1232 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1232 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1232 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5005 | LHG | O10-C23-O8-C6 |
| 18 | G | 5005 | LHG | O10-C23-O8-C6 |
| 18 | e | 5005 | LHG | O10-C23-O8-C6 |
| 15 | B | 2002 | PQN | C25-C26-C27-C28 |
| 15 | H | 2002 | PQN | C25-C26-C27-C28 |
| 15 | f | 2002 | PQN | C25-C26-C27-C28 |
| 18 | G | 5009 | LHG | C10-C11-C12-C13 |
| 18 | e | 5009 | LHG | C10-C11-C12-C13 |
| 20 | B | 5002 | LMG | C16-C17-C18-C19 |
| 20 | H | 5002 | LMG | C16-C17-C18-C19 |
| 20 | f | 5002 | LMG | C16-C17-C18-C19 |
| 21 | L | 5216 | SQD | C13-C14-C15-C16 |
| 21 | V | 5216 | SQD | C13-C14-C15-C16 |
| 21 | n | 5216 | SQD | C13-C14-C15-C16 |
| 14 | A | 1118 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1118 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1118 | CLA | C2-C1-O2A-CGA |
| 18 | A | 5009 | LHG | C10-C11-C12-C13 |
| 14 | A | 1117 | CLA | C13-C15-C16-C17 |
| 14 | G | 1117 | CLA | C13-C15-C16-C17 |
| 14 | e | 1117 | CLA | C13-C15-C16-C17 |
| 14 | A | 1137 | CLA | C3-C5-C6-C7 |
| 14 | G | 1137 | CLA | C3-C5-C6-C7 |
| 14 | e | 1137 | CLA | C3-C5-C6-C7 |
| 17 | A | 4008 | BCR | C23-C24-C25-C30 |
| 17 | A | 4011 | BCR | C23-C24-C25-C26 |
| 17 | A | 4011 | BCR | C23-C24-C25-C30 |
| 17 | B | 4004 | BCR | C1-C6-C7-C8 |
| 17 | B | 4004 | BCR | C5-C6-C7-C8 |
| 17 | B | 4004 | BCR | C23-C24-C25-C26 |
| 17 | B | 4005 | BCR | C23-C24-C25-C26 |
| 17 | B | 4010 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | B | 4017 | BCR | C5-C6-C7-C8 |
| 17 | B | 4014 | BCR | C23-C24-C25-C26 |
| 17 | J | 4015 | BCR | C23-C24-C25-C26 |
| 17 | J | 4012 | BCR | C1-C6-C7-C8 |
| 17 | J | 4012 | BCR | C23-C24-C25-C26 |
| 17 | J | 4012 | BCR | C23-C24-C25-C30 |
| 17 | L | 4019 | BCR | C23-C24-C25-C26 |
| 17 | L | 4019 | BCR | C23-C24-C25-C30 |
| 17 | M | 4021 | BCR | C1-C6-C7-C8 |
| 17 | 1 | 521 | BCR | C1-C6-C7-C8 |
| 17 | 1 | 521 | BCR | C5-C6-C7-C8 |
| 17 | 1 | 521 | BCR | C23-C24-C25-C26 |
| 17 | 1 | 521 | BCR | C23-C24-C25-C30 |
| 17 | 1 | 523 | BCR | C1-C6-C7-C8 |
| 17 | 1 | 523 | BCR | C5-C6-C7-C8 |
| 17 | 1 | 523 | BCR | C23-C24-C25-C26 |
| 17 | 1 | 523 | BCR | C23-C24-C25-C30 |
| 17 | 2 | 521 | BCR | C1-C6-C7-C8 |
| 17 | 2 | 521 | BCR | C5-C6-C7-C8 |
| 17 | 2 | 522 | BCR | C1-C6-C7-C8 |
| 17 | 2 | 523 | BCR | C23-C24-C25-C26 |
| 17 | 2 | 523 | BCR | C23-C24-C25-C30 |
| 17 | 2 | 524 | BCR | C23-C24-C25-C26 |
| 17 | 2 | 524 | BCR | C23-C24-C25-C30 |
| 17 | 3 | 521 | BCR | C1-C6-C7-C8 |
| 17 | 3 | 521 | BCR | C5-C6-C7-C8 |
| 17 | 3 | 523 | BCR | C23-C24-C25-C26 |
| 17 | 3 | 523 | BCR | C23-C24-C25-C30 |
| 17 | 4 | 521 | BCR | C1-C6-C7-C8 |
| 17 | 4 | 521 | BCR | C5-C6-C7-C8 |
| 17 | 4 | 521 | BCR | C23-C24-C25-C26 |
| 17 | 4 | 521 | BCR | C23-C24-C25-C30 |
| 17 | 4 | 522 | BCR | C1-C6-C7-C8 |
| 17 | 4 | 522 | BCR | C5-C6-C7-C8 |
| 17 | 4 | 523 | BCR | C23-C24-C25-C26 |
| 17 | 4 | 523 | BCR | C23-C24-C25-C30 |
| 17 | 4 | 524 | BCR | C23-C24-C25-C26 |
| 17 | 4 | 524 | BCR | C23-C24-C25-C30 |
| 17 | 5 | 522 | BCR | C1-C6-C7-C8 |
| 17 | 5 | 523 | BCR | C23-C24-C25-C26 |
| 17 | 5 | 523 | BCR | C23-C24-C25-C30 |
| 17 | 5 | 524 | BCR | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | 5 | 524 | BCR | C23-C24-C25-C30 |
| 17 | 6 | 521 | BCR | C1-C6-C7-C8 |
| 17 | 6 | 521 | BCR | C5-C6-C7-C8 |
| 17 | 6 | 522 | BCR | C1-C6-C7-C8 |
| 17 | 6 | 523 | BCR | C23-C24-C25-C26 |
| 17 | 6 | 523 | BCR | C23-C24-C25-C30 |
| 17 | G | 4008 | BCR | C23-C24-C25-C30 |
| 17 | G | 4011 | BCR | C23-C24-C25-C26 |
| 17 | G | 4011 | BCR | C23-C24-C25-C30 |
| 17 | H | 4004 | BCR | C1-C6-C7-C8 |
| 17 | H | 4004 | BCR | C5-C6-C7-C8 |
| 17 | H | 4004 | BCR | C23-C24-C25-C26 |
| 17 | H | 4005 | BCR | C23-C24-C25-C26 |
| 17 | H | 4010 | BCR | C23-C24-C25-C30 |
| 17 | H | 4017 | BCR | C5-C6-C7-C8 |
| 17 | H | 4014 | BCR | C23-C24-C25-C26 |
| 17 | T | 4015 | BCR | C23-C24-C25-C26 |
| 17 | T | 4012 | BCR | C1-C6-C7-C8 |
| 17 | T | 4012 | BCR | C23-C24-C25-C26 |
| 17 | T | 4012 | BCR | C23-C24-C25-C30 |
| 17 | V | 4019 | BCR | C23-C24-C25-C26 |
| 17 | V | 4019 | BCR | C23-C24-C25-C30 |
| 17 | W | 4021 | BCR | C1-C6-C7-C8 |
| 17 | Y | 521 | BCR | C1-C6-C7-C8 |
| 17 | Y | 521 | BCR | C5-C6-C7-C8 |
| 17 | Y | 521 | BCR | C23-C24-C25-C26 |
| 17 | Y | 521 | BCR | C23-C24-C25-C30 |
| 17 | Y | 523 | BCR | C1-C6-C7-C8 |
| 17 | Y | 523 | BCR | C5-C6-C7-C8 |
| 17 | Y | 523 | BCR | C23-C24-C25-C26 |
| 17 | Y | 523 | BCR | C23-C24-C25-C30 |
| 17 | Z | 521 | BCR | C1-C6-C7-C8 |
| 17 | Z | 521 | BCR | C5-C6-C7-C8 |
| 17 | Z | 522 | BCR | C1-C6-C7-C8 |
| 17 | Z | 523 | BCR | C23-C24-C25-C26 |
| 17 | Z | 523 | BCR | C23-C24-C25-C30 |
| 17 | Z | 524 | BCR | C23-C24-C25-C26 |
| 17 | Z | 524 | BCR | C23-C24-C25-C30 |
| 17 | a | 521 | BCR | C1-C6-C7-C8 |
| 17 | a | 521 | BCR | C5-C6-C7-C8 |
| 17 | a | 523 | BCR | C23-C24-C25-C26 |
| 17 | a | 523 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | b | 521 | BCR | C1-C6-C7-C8 |
| 17 | b | 521 | BCR | C5-C6-C7-C8 |
| 17 | b | 521 | BCR | C23-C24-C25-C26 |
| 17 | b | 521 | BCR | C23-C24-C25-C30 |
| 17 | b | 522 | BCR | C1-C6-C7-C8 |
| 17 | b | 522 | BCR | C5-C6-C7-C8 |
| 17 | b | 523 | BCR | C23-C24-C25-C26 |
| 17 | b | 523 | BCR | C23-C24-C25-C30 |
| 17 | b | 524 | BCR | C23-C24-C25-C26 |
| 17 | b | 524 | BCR | C23-C24-C25-C30 |
| 17 | c | 522 | BCR | C1-C6-C7-C8 |
| 17 | c | 523 | BCR | C23-C24-C25-C26 |
| 17 | c | 523 | BCR | C23-C24-C25-C30 |
| 17 | c | 524 | BCR | C23-C24-C25-C26 |
| 17 | c | 524 | BCR | C23-C24-C25-C30 |
| 17 | d | 521 | BCR | C1-C6-C7-C8 |
| 17 | d | 521 | BCR | C5-C6-C7-C8 |
| 17 | d | 522 | BCR | C1-C6-C7-C8 |
| 17 | d | 523 | BCR | C23-C24-C25-C26 |
| 17 | d | 523 | BCR | C23-C24-C25-C30 |
| 17 | e | 4008 | BCR | C23-C24-C25-C30 |
| 17 | e | 4011 | BCR | C23-C24-C25-C26 |
| 17 | e | 4011 | BCR | C23-C24-C25-C30 |
| 17 | f | 4004 | BCR | C1-C6-C7-C8 |
| 17 | f | 4004 | BCR | C5-C6-C7-C8 |
| 17 | f | 4004 | BCR | C23-C24-C25-C26 |
| 17 | f | 4005 | BCR | C23-C24-C25-C26 |
| 17 | f | 4010 | BCR | C23-C24-C25-C30 |
| 17 | f | 4017 | BCR | C5-C6-C7-C8 |
| 17 | f | 4014 | BCR | C23-C24-C25-C26 |
| 17 | l | 4015 | BCR | C23-C24-C25-C26 |
| 17 | l | 4012 | BCR | C1-C6-C7-C8 |
| 17 | l | 4012 | BCR | C23-C24-C25-C26 |
| 17 | l | 4012 | BCR | C23-C24-C25-C30 |
| 17 | n | 4019 | BCR | C23-C24-C25-C26 |
| 17 | n | 4019 | BCR | C23-C24-C25-C30 |
| 17 | o | 4021 | BCR | C1-C6-C7-C8 |
| 17 | q | 521 | BCR | C1-C6-C7-C8 |
| 17 | q | 521 | BCR | C5-C6-C7-C8 |
| 17 | q | 521 | BCR | C23-C24-C25-C26 |
| 17 | q | 521 | BCR | C23-C24-C25-C30 |
| 17 | q | 523 | BCR | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | q | 523 | BCR | C5-C6-C7-C8 |
| 17 | q | 523 | BCR | C23-C24-C25-C26 |
| 17 | q | 523 | BCR | C23-C24-C25-C30 |
| 17 | r | 521 | BCR | C1-C6-C7-C8 |
| 17 | r | 521 | BCR | C5-C6-C7-C8 |
| 17 | r | 522 | BCR | C1-C6-C7-C8 |
| 17 | r | 523 | BCR | C23-C24-C25-C26 |
| 17 | r | 523 | BCR | C23-C24-C25-C30 |
| 17 | r | 524 | BCR | C23-C24-C25-C26 |
| 17 | r | 524 | BCR | C23-C24-C25-C30 |
| 17 | s | 521 | BCR | C1-C6-C7-C8 |
| 17 | s | 521 | BCR | C5-C6-C7-C8 |
| 17 | s | 523 | BCR | C23-C24-C25-C26 |
| 17 | s | 523 | BCR | C23-C24-C25-C30 |
| 17 | t | 521 | BCR | C1-C6-C7-C8 |
| 17 | t | 521 | BCR | C5-C6-C7-C8 |
| 17 | t | 521 | BCR | C23-C24-C25-C26 |
| 17 | t | 521 | BCR | C23-C24-C25-C30 |
| 17 | t | 522 | BCR | C1-C6-C7-C8 |
| 17 | t | 522 | BCR | C5-C6-C7-C8 |
| 17 | t | 523 | BCR | C23-C24-C25-C26 |
| 17 | t | 523 | BCR | C23-C24-C25-C30 |
| 17 | t | 524 | BCR | C23-C24-C25-C26 |
| 17 | t | 524 | BCR | C23-C24-C25-C30 |
| 17 | u | 522 | BCR | C1-C6-C7-C8 |
| 17 | u | 523 | BCR | C23-C24-C25-C26 |
| 17 | u | 523 | BCR | C23-C24-C25-C30 |
| 17 | u | 524 | BCR | C23-C24-C25-C26 |
| 17 | u | 524 | BCR | C23-C24-C25-C30 |
| 17 | v | 521 | BCR | C1-C6-C7-C8 |
| 17 | v | 521 | BCR | C5-C6-C7-C8 |
| 17 | v | 522 | BCR | C1-C6-C7-C8 |
| 17 | v | 523 | BCR | C23-C24-C25-C26 |
| 17 | v | 523 | BCR | C23-C24-C25-C30 |
| 18 | L | 5221 | LHG | C32-C33-C34-C35 |
| 14 | B | 1215 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1215 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1215 | CLA | CBA-CGA-O2A-C1 |
| 20 | J | 5104 | LMG | C29-C28-O8-C9 |
| 20 | T | 5104 | LMG | C29-C28-O8-C9 |
| 20 | l | 5104 | LMG | C29-C28-O8-C9 |
| 14 | A | 1133 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1136 | CLA | C13-C15-C16-C17 |
| 14 | 2 | 501 | CLA | C10-C11-C12-C13 |
| 14 | G | 1133 | CLA | C13-C15-C16-C17 |
| 14 | G | 1136 | CLA | C13-C15-C16-C17 |
| 14 | Z | 501 | CLA | C10-C11-C12-C13 |
| 14 | e | 1133 | CLA | C13-C15-C16-C17 |
| 14 | e | 1136 | CLA | C13-C15-C16-C17 |
| 14 | r | 501 | CLA | C10-C11-C12-C13 |
| 18 | L | 5221 | LHG | C27-C28-C29-C30 |
| 18 | V | 5221 | LHG | C27-C28-C29-C30 |
| 18 | V | 5221 | LHG | C32-C33-C34-C35 |
| 18 | n | 5221 | LHG | C27-C28-C29-C30 |
| 18 | n | 5221 | LHG | C32-C33-C34-C35 |
| 14 | A | 1120 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1120 | CLA | O1D-CGD-O2D-CED |
| 14 | j | 1302 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1133 | CLA | C15-C16-C17-C18 |
| 14 | B | 1218 | CLA | C5-C6-C7-C8 |
| 14 | H | 1218 | CLA | C5-C6-C7-C8 |
| 14 | e | 1133 | CLA | C15-C16-C17-C18 |
| 14 | f | 1218 | CLA | C5-C6-C7-C8 |
| 14 | G | 1120 | CLA | O1D-CGD-O2D-CED |
| 21 | 6 | 822 | SQD | C24-C23-O48-C46 |
| 21 | d | 822 | SQD | C24-C23-O48-C46 |
| 21 | v | 822 | SQD | C24-C23-O48-C46 |
| 18 | A | 5009 | LHG | C27-C28-C29-C30 |
| 18 | G | 5009 | LHG | C27-C28-C29-C30 |
| 18 | e | 5009 | LHG | C27-C28-C29-C30 |
| 20 | B | 5002 | LMG | C37-C38-C39-C40 |
| 20 | H | 5002 | LMG | C37-C38-C39-C40 |
| 20 | f | 5002 | LMG | C37-C38-C39-C40 |
| 14 | A | 1117 | CLA | C4-C3-C5-C6 |
| 14 | B | 1227 | CLA | C4-C3-C5-C6 |
| 14 | G | 1117 | CLA | C4-C3-C5-C6 |
| 14 | H | 1227 | CLA | C4-C3-C5-C6 |
| 14 | e | 1117 | CLA | C4-C3-C5-C6 |
| 14 | f | 1227 | CLA | C4-C3-C5-C6 |
| 14 | A | 1103 | CLA | C11-C10-C8-C7 |
| 14 | A | 1110 | CLA | C2-C3-C5-C6 |
| 14 | A | 1117 | CLA | C2-C3-C5-C6 |
| 14 | A | 1132 | CLA | C2-C3-C5-C6 |
| 14 | A | 1133 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1208 | CLA | C2-C3-C5-C6 |
| 14 | B | 1214 | CLA | C12-C13-C15-C16 |
| 14 | B | 1223 | CLA | C12-C13-C15-C16 |
| 14 | B | 1231 | CLA | C2-C3-C5-C6 |
| 14 | B | 1234 | CLA | C11-C12-C13-C15 |
| 14 | B | 1239 | CLA | C6-C7-C8-C10 |
| 14 | L | 1503 | CLA | C6-C7-C8-C10 |
| 14 | G | 1103 | CLA | C11-C10-C8-C7 |
| 14 | G | 1110 | CLA | C2-C3-C5-C6 |
| 14 | G | 1117 | CLA | C2-C3-C5-C6 |
| 14 | G | 1132 | CLA | C2-C3-C5-C6 |
| 14 | G | 1133 | CLA | C11-C12-C13-C15 |
| 14 | H | 1208 | CLA | C2-C3-C5-C6 |
| 14 | H | 1214 | CLA | C12-C13-C15-C16 |
| 14 | H | 1223 | CLA | C12-C13-C15-C16 |
| 14 | H | 1231 | CLA | C2-C3-C5-C6 |
| 14 | H | 1234 | CLA | C11-C12-C13-C15 |
| 14 | H | 1239 | CLA | C6-C7-C8-C10 |
| 14 | V | 1503 | CLA | C6-C7-C8-C10 |
| 14 | e | 1103 | CLA | C11-C10-C8-C7 |
| 14 | e | 1110 | CLA | C2-C3-C5-C6 |
| 14 | e | 1132 | CLA | C2-C3-C5-C6 |
| 14 | e | 1133 | CLA | C11-C12-C13-C15 |
| 14 | f | 1208 | CLA | C2-C3-C5-C6 |
| 14 | f | 1214 | CLA | C12-C13-C15-C16 |
| 14 | f | 1223 | CLA | C12-C13-C15-C16 |
| 14 | f | 1231 | CLA | C2-C3-C5-C6 |
| 14 | f | 1234 | CLA | C11-C12-C13-C15 |
| 14 | f | 1239 | CLA | C6-C7-C8-C10 |
| 14 | n | 1503 | CLA | C6-C7-C8-C10 |
| 14 | A | 1124 | CLA | C3-C5-C6-C7 |
| 14 | G | 1124 | CLA | C3-C5-C6-C7 |
| 14 | e | 1124 | CLA | C3-C5-C6-C7 |
| 14 | A | 1120 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1120 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1120 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5009 | LHG | C11-C12-C13-C14 |
| 18 | G | 5009 | LHG | C11-C12-C13-C14 |
| 18 | e | 5009 | LHG | C11-C12-C13-C14 |
| 14 | A | 1117 | CLA | C8-C10-C11-C12 |
| 14 | A | 1136 | CLA | C10-C11-C12-C13 |
| 14 | A | 1138 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1202 | CLA | C13-C15-C16-C17 |
| 14 | B | 1221 | CLA | C5-C6-C7-C8 |
| 14 | G | 1117 | CLA | C8-C10-C11-C12 |
| 14 | G | 1133 | CLA | C15-C16-C17-C18 |
| 14 | G | 1138 | CLA | C8-C10-C11-C12 |
| 14 | H | 1202 | CLA | C13-C15-C16-C17 |
| 14 | e | 1136 | CLA | C10-C11-C12-C13 |
| 14 | e | 1138 | CLA | C8-C10-C11-C12 |
| 14 | f | 1202 | CLA | C13-C15-C16-C17 |
| 14 | f | 1221 | CLA | C5-C6-C7-C8 |
| 17 | B | 4010 | BCR | C9-C10-C11-C12 |
| 17 | 2 | 522 | BCR | C9-C10-C11-C12 |
| 17 | H | 4010 | BCR | C9-C10-C11-C12 |
| 17 | Z | 522 | BCR | C9-C10-C11-C12 |
| 17 | f | 4010 | BCR | C9-C10-C11-C12 |
| 17 | r | 522 | BCR | C9-C10-C11-C12 |
| 14 | F | 1302 | CLA | CBD-CGD-O2D-CED |
| 14 | R | 1302 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1111 | CLA | C16-C17-C18-C20 |
| 14 | B | 1226 | CLA | C6-C7-C8-C10 |
| 14 | G | 1111 | CLA | C16-C17-C18-C20 |
| 14 | H | 1226 | CLA | C6-C7-C8-C10 |
| 14 | e | 1111 | CLA | C16-C17-C18-C20 |
| 14 | f | 1226 | CLA | C6-C7-C8-C10 |
| 14 | A | 1132 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1201 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1132 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1201 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1132 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1201 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1135 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1023 | CLA | C2A-CAA-CBA-CGA |
| 14 | L | 1501 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | 4 | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1135 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1023 | CLA | C2A-CAA-CBA-CGA |
| 14 | V | 1501 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | b | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1135 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1023 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | n | 1501 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | t | 505 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1210 | CLA | C13-C15-C16-C17 |
| 14 | B | 1207 | CLA | C10-C11-C12-C13 |
| 14 | G | 1136 | CLA | C10-C11-C12-C13 |
| 14 | H | 1210 | CLA | C13-C15-C16-C17 |
| 14 | H | 1221 | CLA | C5-C6-C7-C8 |
| 14 | H | 1207 | CLA | C10-C11-C12-C13 |
| 14 | e | 1117 | CLA | C8-C10-C11-C12 |
| 14 | f | 1210 | CLA | C13-C15-C16-C17 |
| 14 | f | 1207 | CLA | C10-C11-C12-C13 |
| 18 | I | 5001 | LHG | C27-C28-C29-C30 |
| 18 | L | 5220 | LHG | C29-C30-C31-C32 |
| 18 | S | 5001 | LHG | C27-C28-C29-C30 |
| 18 | k | 5001 | LHG | C27-C28-C29-C30 |
| 14 | G | 1103 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1240 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1240 | CLA | CBD-CGD-O2D-CED |
| 18 | V | 5220 | LHG | C29-C30-C31-C32 |
| 18 | n | 5220 | LHG | C29-C30-C31-C32 |
| 14 | A | 1103 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1103 | CLA | O1D-CGD-O2D-CED |
| 20 | T | 5104 | LMG | C31-C32-C33-C34 |
| 20 | l | 5104 | LMG | C31-C32-C33-C34 |
| 19 | A | 1848 | LMU | O5B-C5B-C6B-O6B |
| 19 | G | 1848 | LMU | O5B-C5B-C6B-O6B |
| 19 | e | 1848 | LMU | O5B-C5B-C6B-O6B |
| 14 | H | 1240 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1227 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1105 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1105 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1105 | CLA | CBA-CGA-O2A-C1 |
| 19 | A | 1849 | LMU | O5'-C1'-O1'-C1 |
| 19 | G | 1849 | LMU | O5'-C1'-O1'-C1 |
| 19 | e | 1849 | LMU | O5'-C1'-O1'-C1 |
| 18 | A | 5009 | LHG | C11-C10-C9-C8 |
| 18 | G | 5009 | LHG | C11-C10-C9-C8 |
| 18 | e | 5009 | LHG | C11-C10-C9-C8 |
| 20 | J | 5104 | LMG | C31-C32-C33-C34 |
| 20 | B | 5002 | LMG | C28-C29-C30-C31 |
| 20 | H | 5002 | LMG | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 20 | f | 5002 | LMG | C28-C29-C30-C31 |
| 18 | A | 5001 | LHG | C8-C7-O7-C5 |
| 18 | G | 5001 | LHG | C8-C7-O7-C5 |
| 18 | e | 5001 | LHG | C8-C7-O7-C5 |
| 20 | J | 5104 | LMG | C11-C10-O7-C8 |
| 20 | T | 5104 | LMG | C11-C10-O7-C8 |
| 20 | l | 5104 | LMG | C11-C10-O7-C8 |
| 14 | 2 | 509 | CLA | C5-C6-C7-C8 |
| 14 | B | 1227 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1227 | CLA | CBD-CGD-O2D-CED |
| 18 | A | 5005 | LHG | O9-C7-O7-C5 |
| 18 | G | 5005 | LHG | O9-C7-O7-C5 |
| 18 | e | 5005 | LHG | O9-C7-O7-C5 |
| 14 | B | 1213 | CLA | C3-C5-C6-C7 |
| 14 | H | 1213 | CLA | C3-C5-C6-C7 |
| 14 | f | 1213 | CLA | C3-C5-C6-C7 |
| 18 | A | 5002 | LHG | C25-C26-C27-C28 |
| 18 | G | 5002 | LHG | C25-C26-C27-C28 |
| 18 | e | 5002 | LHG | C25-C26-C27-C28 |
| 14 | Z | 509 | CLA | C5-C6-C7-C8 |
| 14 | r | 509 | CLA | C5-C6-C7-C8 |
| 18 | I | 5001 | LHG | O7-C5-C6-O8 |
| 18 | S | 5001 | LHG | O7-C5-C6-O8 |
| 18 | k | 5001 | LHG | O7-C5-C6-O8 |
| 20 | B | 5002 | LMG | O7-C8-C9-O8 |
| 20 | H | 5002 | LMG | O7-C8-C9-O8 |
| 20 | f | 5002 | LMG | O7-C8-C9-O8 |
| 18 | k | 5001 | LHG | C28-C29-C30-C31 |
| 14 | A | 1125 | CLA | C13-C15-C16-C17 |
| 14 | G | 1125 | CLA | C13-C15-C16-C17 |
| 14 | e | 1125 | CLA | C13-C15-C16-C17 |
| 14 | A | 1110 | CLA | C4-C3-C5-C6 |
| 14 | A | 1101 | CLA | C4-C3-C5-C6 |
| 14 | B | 1231 | CLA | C4-C3-C5-C6 |
| 14 | G | 1110 | CLA | C4-C3-C5-C6 |
| 14 | G | 1101 | CLA | C4-C3-C5-C6 |
| 14 | H | 1231 | CLA | C4-C3-C5-C6 |
| 14 | e | 1110 | CLA | C4-C3-C5-C6 |
| 14 | e | 1101 | CLA | C4-C3-C5-C6 |
| 14 | f | 1231 | CLA | C4-C3-C5-C6 |
| 14 | e | 1117 | CLA | C2-C3-C5-C6 |
| 18 | A | 5009 | LHG | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | I | 5001 | LHG | C28-C29-C30-C31 |
| 18 | G | 5009 | LHG | C28-C29-C30-C31 |
| 18 | S | 5001 | LHG | C28-C29-C30-C31 |
| 18 | e | 5009 | LHG | C28-C29-C30-C31 |
| 14 | A | 1103 | CLA | C11-C10-C8-C9 |
| 14 | A | 1109 | CLA | C11-C12-C13-C14 |
| 14 | A | 1123 | CLA | C11-C10-C8-C9 |
| 14 | A | 1127 | CLA | C14-C13-C15-C16 |
| 14 | A | 1138 | CLA | C11-C10-C8-C9 |
| 14 | A | 1139 | CLA | C11-C10-C8-C9 |
| 14 | B | 1216 | CLA | C6-C7-C8-C9 |
| 14 | B | 1221 | CLA | C11-C10-C8-C9 |
| 14 | B | 1223 | CLA | C11-C12-C13-C14 |
| 14 | 5 | 509 | CLA | C11-C10-C8-C9 |
| 14 | G | 1103 | CLA | C11-C10-C8-C9 |
| 14 | G | 1109 | CLA | C11-C12-C13-C14 |
| 14 | G | 1119 | CLA | C6-C7-C8-C9 |
| 14 | G | 1123 | CLA | C11-C10-C8-C9 |
| 14 | G | 1127 | CLA | C14-C13-C15-C16 |
| 14 | G | 1138 | CLA | C11-C10-C8-C9 |
| 14 | G | 1139 | CLA | C11-C10-C8-C9 |
| 14 | H | 1216 | CLA | C6-C7-C8-C9 |
| 14 | H | 1221 | CLA | C11-C10-C8-C9 |
| 14 | H | 1223 | CLA | C11-C12-C13-C14 |
| 14 | c | 509 | CLA | C11-C10-C8-C9 |
| 14 | e | 1103 | CLA | C11-C10-C8-C9 |
| 14 | e | 1109 | CLA | C11-C12-C13-C14 |
| 14 | e | 1123 | CLA | C11-C10-C8-C9 |
| 14 | e | 1127 | CLA | C14-C13-C15-C16 |
| 14 | e | 1138 | CLA | C11-C10-C8-C9 |
| 14 | e | 1139 | CLA | C11-C10-C8-C9 |
| 14 | f | 1221 | CLA | C11-C10-C8-C9 |
| 14 | f | 1223 | CLA | C11-C12-C13-C14 |
| 14 | u | 509 | CLA | C11-C10-C8-C9 |
| 18 | A | 5001 | LHG | C10-C11-C12-C13 |
| 18 | G | 5001 | LHG | C10-C11-C12-C13 |
| 18 | e | 5001 | LHG | C10-C11-C12-C13 |
| 14 | A | 1118 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1120 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1121 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 512 | CLA | C2A-CAA-CBA-CGA |
| 14 | 5 | 517 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1118 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1120 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1121 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 512 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1118 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1120 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1121 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 512 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 517 | CLA | C2A-CAA-CBA-CGA |
| 19 | B | 1843 | LMU | C7-C8-C9-C10 |
| 19 | f | 1843 | LMU | C7-C8-C9-C10 |
| 17 | e | 4001 | BCR | C11-C12-C13-C35 |
| 14 | G | 1131 | CLA | C13-C15-C16-C17 |
| 19 | H | 1843 | LMU | C7-C8-C9-C10 |
| 17 | 3 | 523 | BCR | C21-C22-C23-C24 |
| 17 | a | 523 | BCR | C21-C22-C23-C24 |
| 17 | s | 523 | BCR | C21-C22-C23-C24 |
| 14 | A | 1102 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1106 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1107 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1109 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1116 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1118 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1120 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1122 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1125 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1129 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1132 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1134 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1135 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1022 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1130 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1101 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1219 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1221 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1225 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1226 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1227 | CLA | C1A-C2A-CAA-CBA |
| 14 | F | 1302 | CLA | C1A-C2A-CAA-CBA |
| 14 | J | 1302 | CLA | C1A-C2A-CAA-CBA |
| 14 | J | 1303 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | K | 1103 | CLA | C1A-C2A-CAA-CBA |
| 14 | K | 1105 | CLA | C1A-C2A-CAA-CBA |
| 14 | L | 1501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 1 | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | 1 | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | 1 | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | 1 | 519 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | 4 | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 4 | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | 4 | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 502 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 513 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1102 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1106 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1107 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1109 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1116 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1118 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1120 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1122 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1125 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1129 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1132 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1134 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1135 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1022 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1130 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1101 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1219 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1221 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1225 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1226 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1227 | CLA | C1A-C2A-CAA-CBA |
| 14 | R | 1302 | CLA | C1A-C2A-CAA-CBA |
| 14 | T | 1302 | CLA | C1A-C2A-CAA-CBA |
| 14 | T | 1303 | CLA | C1A-C2A-CAA-CBA |
| 14 | U | 1103 | CLA | C1A-C2A-CAA-CBA |
| 14 | U | 1105 | CLA | C1A-C2A-CAA-CBA |
| 14 | V | 1501 | CLA | C1A-C2A-CAA-CBA |
| 14 | Y | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | Y | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | Y | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | Y | 519 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | b | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | b | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | b | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 502 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 513 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 518 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1102 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1106 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1107 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1109 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1116 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1118 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1120 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1122 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1125 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1129 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1132 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1134 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1135 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1022 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1130 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1101 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1219 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1221 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1225 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1226 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1227 | CLA | C1A-C2A-CAA-CBA |
| 14 | j | 1302 | CLA | C1A-C2A-CAA-CBA |
| 14 | l | 1302 | CLA | C1A-C2A-CAA-CBA |
| 14 | l | 1303 | CLA | C1A-C2A-CAA-CBA |
| 14 | m | 1103 | CLA | C1A-C2A-CAA-CBA |
| 14 | m | 1105 | CLA | C1A-C2A-CAA-CBA |
| 14 | n | 1501 | CLA | C1A-C2A-CAA-CBA |
| 14 | q | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | q | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | q | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | q | 519 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | t | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | t | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | t | 511 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | u | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 502 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 513 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 505 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 518 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1208 | CLA | C16-C17-C18-C20 |
| 14 | B | 1218 | CLA | C11-C12-C13-C15 |
| 14 | B | 1239 | CLA | C16-C17-C18-C19 |
| 14 | B | 1239 | CLA | C16-C17-C18-C20 |
| 14 | H | 1208 | CLA | C16-C17-C18-C20 |
| 14 | H | 1218 | CLA | C11-C12-C13-C15 |
| 14 | H | 1239 | CLA | C16-C17-C18-C19 |
| 14 | H | 1239 | CLA | C16-C17-C18-C20 |
| 14 | f | 1208 | CLA | C16-C17-C18-C20 |
| 14 | f | 1218 | CLA | C11-C12-C13-C15 |
| 14 | f | 1239 | CLA | C16-C17-C18-C19 |
| 14 | f | 1239 | CLA | C16-C17-C18-C20 |
| 15 | B | 2002 | PQN | C26-C27-C28-C29 |
| 15 | H | 2002 | PQN | C26-C27-C28-C29 |
| 15 | f | 2002 | PQN | C26-C27-C28-C29 |
| 18 | L | 5221 | LHG | C8-C7-O7-C5 |
| 18 | V | 5221 | LHG | C8-C7-O7-C5 |
| 18 | n | 5221 | LHG | C8-C7-O7-C5 |
| 18 | A | 5006 | LHG | C27-C28-C29-C30 |
| 18 | G | 5006 | LHG | C27-C28-C29-C30 |
| 18 | e | 5006 | LHG | C27-C28-C29-C30 |
| 14 | A | 1131 | CLA | C13-C15-C16-C17 |
| 14 | B | 1223 | CLA | C10-C11-C12-C13 |
| 14 | H | 1224 | CLA | C5-C6-C7-C8 |
| 14 | e | 1131 | CLA | C13-C15-C16-C17 |
| 14 | f | 1223 | CLA | C10-C11-C12-C13 |
| 18 | A | 5002 | LHG | C4-O6-P-O3 |
| 18 | I | 5001 | LHG | C3-O3-P-O6 |
| 18 | G | 5002 | LHG | C4-O6-P-O3 |
| 18 | S | 5001 | LHG | C3-O3-P-O6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | e | 5002 | LHG | C4-O6-P-O3 |
| 18 | k | 5001 | LHG | C3-O3-P-O6 |
| 18 | A | 5008 | LHG | C25-C26-C27-C28 |
| 18 | G | 5008 | LHG | C25-C26-C27-C28 |
| 18 | e | 5008 | LHG | C25-C26-C27-C28 |
| 14 | A | 1132 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1132 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1132 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1203 | CLA | C13-C15-C16-C17 |
| 14 | B | 1224 | CLA | C5-C6-C7-C8 |
| 14 | H | 1203 | CLA | C13-C15-C16-C17 |
| 14 | H | 1223 | CLA | C10-C11-C12-C13 |
| 14 | f | 1203 | CLA | C13-C15-C16-C17 |
| 14 | f | 1224 | CLA | C5-C6-C7-C8 |
| 18 | A | 5007 | LHG | O6-C4-C5-C6 |
| 18 | G | 5007 | LHG | O6-C4-C5-C6 |
| 18 | e | 5007 | LHG | O6-C4-C5-C6 |
| 18 | L | 5218 | LHG | C11-C10-C9-C8 |
| 18 | V | 5218 | LHG | C11-C10-C9-C8 |
| 18 | n | 5218 | LHG | C11-C10-C9-C8 |
| 18 | A | 5002 | LHG | C30-C31-C32-C33 |
| 18 | A | 5008 | LHG | C12-C13-C14-C15 |
| 18 | G | 5002 | LHG | C30-C31-C32-C33 |
| 18 | G | 5008 | LHG | C12-C13-C14-C15 |
| 18 | e | 5002 | LHG | C30-C31-C32-C33 |
| 18 | e | 5008 | LHG | C12-C13-C14-C15 |
| 15 | A | 2001 | PQN | C25-C26-C27-C28 |
| 15 | G | 2001 | PQN | C25-C26-C27-C28 |
| 15 | e | 2001 | PQN | C25-C26-C27-C28 |
| 14 | B | 1217 | CLA | C11-C12-C13-C15 |
| 14 | H | 1217 | CLA | C11-C12-C13-C15 |
| 14 | f | 1217 | CLA | C11-C12-C13-C15 |
| 18 | A | 5002 | LHG | C23-C24-C25-C26 |
| 18 | G | 5002 | LHG | C23-C24-C25-C26 |
| 18 | e | 5002 | LHG | C23-C24-C25-C26 |
| 18 | B | 1842 | LHG | C25-C26-C27-C28 |
| 18 | H | 1842 | LHG | C25-C26-C27-C28 |
| 18 | f | 1842 | LHG | C25-C26-C27-C28 |
| 20 | J | 5104 | LMG | C30-C31-C32-C33 |
| 14 | A | 1108 | CLA | C4-C3-C5-C6 |
| 14 | B | 1210 | CLA | C4-C3-C5-C6 |
| 14 | G | 1108 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1210 | CLA | C4-C3-C5-C6 |
| 14 | e | 1108 | CLA | C4-C3-C5-C6 |
| 14 | f | 1210 | CLA | C4-C3-C5-C6 |
| 15 | A | 2001 | PQN | C14-C13-C15-C16 |
| 15 | G | 2001 | PQN | C14-C13-C15-C16 |
| 15 | e | 2001 | PQN | C14-C13-C15-C16 |
| 20 | T | 5104 | LMG | C30-C31-C32-C33 |
| 20 | l | 5104 | LMG | C30-C31-C32-C33 |
| 18 | G | 5003 | LHG | C9-C10-C11-C12 |
| 14 | A | 1105 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1105 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1105 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 5002 | LMG | O10-C28-O8-C9 |
| 20 | H | 5002 | LMG | O10-C28-O8-C9 |
| 20 | f | 5002 | LMG | O10-C28-O8-C9 |
| 18 | A | 5003 | LHG | C9-C10-C11-C12 |
| 18 | B | 1855 | LHG | C27-C28-C29-C30 |
| 18 | H | 1855 | LHG | C27-C28-C29-C30 |
| 18 | e | 5003 | LHG | C9-C10-C11-C12 |
| 18 | f | 1855 | LHG | C27-C28-C29-C30 |
| 14 | A | 1103 | CLA | C16-C17-C18-C20 |
| 14 | L | 1502 | CLA | C16-C17-C18-C19 |
| 14 | 2 | 505 | CLA | C16-C17-C18-C20 |
| 14 | G | 1103 | CLA | C16-C17-C18-C20 |
| 14 | V | 1502 | CLA | C16-C17-C18-C19 |
| 14 | Z | 505 | CLA | C16-C17-C18-C20 |
| 14 | e | 1103 | CLA | C16-C17-C18-C20 |
| 14 | n | 1502 | CLA | C16-C17-C18-C19 |
| 14 | r | 505 | CLA | C16-C17-C18-C20 |
| 18 | A | 5002 | LHG | C4-C5-C6-O8 |
| 18 | A | 5004 | LHG | C4-C5-C6-O8 |
| 18 | A | 5008 | LHG | C4-C5-C6-O8 |
| 18 | L | 5218 | LHG | C4-C5-C6-O8 |
| 18 | L | 5221 | LHG | C4-C5-C6-O8 |
| 18 | G | 5002 | LHG | C4-C5-C6-O8 |
| 18 | G | 5004 | LHG | C4-C5-C6-O8 |
| 18 | G | 5008 | LHG | C4-C5-C6-O8 |
| 18 | S | 5001 | LHG | C31-C32-C33-C34 |
| 18 | V | 5218 | LHG | C4-C5-C6-O8 |
| 18 | V | 5221 | LHG | C4-C5-C6-O8 |
| 18 | e | 5002 | LHG | C4-C5-C6-O8 |
| 18 | e | 5004 | LHG | C4-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | e | 5008 | LHG | C4-C5-C6-O8 |
| 18 | n | 5218 | LHG | C4-C5-C6-O8 |
| 18 | n | 5221 | LHG | C4-C5-C6-O8 |
| 21 | 3 | 822 | SQD | C44-C45-C46-O48 |
| 21 | 6 | 822 | SQD | C44-C45-C46-O48 |
| 21 | a | 822 | SQD | C44-C45-C46-O48 |
| 21 | d | 822 | SQD | C44-C45-C46-O48 |
| 21 | s | 822 | SQD | C44-C45-C46-O48 |
| 21 | v | 822 | SQD | C44-C45-C46-O48 |
| 18 | I | 5001 | LHG | C31-C32-C33-C34 |
| 18 | G | 5007 | LHG | C25-C26-C27-C28 |
| 18 | e | 5005 | LHG | C31-C32-C33-C34 |
| 18 | k | 5001 | LHG | C31-C32-C33-C34 |
| 14 | B | 1215 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1215 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1215 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5005 | LHG | C31-C32-C33-C34 |
| 18 | A | 5007 | LHG | C25-C26-C27-C28 |
| 18 | G | 5005 | LHG | C31-C32-C33-C34 |
| 18 | e | 5007 | LHG | C25-C26-C27-C28 |
| 14 | A | 1137 | CLA | C5-C6-C7-C8 |
| 14 | G | 1137 | CLA | C5-C6-C7-C8 |
| 14 | e | 1137 | CLA | C5-C6-C7-C8 |
| 14 | A | 1108 | CLA | C5-C6-C7-C8 |
| 14 | G | 1108 | CLA | C5-C6-C7-C8 |
| 14 | e | 1108 | CLA | C5-C6-C7-C8 |
| 14 | A | 1135 | CLA | C3-C5-C6-C7 |
| 14 | G | 1135 | CLA | C3-C5-C6-C7 |
| 14 | e | 1135 | CLA | C3-C5-C6-C7 |
| 14 | A | 1127 | CLA | C16-C17-C18-C19 |
| 14 | G | 1127 | CLA | C16-C17-C18-C19 |
| 14 | e | 1127 | CLA | C16-C17-C18-C19 |
| 19 | A | 1849 | LMU | O5'-C5'-C6'-O6' |
| 19 | G | 1849 | LMU | O5'-C5'-C6'-O6' |
| 19 | e | 1849 | LMU | O5'-C5'-C6'-O6' |
| 18 | L | 5220 | LHG | O1-C1-C2-O2 |
| 18 | V | 5220 | LHG | O1-C1-C2-O2 |
| 18 | n | 5220 | LHG | O1-C1-C2-O2 |
| 18 | G | 5001 | LHG | C9-C10-C11-C12 |
| 18 | A | 5001 | LHG | C9-C10-C11-C12 |
| 18 | e | 5001 | LHG | C9-C10-C11-C12 |
| 21 | H | 1852 | SQD | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 2 | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1204 | CLA | C13-C15-C16-C17 |
| 14 | B | 1215 | CLA | C13-C15-C16-C17 |
| 14 | 6 | 505 | CLA | C13-C15-C16-C17 |
| 14 | H | 1215 | CLA | C13-C15-C16-C17 |
| 14 | d | 505 | CLA | C13-C15-C16-C17 |
| 14 | f | 1215 | CLA | C13-C15-C16-C17 |
| 14 | v | 505 | CLA | C13-C15-C16-C17 |
| 14 | A | 1119 | CLA | C4-C3-C5-C6 |
| 14 | G | 1119 | CLA | C4-C3-C5-C6 |
| 14 | e | 1119 | CLA | C4-C3-C5-C6 |
| 21 | B | 1852 | SQD | C28-C29-C30-C31 |
| 21 | f | 1852 | SQD | C28-C29-C30-C31 |
| 14 | r | 518 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1127 | CLA | C16-C17-C18-C20 |
| 14 | B | 1215 | CLA | C16-C17-C18-C20 |
| 14 | G | 1127 | CLA | C16-C17-C18-C20 |
| 14 | H | 1215 | CLA | C16-C17-C18-C20 |
| 14 | e | 1127 | CLA | C16-C17-C18-C20 |
| 14 | f | 1215 | CLA | C16-C17-C18-C20 |
| 14 | A | 1111 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1111 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1111 | CLA | CBA-CGA-O2A-C1 |
| 19 | B | 1843 | LMU | C11-C10-C9-C8 |
| 19 | H | 1843 | LMU | C11-C10-C9-C8 |
| 19 | f | 1843 | LMU | C11-C10-C9-C8 |
| 14 | B | 1226 | CLA | CBD-CGD-O2D-CED |
| 14 | 5 | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1226 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | f | 1226 | CLA | CBD-CGD-O2D-CED |
| 14 | u | 508 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1126 | CLA | C13-C15-C16-C17 |
| 14 | G | 1121 | CLA | C5-C6-C7-C8 |
| 14 | G | 1126 | CLA | C13-C15-C16-C17 |
| 14 | e | 1121 | CLA | C5-C6-C7-C8 |
| 14 | e | 1126 | CLA | C13-C15-C16-C17 |
| 14 | f | 1204 | CLA | C13-C15-C16-C17 |
| 18 | A | 5004 | LHG | C9-C10-C11-C12 |
| 18 | G | 5004 | LHG | C9-C10-C11-C12 |
| 21 | B | 1852 | SQD | C9-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | H | 1852 | SQD | C9-C10-C11-C12 |
| 21 | f | 1852 | SQD | C9-C10-C11-C12 |
| 21 | 4 | 822 | SQD | C46-C45-O47-C7 |
| 21 | b | 822 | SQD | C46-C45-O47-C7 |
| 21 | t | 822 | SQD | C46-C45-O47-C7 |
| 14 | A | 1129 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 504 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1129 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 504 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1129 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 504 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1106 | CLA | C13-C15-C16-C17 |
| 14 | A | 1121 | CLA | C5-C6-C7-C8 |
| 14 | A | 1132 | CLA | C5-C6-C7-C8 |
| 14 | A | 1138 | CLA | C13-C15-C16-C17 |
| 14 | G | 1106 | CLA | C13-C15-C16-C17 |
| 14 | G | 1132 | CLA | C5-C6-C7-C8 |
| 14 | G | 1138 | CLA | C13-C15-C16-C17 |
| 14 | H | 1204 | CLA | C13-C15-C16-C17 |
| 14 | e | 1106 | CLA | C13-C15-C16-C17 |
| 14 | e | 1132 | CLA | C5-C6-C7-C8 |
| 14 | e | 1138 | CLA | C13-C15-C16-C17 |
| 14 | A | 1105 | CLA | C2-C1-O2A-CGA |
| 14 | A | 1120 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1105 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1120 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1105 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1120 | CLA | C2-C1-O2A-CGA |
| 18 | V | 5218 | LHG | C28-C29-C30-C31 |
| 18 | e | 5004 | LHG | C9-C10-C11-C12 |
| 14 | r | 511 | CLA | O1D-CGD-O2D-CED |
| 18 | B | 1842 | LHG | C30-C31-C32-C33 |
| 18 | L | 5218 | LHG | C28-C29-C30-C31 |
| 18 | H | 1842 | LHG | C30-C31-C32-C33 |
| 18 | f | 1842 | LHG | C30-C31-C32-C33 |
| 18 | n | 5218 | LHG | C28-C29-C30-C31 |
| 14 | A | 1109 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 505 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 511 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1109 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 505 | CLA | O1D-CGD-O2D-CED |
| 14 | Z | 511 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1109 | CLA | O1D-CGD-O2D-CED |
| 14 | q | 505 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5006 | LHG | C32-C33-C34-C35 |
| 20 | B | 5002 | LMG | C41-C42-C43-C44 |
| 20 | H | 5002 | LMG | C41-C42-C43-C44 |
| 20 | f | 5002 | LMG | C41-C42-C43-C44 |
| 14 | A | 1103 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1103 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1103 | CLA | CBA-CGA-O2A-C1 |
| 14 | 6 | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | d | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | v | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | 2 | 505 | CLA | C16-C17-C18-C19 |
| 14 | Z | 505 | CLA | C16-C17-C18-C19 |
| 14 | r | 505 | CLA | C16-C17-C18-C19 |
| 18 | G | 5006 | LHG | C32-C33-C34-C35 |
| 18 | e | 5006 | LHG | C32-C33-C34-C35 |
| 14 | B | 1240 | CLA | C8-C10-C11-C12 |
| 18 | H | 1842 | LHG | C32-C33-C34-C35 |
| 18 | f | 1842 | LHG | C32-C33-C34-C35 |
| 14 | A | 1103 | CLA | C13-C15-C16-C17 |
| 14 | A | 1140 | CLA | C15-C16-C17-C18 |
| 14 | G | 1103 | CLA | C13-C15-C16-C17 |
| 14 | G | 1140 | CLA | C15-C16-C17-C18 |
| 14 | H | 1240 | CLA | C8-C10-C11-C12 |
| 14 | e | 1140 | CLA | C15-C16-C17-C18 |
| 14 | f | 1240 | CLA | C8-C10-C11-C12 |
| 18 | B | 1842 | LHG | C32-C33-C34-C35 |
| 18 | A | 5001 | LHG | O7-C5-C6-O8 |
| 18 | G | 5001 | LHG | O7-C5-C6-O8 |
| 18 | e | 5001 | LHG | O7-C5-C6-O8 |
| 21 | 2 | 822 | SQD | O47-C45-C46-O48 |
| 21 | Z | 822 | SQD | O47-C45-C46-O48 |
| 21 | r | 822 | SQD | O47-C45-C46-O48 |
| 18 | e | 5008 | LHG | C26-C27-C28-C29 |
| 14 | e | 1103 | CLA | C13-C15-C16-C17 |
| 14 | G | 1111 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5008 | LHG | C26-C27-C28-C29 |
| 18 | G | 5008 | LHG | C26-C27-C28-C29 |
| 20 | B | 5002 | LMG | C35-C36-C37-C38 |
| 20 | H | 5002 | LMG | C35-C36-C37-C38 |
| 20 | f | 5002 | LMG | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | f | 1852 | SQD | C24-C25-C26-C27 |
| 21 | B | 1852 | SQD | C24-C25-C26-C27 |
| 21 | H | 1852 | SQD | C24-C25-C26-C27 |
| 14 | A | 1106 | CLA | C11-C12-C13-C15 |
| 14 | A | 1116 | CLA | C6-C7-C8-C10 |
| 14 | A | 1119 | CLA | C2-C3-C5-C6 |
| 14 | A | 1123 | CLA | C11-C10-C8-C7 |
| 14 | A | 1127 | CLA | C11-C12-C13-C15 |
| 14 | A | 1127 | CLA | C12-C13-C15-C16 |
| 14 | A | 1138 | CLA | C11-C10-C8-C7 |
| 14 | A | 1139 | CLA | C12-C13-C15-C16 |
| 14 | A | 1237 | CLA | C11-C10-C8-C7 |
| 14 | A | 1237 | CLA | C12-C13-C15-C16 |
| 14 | A | 1101 | CLA | C11-C12-C13-C15 |
| 14 | B | 1012 | CLA | C11-C10-C8-C7 |
| 14 | B | 1225 | CLA | C12-C13-C15-C16 |
| 14 | B | 1231 | CLA | C6-C7-C8-C10 |
| 14 | L | 1502 | CLA | C11-C10-C8-C7 |
| 14 | 2 | 503 | CLA | C12-C13-C15-C16 |
| 14 | 5 | 509 | CLA | C11-C10-C8-C7 |
| 14 | 5 | 509 | CLA | C12-C13-C15-C16 |
| 14 | G | 1106 | CLA | C11-C12-C13-C15 |
| 14 | G | 1116 | CLA | C6-C7-C8-C10 |
| 14 | G | 1119 | CLA | C2-C3-C5-C6 |
| 14 | G | 1123 | CLA | C11-C10-C8-C7 |
| 14 | G | 1127 | CLA | C11-C12-C13-C15 |
| 14 | G | 1127 | CLA | C12-C13-C15-C16 |
| 14 | G | 1138 | CLA | C11-C10-C8-C7 |
| 14 | G | 1139 | CLA | C12-C13-C15-C16 |
| 14 | G | 1237 | CLA | C11-C10-C8-C7 |
| 14 | G | 1237 | CLA | C12-C13-C15-C16 |
| 14 | G | 1101 | CLA | C11-C12-C13-C15 |
| 14 | H | 1012 | CLA | C11-C10-C8-C7 |
| 14 | H | 1225 | CLA | C12-C13-C15-C16 |
| 14 | H | 1231 | CLA | C6-C7-C8-C10 |
| 14 | V | 1502 | CLA | C11-C10-C8-C7 |
| 14 | Z | 503 | CLA | C12-C13-C15-C16 |
| 14 | c | 509 | CLA | C11-C10-C8-C7 |
| 14 | c | 509 | CLA | C12-C13-C15-C16 |
| 14 | e | 1106 | CLA | C11-C12-C13-C15 |
| 14 | e | 1116 | CLA | C6-C7-C8-C10 |
| 14 | e | 1119 | CLA | C2-C3-C5-C6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1123 | CLA | C11-C10-C8-C7 |
| 14 | e | 1127 | CLA | C11-C12-C13-C15 |
| 14 | e | 1127 | CLA | C12-C13-C15-C16 |
| 14 | e | 1138 | CLA | C11-C10-C8-C7 |
| 14 | e | 1139 | CLA | C12-C13-C15-C16 |
| 14 | e | 1237 | CLA | C11-C10-C8-C7 |
| 14 | e | 1237 | CLA | C12-C13-C15-C16 |
| 14 | e | 1101 | CLA | C11-C12-C13-C15 |
| 14 | f | 1012 | CLA | C11-C10-C8-C7 |
| 14 | f | 1225 | CLA | C12-C13-C15-C16 |
| 14 | f | 1231 | CLA | C6-C7-C8-C10 |
| 14 | n | 1502 | CLA | C11-C10-C8-C7 |
| 14 | r | 503 | CLA | C12-C13-C15-C16 |
| 14 | u | 509 | CLA | C11-C10-C8-C7 |
| 14 | u | 509 | CLA | C12-C13-C15-C16 |
| 15 | A | 2001 | PQN | C17-C18-C20-C21 |
| 15 | A | 2001 | PQN | C22-C23-C25-C26 |
| 15 | G | 2001 | PQN | C17-C18-C20-C21 |
| 15 | G | 2001 | PQN | C22-C23-C25-C26 |
| 15 | e | 2001 | PQN | C17-C18-C20-C21 |
| 15 | e | 2001 | PQN | C22-C23-C25-C26 |
| 14 | e | 1111 | CLA | O1A-CGA-O2A-C1 |
| 14 | A | 1106 | CLA | C11-C12-C13-C14 |
| 14 | A | 1107 | CLA | C11-C12-C13-C14 |
| 14 | A | 1111 | CLA | C11-C12-C13-C14 |
| 14 | A | 1119 | CLA | C6-C7-C8-C9 |
| 14 | A | 1124 | CLA | C11-C10-C8-C9 |
| 14 | A | 1127 | CLA | C11-C12-C13-C14 |
| 14 | A | 1128 | CLA | C6-C7-C8-C9 |
| 14 | A | 1132 | CLA | C14-C13-C15-C16 |
| 14 | A | 1136 | CLA | C11-C12-C13-C14 |
| 14 | A | 1138 | CLA | C14-C13-C15-C16 |
| 14 | A | 1237 | CLA | C11-C10-C8-C9 |
| 14 | B | 1012 | CLA | C14-C13-C15-C16 |
| 14 | B | 1206 | CLA | C6-C7-C8-C9 |
| 14 | B | 1210 | CLA | C6-C7-C8-C9 |
| 14 | B | 1214 | CLA | C11-C10-C8-C9 |
| 14 | B | 1214 | CLA | C14-C13-C15-C16 |
| 14 | B | 1219 | CLA | C11-C12-C13-C14 |
| 14 | B | 1231 | CLA | C6-C7-C8-C9 |
| 14 | B | 1234 | CLA | C11-C10-C8-C9 |
| 14 | B | 1239 | CLA | C6-C7-C8-C9 |

Continued on next page...

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 5 | 509 | CLA | C14-C13-C15-C16 |
| 14 | G | 1106 | CLA | C11-C12-C13-C14 |
| 14 | G | 1107 | CLA | C11-C12-C13-C14 |
| 14 | G | 1111 | CLA | C11-C12-C13-C14 |
| 14 | G | 1124 | CLA | C11-C10-C8-C9 |
| 14 | G | 1127 | CLA | C11-C12-C13-C14 |
| 14 | G | 1128 | CLA | C6-C7-C8-C9 |
| 14 | G | 1132 | CLA | C14-C13-C15-C16 |
| 14 | G | 1136 | CLA | C11-C12-C13-C14 |
| 14 | G | 1138 | CLA | C14-C13-C15-C16 |
| 14 | G | 1237 | CLA | C11-C10-C8-C9 |
| 14 | H | 1012 | CLA | C14-C13-C15-C16 |
| 14 | H | 1206 | CLA | C6-C7-C8-C9 |
| 14 | H | 1210 | CLA | C6-C7-C8-C9 |
| 14 | H | 1214 | CLA | C11-C10-C8-C9 |
| 14 | H | 1214 | CLA | C14-C13-C15-C16 |
| 14 | H | 1219 | CLA | C11-C12-C13-C14 |
| 14 | H | 1231 | CLA | C6-C7-C8-C9 |
| 14 | H | 1234 | CLA | C11-C10-C8-C9 |
| 14 | H | 1239 | CLA | C6-C7-C8-C9 |
| 14 | c | 509 | CLA | C14-C13-C15-C16 |
| 14 | e | 1106 | CLA | C11-C12-C13-C14 |
| 14 | e | 1107 | CLA | C11-C12-C13-C14 |
| 14 | e | 1111 | CLA | C11-C12-C13-C14 |
| 14 | e | 1119 | CLA | C6-C7-C8-C9 |
| 14 | e | 1124 | CLA | C11-C10-C8-C9 |
| 14 | e | 1127 | CLA | C11-C12-C13-C14 |
| 14 | e | 1128 | CLA | C6-C7-C8-C9 |
| 14 | e | 1132 | CLA | C14-C13-C15-C16 |
| 14 | e | 1136 | CLA | C11-C12-C13-C14 |
| 14 | e | 1138 | CLA | C14-C13-C15-C16 |
| 14 | e | 1237 | CLA | C11-C10-C8-C9 |
| 14 | f | 1012 | CLA | C14-C13-C15-C16 |
| 14 | f | 1206 | CLA | C6-C7-C8-C9 |
| 14 | f | 1210 | CLA | C6-C7-C8-C9 |
| 14 | f | 1214 | CLA | C11-C10-C8-C9 |
| 14 | f | 1214 | CLA | C14-C13-C15-C16 |
| 14 | f | 1216 | CLA | C6-C7-C8-C9 |
| 14 | f | 1219 | CLA | C11-C12-C13-C14 |
| 14 | f | 1231 | CLA | C6-C7-C8-C9 |
| 14 | f | 1234 | CLA | C11-C10-C8-C9 |
| 14 | f | 1239 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | u | 509 | CLA | C14-C13-C15-C16 |
| 15 | A | 2001 | PQN | C19-C18-C20-C21 |
| 15 | A | 2001 | PQN | C24-C23-C25-C26 |
| 15 | G | 2001 | PQN | C19-C18-C20-C21 |
| 15 | G | 2001 | PQN | C24-C23-C25-C26 |
| 15 | e | 2001 | PQN | C19-C18-C20-C21 |
| 15 | e | 2001 | PQN | C24-C23-C25-C26 |
| 17 | 1 | 522 | BCR | C9-C10-C11-C12 |
| 17 | Y | 522 | BCR | C9-C10-C11-C12 |
| 17 | q | 522 | BCR | C9-C10-C11-C12 |
| 18 | G | 5006 | LHG | C7-C8-C9-C10 |
| 18 | G | 5003 | LHG | C15-C16-C17-C18 |
| 18 | e | 5003 | LHG | C15-C16-C17-C18 |
| 14 | e | 1111 | CLA | C2A-CAA-CBA-CGA |
| 18 | A | 5003 | LHG | C15-C16-C17-C18 |
| 14 | A | 1111 | CLA | O1A-CGA-O2A-C1 |
| 17 | 2 | 523 | BCR | C7-C8-C9-C34 |
| 17 | Z | 523 | BCR | C7-C8-C9-C34 |
| 17 | r | 523 | BCR | C7-C8-C9-C34 |
| 14 | A | 1126 | CLA | C16-C17-C18-C19 |
| 14 | A | 1133 | CLA | C16-C17-C18-C20 |
| 14 | G | 1126 | CLA | C16-C17-C18-C19 |
| 14 | G | 1133 | CLA | C16-C17-C18-C20 |
| 14 | e | 1126 | CLA | C16-C17-C18-C19 |
| 14 | e | 1133 | CLA | C16-C17-C18-C20 |
| 18 | n | 5221 | LHG | C15-C16-C17-C18 |
| 17 | A | 4001 | BCR | C21-C22-C23-C24 |
| 17 | G | 4001 | BCR | C21-C22-C23-C24 |
| 17 | e | 4001 | BCR | C21-C22-C23-C24 |
| 18 | B | 1855 | LHG | C13-C14-C15-C16 |
| 18 | L | 5221 | LHG | C15-C16-C17-C18 |
| 18 | H | 1855 | LHG | C13-C14-C15-C16 |
| 18 | V | 5221 | LHG | C15-C16-C17-C18 |
| 18 | f | 1855 | LHG | C13-C14-C15-C16 |
| 20 | B | 5002 | LMG | C30-C31-C32-C33 |
| 20 | f | 5002 | LMG | C30-C31-C32-C33 |
| 14 | A | 1117 | CLA | C15-C16-C17-C18 |
| 14 | A | 1136 | CLA | C15-C16-C17-C18 |
| 14 | B | 1231 | CLA | C5-C6-C7-C8 |
| 14 | G | 1117 | CLA | C15-C16-C17-C18 |
| 14 | G | 1136 | CLA | C15-C16-C17-C18 |
| 14 | H | 1231 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1117 | CLA | C15-C16-C17-C18 |
| 14 | e | 1136 | CLA | C15-C16-C17-C18 |
| 20 | H | 5002 | LMG | C30-C31-C32-C33 |
| 14 | 2 | 518 | CLA | CBA-CGA-O2A-C1 |
| 14 | Z | 518 | CLA | CBA-CGA-O2A-C1 |
| 14 | r | 518 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1023 | CLA | C4C-C3C-CAC-CBC |
| 14 | f | 1023 | CLA | C4C-C3C-CAC-CBC |
| 18 | A | 5006 | LHG | C7-C8-C9-C10 |
| 18 | e | 5006 | LHG | C7-C8-C9-C10 |
| 14 | B | 1230 | CLA | C5-C6-C7-C8 |
| 14 | H | 1230 | CLA | C5-C6-C7-C8 |
| 14 | f | 1231 | CLA | C5-C6-C7-C8 |
| 14 | f | 1230 | CLA | C5-C6-C7-C8 |
| 14 | B | 1023 | CLA | C4C-C3C-CAC-CBC |
| 18 | B | 1842 | LHG | C28-C29-C30-C31 |
| 18 | H | 1842 | LHG | C28-C29-C30-C31 |
| 18 | f | 1842 | LHG | C28-C29-C30-C31 |
| 18 | A | 5005 | LHG | O6-C4-C5-C6 |
| 18 | G | 5005 | LHG | O6-C4-C5-C6 |
| 18 | e | 5005 | LHG | O6-C4-C5-C6 |
| 18 | L | 5220 | LHG | C28-C29-C30-C31 |
| 19 | l | 5105 | LMU | C3-C4-C5-C6 |
| 18 | G | 5004 | LHG | C11-C10-C9-C8 |
| 18 | V | 5220 | LHG | C28-C29-C30-C31 |
| 18 | n | 5220 | LHG | C28-C29-C30-C31 |
| 19 | J | 5105 | LMU | C3-C4-C5-C6 |
| 19 | T | 5105 | LMU | C3-C4-C5-C6 |
| 14 | A | 1125 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1125 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1125 | CLA | CBA-CGA-O2A-C1 |
| 18 | A | 5004 | LHG | C11-C10-C9-C8 |
| 18 | e | 5004 | LHG | C11-C10-C9-C8 |
| 18 | A | 5009 | LHG | O2-C2-C3-O3 |
| 18 | G | 5009 | LHG | O2-C2-C3-O3 |
| 18 | e | 5009 | LHG | O2-C2-C3-O3 |
| 14 | A | 1134 | CLA | C11-C10-C8-C9 |
| 14 | B | 1213 | CLA | C14-C13-C15-C16 |
| 14 | G | 1134 | CLA | C11-C10-C8-C9 |
| 14 | H | 1213 | CLA | C14-C13-C15-C16 |
| 14 | e | 1134 | CLA | C11-C10-C8-C9 |
| 14 | f | 1213 | CLA | C14-C13-C15-C16 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 20 | H | 5002 | LMG | C23-C24-C25-C26 |
| 21 | L | 5216 | SQD | C14-C15-C16-C17 |
| 21 | n | 5216 | SQD | C14-C15-C16-C17 |
| 18 | A | 5003 | LHG | C25-C26-C27-C28 |
| 18 | G | 5003 | LHG | C25-C26-C27-C28 |
| 18 | e | 5003 | LHG | C25-C26-C27-C28 |
| 21 | V | 5216 | SQD | C14-C15-C16-C17 |
| 14 | q | 519 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5006 | LHG | C8-C7-O7-C5 |
| 18 | G | 5006 | LHG | C8-C7-O7-C5 |
| 18 | e | 5006 | LHG | C8-C7-O7-C5 |
| 18 | G | 5001 | LHG | C31-C32-C33-C34 |
| 18 | V | 5221 | LHG | C13-C14-C15-C16 |
| 18 | e | 5001 | LHG | C31-C32-C33-C34 |
| 20 | B | 5002 | LMG | C23-C24-C25-C26 |
| 20 | f | 5002 | LMG | C23-C24-C25-C26 |
| 21 | L | 5216 | SQD | C25-C26-C27-C28 |
| 21 | V | 5216 | SQD | C25-C26-C27-C28 |
| 18 | L | 5221 | LHG | C5-C4-O6-P |
| 18 | V | 5221 | LHG | C5-C4-O6-P |
| 18 | n | 5221 | LHG | C5-C4-O6-P |
| 14 | l | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 519 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1227 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1240 | CLA | C3A-C2A-CAA-CBA |
| 14 | K | 1401 | CLA | C3A-C2A-CAA-CBA |
| 14 | 6 | 517 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1227 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1240 | CLA | C3A-C2A-CAA-CBA |
| 14 | U | 1401 | CLA | C3A-C2A-CAA-CBA |
| 14 | d | 517 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1227 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1240 | CLA | C3A-C2A-CAA-CBA |
| 14 | m | 1401 | CLA | C3A-C2A-CAA-CBA |
| 14 | v | 517 | CLA | C3A-C2A-CAA-CBA |
| 18 | A | 5005 | LHG | C29-C30-C31-C32 |
| 18 | A | 5001 | LHG | C31-C32-C33-C34 |
| 18 | L | 5221 | LHG | C13-C14-C15-C16 |
| 18 | G | 5005 | LHG | C29-C30-C31-C32 |
| 18 | e | 5005 | LHG | C29-C30-C31-C32 |
| 18 | n | 5221 | LHG | C13-C14-C15-C16 |
| 21 | n | 5216 | SQD | C25-C26-C27-C28 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1108 | CLA | C6-C7-C8-C9 |
| 14 | G | 1108 | CLA | C6-C7-C8-C9 |
| 14 | e | 1108 | CLA | C6-C7-C8-C9 |
| 18 | G | 5007 | LHG | C34-C35-C36-C37 |
| 18 | e | 5007 | LHG | C34-C35-C36-C37 |
| 18 | A | 5007 | LHG | C34-C35-C36-C37 |
| 18 | A | 5006 | LHG | C12-C13-C14-C15 |
| 18 | G | 5006 | LHG | C12-C13-C14-C15 |
| 18 | e | 5006 | LHG | C12-C13-C14-C15 |
| 14 | A | 1139 | CLA | C10-C11-C12-C13 |
| 14 | B | 1206 | CLA | C13-C15-C16-C17 |
| 14 | G | 1139 | CLA | C10-C11-C12-C13 |
| 14 | H | 1206 | CLA | C13-C15-C16-C17 |
| 14 | e | 1139 | CLA | C10-C11-C12-C13 |
| 14 | f | 1206 | CLA | C13-C15-C16-C17 |
| 18 | A | 5005 | LHG | C4-C5-C6-O8 |
| 18 | A | 5006 | LHG | C4-C5-C6-O8 |
| 18 | A | 5007 | LHG | C4-C5-C6-O8 |
| 18 | L | 5220 | LHG | C4-C5-C6-O8 |
| 18 | G | 5005 | LHG | C4-C5-C6-O8 |
| 18 | G | 5006 | LHG | C4-C5-C6-O8 |
| 18 | G | 5007 | LHG | C4-C5-C6-O8 |
| 18 | V | 5220 | LHG | C4-C5-C6-O8 |
| 18 | e | 5005 | LHG | C4-C5-C6-O8 |
| 18 | e | 5006 | LHG | C4-C5-C6-O8 |
| 18 | e | 5007 | LHG | C4-C5-C6-O8 |
| 18 | n | 5220 | LHG | C4-C5-C6-O8 |
| 21 | L | 5216 | SQD | C44-C45-C46-O48 |
| 21 | l | 822 | SQD | C44-C45-C46-O48 |
| 21 | V | 5216 | SQD | C44-C45-C46-O48 |
| 21 | Y | 822 | SQD | C44-C45-C46-O48 |
| 21 | n | 5216 | SQD | C44-C45-C46-O48 |
| 21 | q | 822 | SQD | C44-C45-C46-O48 |
| 18 | G | 5009 | LHG | C32-C33-C34-C35 |
| 20 | f | 5002 | LMG | C34-C35-C36-C37 |
| 14 | H | 1209 | CLA | C5-C6-C7-C8 |
| 14 | f | 1209 | CLA | C5-C6-C7-C8 |
| 18 | A | 5009 | LHG | C32-C33-C34-C35 |
| 18 | G | 5004 | LHG | C25-C26-C27-C28 |
| 18 | e | 5004 | LHG | C25-C26-C27-C28 |
| 18 | e | 5009 | LHG | C32-C33-C34-C35 |
| 20 | B | 5002 | LMG | C34-C35-C36-C37 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 20 | H | 5002 | LMG | C34-C35-C36-C37 |
| 14 | B | 1209 | CLA | C5-C6-C7-C8 |
| 18 | A | 5004 | LHG | C25-C26-C27-C28 |
| 18 | G | 5007 | LHG | C15-C16-C17-C18 |
| 18 | e | 5007 | LHG | C15-C16-C17-C18 |
| 18 | A | 5007 | LHG | C15-C16-C17-C18 |
| 14 | A | 1110 | CLA | O1D-CGD-O2D-CED |
| 18 | L | 5220 | LHG | C11-C10-C9-C8 |
| 18 | V | 5220 | LHG | C11-C10-C9-C8 |
| 18 | n | 5220 | LHG | C11-C10-C9-C8 |
| 14 | G | 1110 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1110 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5006 | LHG | C3-O3-P-O6 |
| 18 | G | 5006 | LHG | C3-O3-P-O6 |
| 18 | e | 5006 | LHG | C3-O3-P-O6 |
| 14 | B | 1201 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1201 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1201 | CLA | O1A-CGA-O2A-C1 |
| 18 | L | 5221 | LHG | C17-C18-C19-C20 |
| 14 | A | 1104 | CLA | C3-C5-C6-C7 |
| 14 | B | 1012 | CLA | C3-C5-C6-C7 |
| 14 | B | 1227 | CLA | C3-C5-C6-C7 |
| 14 | G | 1104 | CLA | C3-C5-C6-C7 |
| 14 | H | 1012 | CLA | C3-C5-C6-C7 |
| 14 | H | 1227 | CLA | C3-C5-C6-C7 |
| 14 | e | 1104 | CLA | C3-C5-C6-C7 |
| 14 | f | 1227 | CLA | C3-C5-C6-C7 |
| 14 | A | 1111 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1111 | CLA | C2A-CAA-CBA-CGA |
| 18 | A | 5007 | LHG | O1-C1-C2-O2 |
| 18 | A | 5008 | LHG | O1-C1-C2-O2 |
| 18 | G | 5007 | LHG | O1-C1-C2-O2 |
| 18 | G | 5008 | LHG | O1-C1-C2-O2 |
| 18 | e | 5007 | LHG | O1-C1-C2-O2 |
| 18 | e | 5008 | LHG | O1-C1-C2-O2 |
| 18 | V | 5221 | LHG | C17-C18-C19-C20 |
| 18 | n | 5221 | LHG | C17-C18-C19-C20 |
| 21 | L | 5216 | SQD | C9-C10-C11-C12 |
| 21 | V | 5216 | SQD | C9-C10-C11-C12 |
| 14 | H | 1221 | CLA | C13-C15-C16-C17 |
| 18 | B | 1855 | LHG | O6-C4-C5-O7 |
| 18 | H | 1855 | LHG | O6-C4-C5-O7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | f | 1855 | LHG | O6-C4-C5-O7 |
| 14 | B | 1021 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1021 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1021 | CLA | CBA-CGA-O2A-C1 |
| 21 | n | 5216 | SQD | C9-C10-C11-C12 |
| 18 | I | 5001 | LHG | C7-C8-C9-C10 |
| 18 | S | 5001 | LHG | C7-C8-C9-C10 |
| 18 | k | 5001 | LHG | C7-C8-C9-C10 |
| 14 | B | 1226 | CLA | C6-C7-C8-C9 |
| 14 | H | 1226 | CLA | C6-C7-C8-C9 |
| 14 | f | 1226 | CLA | C6-C7-C8-C9 |
| 18 | f | 1855 | LHG | C24-C25-C26-C27 |
| 18 | A | 5002 | LHG | C29-C30-C31-C32 |
| 18 | B | 1855 | LHG | C24-C25-C26-C27 |
| 18 | G | 5002 | LHG | C29-C30-C31-C32 |
| 14 | A | 1125 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1125 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1125 | CLA | O1A-CGA-O2A-C1 |
| 18 | H | 1855 | LHG | C24-C25-C26-C27 |
| 18 | e | 5002 | LHG | C29-C30-C31-C32 |
| 14 | f | 1012 | CLA | C3-C5-C6-C7 |
| 18 | A | 5006 | LHG | O7-C5-C6-O8 |
| 18 | B | 1842 | LHG | O7-C5-C6-O8 |
| 18 | G | 5006 | LHG | O7-C5-C6-O8 |
| 18 | H | 1842 | LHG | O7-C5-C6-O8 |
| 18 | e | 5006 | LHG | O7-C5-C6-O8 |
| 18 | f | 1842 | LHG | O7-C5-C6-O8 |
| 21 | l | 822 | SQD | O6-C44-C45-O47 |
| 21 | Y | 822 | SQD | O6-C44-C45-O47 |
| 21 | f | 1852 | SQD | O6-C44-C45-O47 |
| 21 | q | 822 | SQD | O6-C44-C45-O47 |
| 14 | G | 1122 | CLA | C10-C11-C12-C13 |
| 14 | G | 1132 | CLA | C13-C15-C16-C17 |
| 14 | B | 1226 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1226 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1221 | CLA | C13-C15-C16-C17 |
| 14 | f | 1221 | CLA | C13-C15-C16-C17 |
| 14 | L | 1502 | CLA | C16-C17-C18-C20 |
| 14 | V | 1502 | CLA | C16-C17-C18-C20 |
| 14 | n | 1502 | CLA | C16-C17-C18-C20 |
| 15 | A | 2001 | PQN | C26-C27-C28-C30 |
| 15 | G | 2001 | PQN | C26-C27-C28-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 15 | e | 2001 | PQN | C26-C27-C28-C30 |
| 14 | A | 1122 | CLA | C10-C11-C12-C13 |
| 14 | A | 1128 | CLA | C5-C6-C7-C8 |
| 14 | A | 1132 | CLA | C13-C15-C16-C17 |
| 14 | A | 1237 | CLA | C10-C11-C12-C13 |
| 14 | G | 1128 | CLA | C5-C6-C7-C8 |
| 14 | G | 1237 | CLA | C10-C11-C12-C13 |
| 14 | e | 1122 | CLA | C10-C11-C12-C13 |
| 14 | e | 1128 | CLA | C5-C6-C7-C8 |
| 14 | e | 1132 | CLA | C13-C15-C16-C17 |
| 18 | A | 5004 | LHG | C1-C2-C3-O3 |
| 18 | G | 5004 | LHG | C1-C2-C3-O3 |
| 18 | e | 5004 | LHG | C1-C2-C3-O3 |
| 14 | B | 1223 | CLA | C2-C1-O2A-CGA |
| 14 | L | 1501 | CLA | C2-C1-O2A-CGA |
| 14 | H | 1223 | CLA | C2-C1-O2A-CGA |
| 14 | V | 1501 | CLA | C2-C1-O2A-CGA |
| 14 | f | 1223 | CLA | C2-C1-O2A-CGA |
| 14 | n | 1501 | CLA | C2-C1-O2A-CGA |
| 18 | B | 1855 | LHG | C14-C15-C16-C17 |
| 18 | H | 1855 | LHG | C14-C15-C16-C17 |
| 18 | V | 5220 | LHG | C30-C31-C32-C33 |
| 14 | e | 1237 | CLA | C10-C11-C12-C13 |
| 14 | A | 1117 | CLA | C11-C12-C13-C14 |
| 14 | A | 1140 | CLA | C6-C7-C8-C9 |
| 14 | A | 1237 | CLA | C6-C7-C8-C9 |
| 14 | A | 1130 | CLA | C6-C7-C8-C9 |
| 14 | A | 1101 | CLA | C11-C12-C13-C14 |
| 14 | B | 1203 | CLA | C11-C12-C13-C14 |
| 14 | B | 1205 | CLA | C14-C13-C15-C16 |
| 14 | B | 1215 | CLA | C11-C10-C8-C9 |
| 14 | B | 1217 | CLA | C11-C10-C8-C9 |
| 14 | B | 1219 | CLA | C14-C13-C15-C16 |
| 14 | L | 1501 | CLA | C11-C10-C8-C9 |
| 14 | G | 1117 | CLA | C11-C12-C13-C14 |
| 14 | G | 1140 | CLA | C6-C7-C8-C9 |
| 14 | G | 1237 | CLA | C6-C7-C8-C9 |
| 14 | G | 1130 | CLA | C6-C7-C8-C9 |
| 14 | G | 1101 | CLA | C11-C12-C13-C14 |
| 14 | H | 1203 | CLA | C11-C12-C13-C14 |
| 14 | H | 1205 | CLA | C14-C13-C15-C16 |
| 14 | H | 1215 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1217 | CLA | C11-C10-C8-C9 |
| 14 | H | 1219 | CLA | C14-C13-C15-C16 |
| 14 | V | 1501 | CLA | C11-C10-C8-C9 |
| 14 | e | 1117 | CLA | C11-C12-C13-C14 |
| 14 | e | 1140 | CLA | C6-C7-C8-C9 |
| 14 | e | 1237 | CLA | C6-C7-C8-C9 |
| 14 | e | 1130 | CLA | C6-C7-C8-C9 |
| 14 | e | 1101 | CLA | C11-C12-C13-C14 |
| 14 | f | 1203 | CLA | C11-C12-C13-C14 |
| 14 | f | 1205 | CLA | C14-C13-C15-C16 |
| 14 | f | 1215 | CLA | C11-C10-C8-C9 |
| 14 | f | 1217 | CLA | C11-C10-C8-C9 |
| 14 | n | 1501 | CLA | C11-C10-C8-C9 |
| 18 | L | 5220 | LHG | C30-C31-C32-C33 |
| 18 | f | 1855 | LHG | C14-C15-C16-C17 |
| 18 | n | 5220 | LHG | C30-C31-C32-C33 |
| 18 | A | 5004 | LHG | C2-C3-O3-P |
| 18 | A | 5005 | LHG | C2-C3-O3-P |
| 18 | L | 5218 | LHG | C2-C3-O3-P |
| 18 | L | 5221 | LHG | C2-C3-O3-P |
| 18 | G | 5004 | LHG | C2-C3-O3-P |
| 18 | G | 5005 | LHG | C2-C3-O3-P |
| 18 | V | 5218 | LHG | C2-C3-O3-P |
| 18 | V | 5221 | LHG | C2-C3-O3-P |
| 18 | e | 5004 | LHG | C2-C3-O3-P |
| 18 | e | 5005 | LHG | C2-C3-O3-P |
| 18 | n | 5218 | LHG | C2-C3-O3-P |
| 18 | n | 5221 | LHG | C2-C3-O3-P |
| 20 | J | 5104 | LMG | C32-C33-C34-C35 |
| 20 | T | 5104 | LMG | C32-C33-C34-C35 |
| 20 | l | 5104 | LMG | C32-C33-C34-C35 |
| 14 | A | 1106 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1115 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1106 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1115 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1106 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1115 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1226 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1103 | CLA | C16-C17-C18-C19 |
| 14 | B | 1210 | CLA | C16-C17-C18-C20 |
| 14 | B | 1211 | CLA | C6-C7-C8-C10 |
| 14 | B | 1215 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1103 | CLA | C16-C17-C18-C19 |
| 14 | H | 1210 | CLA | C16-C17-C18-C20 |
| 14 | H | 1211 | CLA | C6-C7-C8-C10 |
| 14 | H | 1215 | CLA | C16-C17-C18-C19 |
| 14 | e | 1103 | CLA | C16-C17-C18-C19 |
| 14 | f | 1210 | CLA | C16-C17-C18-C20 |
| 14 | f | 1211 | CLA | C6-C7-C8-C10 |
| 14 | f | 1215 | CLA | C16-C17-C18-C19 |
| 14 | A | 1237 | CLA | C3-C5-C6-C7 |
| 14 | G | 1237 | CLA | C3-C5-C6-C7 |
| 14 | e | 1237 | CLA | C3-C5-C6-C7 |
| 17 | 3 | 521 | BCR | C23-C24-C25-C26 |
| 17 | 3 | 521 | BCR | C23-C24-C25-C30 |
| 17 | 3 | 522 | BCR | C5-C6-C7-C8 |
| 17 | 5 | 521 | BCR | C5-C6-C7-C8 |
| 17 | 6 | 524 | BCR | C5-C6-C7-C8 |
| 17 | a | 521 | BCR | C23-C24-C25-C26 |
| 17 | a | 521 | BCR | C23-C24-C25-C30 |
| 17 | a | 522 | BCR | C5-C6-C7-C8 |
| 17 | c | 521 | BCR | C5-C6-C7-C8 |
| 17 | d | 524 | BCR | C5-C6-C7-C8 |
| 17 | s | 521 | BCR | C23-C24-C25-C26 |
| 17 | s | 521 | BCR | C23-C24-C25-C30 |
| 17 | s | 522 | BCR | C5-C6-C7-C8 |
| 17 | u | 521 | BCR | C5-C6-C7-C8 |
| 17 | v | 524 | BCR | C5-C6-C7-C8 |
| 18 | A | 5005 | LHG | C33-C34-C35-C36 |
| 18 | e | 5005 | LHG | C33-C34-C35-C36 |
| 14 | j | 1302 | CLA | O1D-CGD-O2D-CED |
| 17 | B | 4010 | BCR | C37-C22-C23-C24 |
| 17 | J | 4015 | BCR | C7-C8-C9-C34 |
| 17 | T | 4015 | BCR | C7-C8-C9-C34 |
| 17 | f | 4010 | BCR | C37-C22-C23-C24 |
| 17 | l | 4015 | BCR | C7-C8-C9-C34 |
| 18 | A | 5004 | LHG | C30-C31-C32-C33 |
| 18 | L | 5221 | LHG | C18-C19-C20-C21 |
| 18 | G | 5004 | LHG | C30-C31-C32-C33 |
| 18 | G | 5005 | LHG | C33-C34-C35-C36 |
| 18 | V | 5221 | LHG | C18-C19-C20-C21 |
| 18 | e | 5004 | LHG | C30-C31-C32-C33 |
| 14 | F | 1302 | CLA | O1D-CGD-O2D-CED |
| 14 | R | 1302 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | A | 4001 | BCR | C7-C8-C9-C10 |
| 17 | A | 4011 | BCR | C17-C18-C19-C20 |
| 17 | M | 4021 | BCR | C11-C12-C13-C14 |
| 17 | 3 | 524 | BCR | C7-C8-C9-C10 |
| 17 | 4 | 524 | BCR | C7-C8-C9-C10 |
| 17 | 6 | 522 | BCR | C7-C8-C9-C10 |
| 17 | G | 4001 | BCR | C7-C8-C9-C10 |
| 17 | G | 4011 | BCR | C17-C18-C19-C20 |
| 17 | W | 4021 | BCR | C11-C12-C13-C14 |
| 17 | a | 524 | BCR | C7-C8-C9-C10 |
| 17 | a | 524 | BCR | C21-C22-C23-C24 |
| 17 | b | 524 | BCR | C7-C8-C9-C10 |
| 17 | d | 522 | BCR | C7-C8-C9-C10 |
| 17 | e | 4001 | BCR | C7-C8-C9-C10 |
| 17 | e | 4011 | BCR | C17-C18-C19-C20 |
| 17 | o | 4021 | BCR | C11-C12-C13-C14 |
| 17 | s | 524 | BCR | C7-C8-C9-C10 |
| 17 | s | 524 | BCR | C21-C22-C23-C24 |
| 17 | t | 524 | BCR | C7-C8-C9-C10 |
| 17 | v | 522 | BCR | C7-C8-C9-C10 |
| 18 | n | 5221 | LHG | C18-C19-C20-C21 |
| 18 | A | 5002 | LHG | C13-C14-C15-C16 |
| 18 | G | 5002 | LHG | C13-C14-C15-C16 |
| 18 | e | 5002 | LHG | C13-C14-C15-C16 |
| 14 | A | 1111 | CLA | C16-C17-C18-C19 |
| 14 | G | 1111 | CLA | C16-C17-C18-C19 |
| 14 | e | 1111 | CLA | C16-C17-C18-C19 |
| 18 | f | 1842 | LHG | C26-C27-C28-C29 |
| 18 | B | 1842 | LHG | C26-C27-C28-C29 |
| 18 | H | 1842 | LHG | C26-C27-C28-C29 |
| 14 | A | 1013 | CLA | C11-C12-C13-C15 |
| 14 | A | 1104 | CLA | C12-C13-C15-C16 |
| 14 | A | 1107 | CLA | C11-C12-C13-C15 |
| 14 | A | 1109 | CLA | C12-C13-C15-C16 |
| 14 | A | 1111 | CLA | C11-C12-C13-C15 |
| 14 | A | 1124 | CLA | C11-C10-C8-C7 |
| 14 | A | 1128 | CLA | C6-C7-C8-C10 |
| 14 | A | 1131 | CLA | C12-C13-C15-C16 |
| 14 | A | 1132 | CLA | C12-C13-C15-C16 |
| 14 | A | 1136 | CLA | C11-C12-C13-C15 |
| 14 | A | 1138 | CLA | C12-C13-C15-C16 |
| 14 | A | 1139 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1012 | CLA | C12-C13-C15-C16 |
| 14 | B | 1203 | CLA | C6-C7-C8-C10 |
| 14 | B | 1206 | CLA | C6-C7-C8-C10 |
| 14 | B | 1215 | CLA | C11-C10-C8-C7 |
| 14 | B | 1217 | CLA | C11-C10-C8-C7 |
| 14 | B | 1219 | CLA | C11-C10-C8-C7 |
| 14 | B | 1219 | CLA | C11-C12-C13-C15 |
| 14 | B | 1219 | CLA | C12-C13-C15-C16 |
| 14 | B | 1234 | CLA | C11-C10-C8-C7 |
| 14 | B | 1239 | CLA | C12-C13-C15-C16 |
| 14 | B | 1240 | CLA | C11-C12-C13-C15 |
| 14 | 5 | 509 | CLA | C11-C12-C13-C15 |
| 14 | 6 | 505 | CLA | C6-C7-C8-C10 |
| 14 | G | 1013 | CLA | C11-C12-C13-C15 |
| 14 | G | 1104 | CLA | C12-C13-C15-C16 |
| 14 | G | 1107 | CLA | C11-C12-C13-C15 |
| 14 | G | 1109 | CLA | C12-C13-C15-C16 |
| 14 | G | 1111 | CLA | C11-C12-C13-C15 |
| 14 | G | 1124 | CLA | C11-C10-C8-C7 |
| 14 | G | 1128 | CLA | C6-C7-C8-C10 |
| 14 | G | 1131 | CLA | C12-C13-C15-C16 |
| 14 | G | 1132 | CLA | C12-C13-C15-C16 |
| 14 | G | 1136 | CLA | C11-C12-C13-C15 |
| 14 | G | 1138 | CLA | C12-C13-C15-C16 |
| 14 | G | 1139 | CLA | C6-C7-C8-C10 |
| 14 | H | 1012 | CLA | C12-C13-C15-C16 |
| 14 | H | 1203 | CLA | C6-C7-C8-C10 |
| 14 | H | 1206 | CLA | C6-C7-C8-C10 |
| 14 | H | 1215 | CLA | C11-C10-C8-C7 |
| 14 | H | 1217 | CLA | C11-C10-C8-C7 |
| 14 | H | 1219 | CLA | C11-C10-C8-C7 |
| 14 | H | 1219 | CLA | C11-C12-C13-C15 |
| 14 | H | 1219 | CLA | C12-C13-C15-C16 |
| 14 | H | 1234 | CLA | C11-C10-C8-C7 |
| 14 | H | 1239 | CLA | C12-C13-C15-C16 |
| 14 | H | 1240 | CLA | C11-C12-C13-C15 |
| 14 | c | 509 | CLA | C11-C12-C13-C15 |
| 14 | d | 505 | CLA | C6-C7-C8-C10 |
| 14 | e | 1013 | CLA | C11-C12-C13-C15 |
| 14 | e | 1104 | CLA | C12-C13-C15-C16 |
| 14 | e | 1107 | CLA | C11-C12-C13-C15 |
| 14 | e | 1109 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1111 | CLA | C11-C12-C13-C15 |
| 14 | e | 1124 | CLA | C11-C10-C8-C7 |
| 14 | e | 1128 | CLA | C6-C7-C8-C10 |
| 14 | e | 1131 | CLA | C12-C13-C15-C16 |
| 14 | e | 1132 | CLA | C12-C13-C15-C16 |
| 14 | e | 1136 | CLA | C11-C12-C13-C15 |
| 14 | e | 1138 | CLA | C12-C13-C15-C16 |
| 14 | e | 1139 | CLA | C6-C7-C8-C10 |
| 14 | f | 1012 | CLA | C12-C13-C15-C16 |
| 14 | f | 1203 | CLA | C6-C7-C8-C10 |
| 14 | f | 1206 | CLA | C6-C7-C8-C10 |
| 14 | f | 1215 | CLA | C11-C10-C8-C7 |
| 14 | f | 1217 | CLA | C11-C10-C8-C7 |
| 14 | f | 1219 | CLA | C11-C10-C8-C7 |
| 14 | f | 1219 | CLA | C11-C12-C13-C15 |
| 14 | f | 1219 | CLA | C12-C13-C15-C16 |
| 14 | f | 1234 | CLA | C11-C10-C8-C7 |
| 14 | f | 1239 | CLA | C12-C13-C15-C16 |
| 14 | f | 1240 | CLA | C11-C12-C13-C15 |
| 14 | u | 509 | CLA | C11-C12-C13-C15 |
| 14 | v | 505 | CLA | C6-C7-C8-C10 |
| 14 | G | 1103 | CLA | C3-C5-C6-C7 |
| 18 | A | 5002 | LHG | C12-C13-C14-C15 |
| 18 | A | 5007 | LHG | C10-C11-C12-C13 |
| 18 | G | 5002 | LHG | C12-C13-C14-C15 |
| 18 | G | 5007 | LHG | C10-C11-C12-C13 |
| 18 | e | 5002 | LHG | C12-C13-C14-C15 |
| 18 | e | 5007 | LHG | C10-C11-C12-C13 |
| 17 | 5 | 522 | BCR | C9-C10-C11-C12 |
| 17 | c | 522 | BCR | C9-C10-C11-C12 |
| 17 | u | 522 | BCR | C9-C10-C11-C12 |
| 14 | B | 1208 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1208 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1208 | CLA | CBA-CGA-O2A-C1 |
| 18 | B | 1855 | LHG | C24-C23-O8-C6 |
| 18 | H | 1855 | LHG | C24-C23-O8-C6 |
| 18 | f | 1855 | LHG | C24-C23-O8-C6 |
| 14 | G | 1121 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1121 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 518 | CLA | O1A-CGA-O2A-C1 |
| 14 | Z | 518 | CLA | O1A-CGA-O2A-C1 |
| 14 | r | 518 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 1 | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 503 | CLA | C2A-CAA-CBA-CGA |
| 18 | A | 5008 | LHG | C11-C12-C13-C14 |
| 18 | G | 5008 | LHG | C11-C12-C13-C14 |
| 18 | e | 5008 | LHG | C11-C12-C13-C14 |
| 18 | e | 5003 | LHG | C23-C24-C25-C26 |
| 14 | A | 1103 | CLA | C3-C5-C6-C7 |
| 14 | e | 1103 | CLA | C3-C5-C6-C7 |
| 14 | e | 1140 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1133 | CLA | C16-C17-C18-C19 |
| 14 | G | 1133 | CLA | C16-C17-C18-C19 |
| 14 | e | 1133 | CLA | C16-C17-C18-C19 |
| 14 | A | 1121 | CLA | CAA-CBA-CGA-O2A |
| 18 | e | 5003 | LHG | C13-C14-C15-C16 |
| 18 | A | 5003 | LHG | C23-C24-C25-C26 |
| 18 | G | 5003 | LHG | C23-C24-C25-C26 |
| 18 | A | 5003 | LHG | C13-C14-C15-C16 |
| 18 | G | 5003 | LHG | C13-C14-C15-C16 |
| 14 | A | 1101 | CLA | C5-C6-C7-C8 |
| 14 | A | 1140 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1140 | CLA | CBD-CGD-O2D-CED |
| 14 | H | 1212 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1103 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1105 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1107 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1118 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1124 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1202 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1208 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1216 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1218 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1238 | CLA | CAD-CBD-CGD-O2D |
| 14 | J | 1303 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 512 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 513 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 516 | CLA | CAD-CBD-CGD-O2D |
| 14 | 2 | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | 2 | 511 | CLA | CAD-CBD-CGD-O2D |
| 14 | 3 | 508 | CLA | CAD-CBD-CGD-O2D |
| 14 | 4 | 518 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 5 | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | 6 | 506 | CLA | CAD-CBD-CGD-O2D |
| 14 | 6 | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1103 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1105 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1107 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1118 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1124 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1202 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1208 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1216 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1218 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1238 | CLA | CAD-CBD-CGD-O2D |
| 14 | T | 1303 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 512 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 513 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 516 | CLA | CAD-CBD-CGD-O2D |
| 14 | Z | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | Z | 511 | CLA | CAD-CBD-CGD-O2D |
| 14 | a | 508 | CLA | CAD-CBD-CGD-O2D |
| 14 | b | 518 | CLA | CAD-CBD-CGD-O2D |
| 14 | c | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | d | 506 | CLA | CAD-CBD-CGD-O2D |
| 14 | d | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1103 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1105 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1107 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1118 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1124 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1202 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1208 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1216 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1218 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1238 | CLA | CAD-CBD-CGD-O2D |
| 14 | l | 1303 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 512 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 513 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 516 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 511 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | s | 508 | CLA | CAD-CBD-CGD-O2D |
| 14 | t | 518 | CLA | CAD-CBD-CGD-O2D |
| 14 | u | 517 | CLA | CAD-CBD-CGD-O2D |
| 14 | v | 506 | CLA | CAD-CBD-CGD-O2D |
| 14 | v | 517 | CLA | CAD-CBD-CGD-O2D |
| 18 | B | 1855 | LHG | C6-C5-O7-C7 |
| 18 | H | 1855 | LHG | C6-C5-O7-C7 |
| 18 | f | 1855 | LHG | C6-C5-O7-C7 |
| 14 | G | 1101 | CLA | C5-C6-C7-C8 |
| 14 | e | 1101 | CLA | C5-C6-C7-C8 |
| 14 | f | 1227 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1212 | CLA | CBD-CGD-O2D-CED |
| 14 | B | 1220 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1220 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1220 | CLA | CBA-CGA-O2A-C1 |
| 14 | B | 1227 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1219 | CLA | C4-C3-C5-C6 |
| 14 | H | 1219 | CLA | C4-C3-C5-C6 |
| 14 | f | 1219 | CLA | C4-C3-C5-C6 |
| 14 | A | 1013 | CLA | C16-C17-C18-C20 |
| 14 | A | 1137 | CLA | C11-C12-C13-C15 |
| 14 | e | 1013 | CLA | C16-C17-C18-C20 |
| 14 | e | 1137 | CLA | C11-C12-C13-C15 |
| 14 | B | 1219 | CLA | C2-C3-C5-C6 |
| 14 | H | 1219 | CLA | C2-C3-C5-C6 |
| 14 | f | 1219 | CLA | C2-C3-C5-C6 |
| 18 | A | 5009 | LHG | C5-C4-O6-P |
| 18 | I | 5001 | LHG | C4-C5-C6-O8 |
| 18 | G | 5009 | LHG | C5-C4-O6-P |
| 18 | S | 5001 | LHG | C4-C5-C6-O8 |
| 18 | e | 5009 | LHG | C5-C4-O6-P |
| 18 | k | 5001 | LHG | C4-C5-C6-O8 |
| 21 | B | 1852 | SQD | O6-C44-C45-C46 |
| 21 | H | 1852 | SQD | O6-C44-C45-C46 |
| 21 | f | 1852 | SQD | O6-C44-C45-C46 |
| 14 | f | 1212 | CLA | CBD-CGD-O2D-CED |
| 14 | c | 509 | CLA | C5-C6-C7-C8 |
| 14 | u | 509 | CLA | C5-C6-C7-C8 |
| 18 | A | 5001 | LHG | C14-C15-C16-C17 |
| 18 | e | 5001 | LHG | C14-C15-C16-C17 |
| 14 | F | 1302 | CLA | C2A-CAA-CBA-CGA |
| 14 | R | 1302 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | j | 1302 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1227 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 509 | CLA | C5-C6-C7-C8 |
| 14 | f | 1215 | CLA | C5-C6-C7-C8 |
| 18 | G | 5001 | LHG | C14-C15-C16-C17 |
| 18 | e | 5009 | LHG | C34-C35-C36-C37 |
| 14 | G | 1013 | CLA | C16-C17-C18-C20 |
| 14 | G | 1137 | CLA | C11-C12-C13-C15 |
| 18 | A | 5009 | LHG | C34-C35-C36-C37 |
| 18 | A | 5005 | LHG | C1-C2-C3-O3 |
| 18 | A | 5009 | LHG | C1-C2-C3-O3 |
| 18 | L | 5220 | LHG | C1-C2-C3-O3 |
| 18 | G | 5005 | LHG | C1-C2-C3-O3 |
| 18 | G | 5009 | LHG | C1-C2-C3-O3 |
| 18 | V | 5220 | LHG | C1-C2-C3-O3 |
| 18 | e | 5005 | LHG | C1-C2-C3-O3 |
| 18 | e | 5009 | LHG | C1-C2-C3-O3 |
| 18 | n | 5220 | LHG | C1-C2-C3-O3 |
| 14 | A | 1102 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1102 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1111 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1120 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1122 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1122 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1134 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1137 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1137 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1139 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1209 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1213 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1213 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1221 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1221 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1226 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1226 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1232 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1232 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1234 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1207 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1207 | CLA | CHA-CBD-CGD-O2D |
| 14 | K | 1103 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 501 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 1 | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | 2 | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | 2 | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | 2 | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | 4 | 502 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 502 | CLA | CHA-CBD-CGD-O2D |
| 14 | 4 | 505 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | 4 | 509 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 509 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 519 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1102 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1102 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1111 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1120 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1122 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1122 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1134 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1137 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1137 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1139 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1209 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1213 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1213 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1221 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1221 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1226 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1226 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1232 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1232 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1234 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1207 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1207 | CLA | CHA-CBD-CGD-O2D |
| 14 | U | 1103 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 501 | CLA | CHA-CBD-CGD-O2D |
| 14 | Y | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | Z | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | Z | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | Z | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | b | 502 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 502 | CLA | CHA-CBD-CGD-O2D |
| 14 | b | 505 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | b | 509 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 509 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 519 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1102 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1102 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1111 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1120 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1122 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1122 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1134 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1137 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1137 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1139 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1209 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1213 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1213 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1221 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1221 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1226 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1226 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1232 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1232 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1234 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1207 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1207 | CLA | CHA-CBD-CGD-O2D |
| 14 | m | 1103 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 501 | CLA | CHA-CBD-CGD-O2D |
| 14 | q | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | r | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 504 | CLA | CHA-CBD-CGD-O1D |
| 14 | r | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | r | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 510 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 510 | CLA | CHA-CBD-CGD-O2D |
| 14 | t | 502 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 502 | CLA | CHA-CBD-CGD-O2D |
| 14 | t | 505 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | t | 509 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 509 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 503 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | u | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 516 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 519 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 503 | CLA | CHA-CBD-CGD-O2D |
| 18 | G | 5009 | LHG | C34-C35-C36-C37 |
| 14 | B | 1215 | CLA | C5-C6-C7-C8 |
| 14 | H | 1215 | CLA | C5-C6-C7-C8 |
| 21 | L | 5216 | SQD | C19-C20-C21-C22 |
| 21 | V | 5216 | SQD | C19-C20-C21-C22 |
| 21 | n | 5216 | SQD | C19-C20-C21-C22 |
| 18 | L | 5220 | LHG | O7-C5-C6-O8 |
| 18 | L | 5221 | LHG | O7-C5-C6-O8 |
| 18 | V | 5220 | LHG | O7-C5-C6-O8 |
| 18 | V | 5221 | LHG | O7-C5-C6-O8 |
| 18 | n | 5220 | LHG | O7-C5-C6-O8 |
| 18 | n | 5221 | LHG | O7-C5-C6-O8 |
| 21 | B | 1852 | SQD | O6-C44-C45-O47 |
| 21 | 3 | 822 | SQD | O6-C44-C45-O47 |
| 21 | 4 | 822 | SQD | O47-C45-C46-O48 |
| 21 | H | 1852 | SQD | O6-C44-C45-O47 |
| 21 | a | 822 | SQD | O6-C44-C45-O47 |
| 21 | b | 822 | SQD | O47-C45-C46-O48 |
| 21 | s | 822 | SQD | O6-C44-C45-O47 |
| 21 | t | 822 | SQD | O47-C45-C46-O48 |
| 14 | B | 1223 | CLA | C5-C6-C7-C8 |
| 14 | H | 1223 | CLA | C5-C6-C7-C8 |
| 14 | f | 1223 | CLA | C5-C6-C7-C8 |
| 14 | A | 1103 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1103 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1103 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5007 | LHG | C33-C34-C35-C36 |
| 14 | A | 1137 | CLA | C11-C12-C13-C14 |
| 14 | G | 1137 | CLA | C11-C12-C13-C14 |
| 14 | e | 1137 | CLA | C11-C12-C13-C14 |
| 18 | A | 5004 | LHG | O1-C1-C2-O2 |
| 18 | A | 5006 | LHG | O1-C1-C2-O2 |
| 18 | G | 5004 | LHG | O1-C1-C2-O2 |
| 18 | G | 5006 | LHG | O1-C1-C2-O2 |
| 18 | e | 5004 | LHG | O1-C1-C2-O2 |
| 18 | e | 5006 | LHG | O1-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | B | 1842 | LHG | C27-C28-C29-C30 |
| 18 | G | 5007 | LHG | C33-C34-C35-C36 |
| 18 | f | 1842 | LHG | C27-C28-C29-C30 |
| 14 | B | 1204 | CLA | C4-C3-C5-C6 |
| 14 | H | 1204 | CLA | C4-C3-C5-C6 |
| 14 | f | 1204 | CLA | C4-C3-C5-C6 |
| 18 | L | 5218 | LHG | C29-C30-C31-C32 |
| 18 | H | 1842 | LHG | C27-C28-C29-C30 |
| 18 | e | 5007 | LHG | C33-C34-C35-C36 |
| 18 | V | 5218 | LHG | C29-C30-C31-C32 |
| 18 | n | 5218 | LHG | C29-C30-C31-C32 |
| 14 | H | 1202 | CLA | C15-C16-C17-C18 |
| 14 | f | 1202 | CLA | C15-C16-C17-C18 |
| 14 | f | 1234 | CLA | C15-C16-C17-C18 |
| 14 | B | 1203 | CLA | C6-C7-C8-C9 |
| 14 | B | 1206 | CLA | C11-C10-C8-C9 |
| 14 | 5 | 509 | CLA | C11-C12-C13-C14 |
| 14 | H | 1203 | CLA | C6-C7-C8-C9 |
| 14 | H | 1206 | CLA | C11-C10-C8-C9 |
| 14 | c | 509 | CLA | C11-C12-C13-C14 |
| 14 | f | 1203 | CLA | C6-C7-C8-C9 |
| 14 | f | 1206 | CLA | C11-C10-C8-C9 |
| 14 | f | 1219 | CLA | C14-C13-C15-C16 |
| 14 | u | 509 | CLA | C11-C12-C13-C14 |
| 18 | A | 5005 | LHG | C25-C26-C27-C28 |
| 18 | G | 5005 | LHG | C25-C26-C27-C28 |
| 14 | B | 1202 | CLA | C15-C16-C17-C18 |
| 21 | 4 | 822 | SQD | C5-C6-S-O8 |
| 21 | b | 822 | SQD | C5-C6-S-O8 |
| 21 | t | 822 | SQD | C5-C6-S-O8 |
| 18 | e | 5005 | LHG | C25-C26-C27-C28 |
| 14 | 2 | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1224 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1224 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1224 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1234 | CLA | C15-C16-C17-C18 |
| 14 | G | 1140 | CLA | O1D-CGD-O2D-CED |
| 14 | c | 508 | CLA | O1D-CGD-O2D-CED |
| 17 | H | 4010 | BCR | C37-C22-C23-C24 |
| 17 | v | 521 | BCR | C7-C8-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | A | 5006 | LHG | O1-C1-C2-C3 |
| 18 | G | 5006 | LHG | O1-C1-C2-C3 |
| 18 | e | 5006 | LHG | O1-C1-C2-C3 |
| 14 | H | 1234 | CLA | C15-C16-C17-C18 |
| 17 | B | 4010 | BCR | C21-C22-C23-C24 |
| 17 | B | 4014 | BCR | C7-C8-C9-C10 |
| 17 | 3 | 524 | BCR | C21-C22-C23-C24 |
| 17 | 4 | 521 | BCR | C17-C18-C19-C20 |
| 17 | H | 4010 | BCR | C21-C22-C23-C24 |
| 17 | H | 4014 | BCR | C7-C8-C9-C10 |
| 17 | b | 521 | BCR | C17-C18-C19-C20 |
| 17 | f | 4010 | BCR | C21-C22-C23-C24 |
| 17 | f | 4014 | BCR | C7-C8-C9-C10 |
| 17 | t | 521 | BCR | C17-C18-C19-C20 |
| 14 | B | 1240 | CLA | O1D-CGD-O2D-CED |
| 14 | 5 | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1113 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1208 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1212 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1229 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1236 | CLA | C1A-C2A-CAA-CBA |
| 14 | 1 | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | 4 | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1113 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1208 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1212 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1229 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1236 | CLA | C1A-C2A-CAA-CBA |
| 14 | Y | 501 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | b | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 503 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1113 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1208 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1212 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1229 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1236 | CLA | C1A-C2A-CAA-CBA |
| 14 | q | 501 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | r | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | t | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 503 | CLA | C1A-C2A-CAA-CBA |
| 21 | L | 5216 | SQD | C23-C24-C25-C26 |
| 21 | V | 5216 | SQD | C23-C24-C25-C26 |
| 14 | A | 1115 | CLA | C11-C12-C13-C14 |
| 14 | G | 1115 | CLA | C11-C12-C13-C14 |
| 14 | e | 1115 | CLA | C11-C12-C13-C14 |
| 14 | G | 1123 | CLA | C15-C16-C17-C18 |
| 14 | e | 1123 | CLA | C15-C16-C17-C18 |
| 14 | A | 1140 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1124 | CLA | CBD-CGD-O2D-CED |
| 18 | L | 5221 | LHG | C24-C25-C26-C27 |
| 18 | V | 5221 | LHG | C24-C25-C26-C27 |
| 18 | n | 5221 | LHG | C24-C25-C26-C27 |
| 17 | J | 4015 | BCR | C15-C16-C17-C18 |
| 17 | 3 | 522 | BCR | C9-C10-C11-C12 |
| 17 | T | 4015 | BCR | C15-C16-C17-C18 |
| 17 | a | 522 | BCR | C9-C10-C11-C12 |
| 17 | s | 522 | BCR | C9-C10-C11-C12 |
| 14 | H | 1240 | CLA | O1D-CGD-O2D-CED |
| 14 | e | 1140 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1240 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1123 | CLA | C15-C16-C17-C18 |
| 18 | B | 1855 | LHG | O2-C2-C3-O3 |
| 18 | H | 1855 | LHG | O2-C2-C3-O3 |
| 18 | f | 1855 | LHG | O2-C2-C3-O3 |
| 14 | u | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1124 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | s | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1108 | CLA | C2-C3-C5-C6 |
| 14 | A | 1101 | CLA | C2-C3-C5-C6 |
| 14 | G | 1108 | CLA | C2-C3-C5-C6 |
| 14 | G | 1101 | CLA | C2-C3-C5-C6 |
| 14 | e | 1108 | CLA | C2-C3-C5-C6 |
| 14 | e | 1101 | CLA | C2-C3-C5-C6 |
| 18 | A | 5002 | LHG | C4-O6-P-O5 |
| 18 | A | 5005 | LHG | C3-O3-P-O5 |
| 18 | A | 5008 | LHG | C4-O6-P-O4 |
| 18 | A | 5003 | LHG | C4-O6-P-O5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | B | 1842 | LHG | C3-O3-P-O4 |
| 18 | B | 1855 | LHG | C3-O3-P-O5 |
| 18 | B | 1855 | LHG | C4-O6-P-O4 |
| 18 | I | 5001 | LHG | C3-O3-P-O5 |
| 18 | L | 5220 | LHG | C4-O6-P-O4 |
| 18 | L | 5221 | LHG | C3-O3-P-O4 |
| 18 | L | 5221 | LHG | C4-O6-P-O4 |
| 18 | G | 5002 | LHG | C4-O6-P-O5 |
| 18 | G | 5005 | LHG | C3-O3-P-O5 |
| 18 | G | 5008 | LHG | C4-O6-P-O4 |
| 18 | G | 5003 | LHG | C4-O6-P-O5 |
| 18 | H | 1842 | LHG | C3-O3-P-O4 |
| 18 | H | 1855 | LHG | C3-O3-P-O5 |
| 18 | H | 1855 | LHG | C4-O6-P-O4 |
| 18 | S | 5001 | LHG | C3-O3-P-O5 |
| 18 | V | 5220 | LHG | C4-O6-P-O4 |
| 18 | V | 5221 | LHG | C3-O3-P-O4 |
| 18 | V | 5221 | LHG | C4-O6-P-O4 |
| 18 | e | 5002 | LHG | C4-O6-P-O5 |
| 18 | e | 5005 | LHG | C3-O3-P-O5 |
| 18 | e | 5008 | LHG | C4-O6-P-O4 |
| 18 | e | 5003 | LHG | C4-O6-P-O5 |
| 18 | f | 1842 | LHG | C3-O3-P-O4 |
| 18 | f | 1855 | LHG | C3-O3-P-O5 |
| 18 | f | 1855 | LHG | C4-O6-P-O4 |
| 18 | k | 5001 | LHG | C3-O3-P-O5 |
| 18 | n | 5220 | LHG | C4-O6-P-O4 |
| 18 | n | 5221 | LHG | C3-O3-P-O4 |
| 18 | n | 5221 | LHG | C4-O6-P-O4 |
| 14 | A | 1117 | CLA | C16-C17-C18-C20 |
| 14 | G | 1117 | CLA | C16-C17-C18-C20 |
| 14 | e | 1117 | CLA | C16-C17-C18-C20 |
| 21 | n | 5216 | SQD | C23-C24-C25-C26 |
| 14 | B | 1205 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1205 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1205 | CLA | CBA-CGA-O2A-C1 |
| 14 | 3 | 510 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1124 | CLA | CBD-CGD-O2D-CED |
| 18 | B | 1855 | LHG | O6-C4-C5-C6 |
| 18 | H | 1855 | LHG | O6-C4-C5-C6 |
| 18 | f | 1855 | LHG | O6-C4-C5-C6 |
| 14 | B | 1228 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1228 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1228 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1213 | CLA | C2A-CAA-CBA-CGA |
| 14 | 2 | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1213 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1213 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 517 | CLA | C2A-CAA-CBA-CGA |
| 14 | L | 1502 | CLA | C3-C5-C6-C7 |
| 14 | V | 1502 | CLA | C3-C5-C6-C7 |
| 14 | n | 1502 | CLA | C3-C5-C6-C7 |
| 18 | A | 5007 | LHG | C28-C29-C30-C31 |
| 18 | G | 5007 | LHG | C28-C29-C30-C31 |
| 18 | e | 5007 | LHG | C28-C29-C30-C31 |
| 14 | A | 1111 | CLA | CAD-CBD-CGD-O1D |
| 14 | A | 1113 | CLA | CAD-CBD-CGD-O1D |
| 14 | A | 1801 | CLA | CAD-CBD-CGD-O1D |
| 14 | B | 1012 | CLA | CAD-CBD-CGD-O1D |
| 14 | B | 1234 | CLA | CAD-CBD-CGD-O1D |
| 14 | B | 1207 | CLA | CAD-CBD-CGD-O1D |
| 14 | K | 1103 | CLA | CAD-CBD-CGD-O1D |
| 14 | K | 1105 | CLA | CAD-CBD-CGD-O1D |
| 14 | 1 | 501 | CLA | CAD-CBD-CGD-O1D |
| 14 | 1 | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | 1 | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | 2 | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | 2 | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | 2 | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | 2 | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | 2 | 518 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | 3 | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | 4 | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | 5 | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | 5 | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | 5 | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | 5 | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | 6 | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1111 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1113 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1801 | CLA | CAD-CBD-CGD-O1D |
| 14 | H | 1012 | CLA | CAD-CBD-CGD-O1D |
| 14 | H | 1234 | CLA | CAD-CBD-CGD-O1D |
| 14 | H | 1207 | CLA | CAD-CBD-CGD-O1D |
| 14 | U | 1103 | CLA | CAD-CBD-CGD-O1D |
| 14 | U | 1105 | CLA | CAD-CBD-CGD-O1D |
| 14 | Y | 501 | CLA | CAD-CBD-CGD-O1D |
| 14 | Y | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | Y | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | Z | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | Z | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | Z | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | Z | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | Z | 518 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | a | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | b | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | c | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | c | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | c | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | c | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1111 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1113 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1801 | CLA | CAD-CBD-CGD-O1D |
| 14 | f | 1012 | CLA | CAD-CBD-CGD-O1D |
| 14 | f | 1234 | CLA | CAD-CBD-CGD-O1D |
| 14 | f | 1207 | CLA | CAD-CBD-CGD-O1D |
| 14 | m | 1103 | CLA | CAD-CBD-CGD-O1D |
| 14 | m | 1105 | CLA | CAD-CBD-CGD-O1D |
| 14 | q | 501 | CLA | CAD-CBD-CGD-O1D |
| 14 | q | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | q | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | r | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | r | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | r | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | r | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | r | 518 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | s | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | s | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | s | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | s | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | s | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | t | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | u | 503 | CLA | CAD-CBD-CGD-O1D |
| 14 | u | 506 | CLA | CAD-CBD-CGD-O1D |
| 14 | u | 510 | CLA | CAD-CBD-CGD-O1D |
| 14 | u | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | v | 503 | CLA | CAD-CBD-CGD-O1D |
| 18 | B | 1842 | LHG | O10-C23-O8-C6 |
| 18 | f | 1842 | LHG | O10-C23-O8-C6 |
| 18 | A | 5002 | LHG | C26-C27-C28-C29 |
| 18 | G | 5002 | LHG | C26-C27-C28-C29 |
| 18 | e | 5002 | LHG | C26-C27-C28-C29 |
| 18 | n | 5218 | LHG | C23-C24-C25-C26 |
| 20 | f | 5002 | LMG | C39-C40-C41-C42 |
| 18 | A | 5005 | LHG | C24-C23-O8-C6 |
| 18 | G | 5005 | LHG | C24-C23-O8-C6 |
| 18 | e | 5005 | LHG | C24-C23-O8-C6 |
| 18 | H | 1842 | LHG | O10-C23-O8-C6 |
| 20 | B | 5002 | LMG | C39-C40-C41-C42 |
| 20 | H | 5002 | LMG | C39-C40-C41-C42 |
| 14 | A | 1104 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1111 | CLA | C12-C13-C15-C16 |
| 14 | A | 1117 | CLA | C11-C12-C13-C15 |
| 14 | B | 1203 | CLA | C11-C12-C13-C15 |
| 14 | B | 1206 | CLA | C11-C10-C8-C7 |
| 14 | B | 1208 | CLA | C6-C7-C8-C10 |
| 14 | B | 1210 | CLA | C2-C3-C5-C6 |
| 14 | B | 1210 | CLA | C6-C7-C8-C10 |
| 14 | B | 1213 | CLA | C11-C12-C13-C15 |
| 14 | B | 1214 | CLA | C11-C12-C13-C15 |
| 14 | B | 1217 | CLA | C6-C7-C8-C10 |
| 14 | B | 1219 | CLA | C6-C7-C8-C10 |
| 14 | B | 1227 | CLA | C6-C7-C8-C10 |
| 14 | G | 1104 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1111 | CLA | C12-C13-C15-C16 |
| 14 | G | 1117 | CLA | C11-C12-C13-C15 |
| 14 | H | 1203 | CLA | C11-C12-C13-C15 |
| 14 | H | 1206 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1208 | CLA | C6-C7-C8-C10 |
| 14 | H | 1210 | CLA | C2-C3-C5-C6 |
| 14 | H | 1210 | CLA | C6-C7-C8-C10 |
| 14 | H | 1213 | CLA | C11-C12-C13-C15 |
| 14 | H | 1214 | CLA | C11-C12-C13-C15 |
| 14 | H | 1217 | CLA | C6-C7-C8-C10 |
| 14 | H | 1219 | CLA | C6-C7-C8-C10 |
| 14 | H | 1227 | CLA | C6-C7-C8-C10 |
| 14 | e | 1104 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1111 | CLA | C12-C13-C15-C16 |
| 14 | e | 1117 | CLA | C11-C12-C13-C15 |
| 14 | f | 1203 | CLA | C11-C12-C13-C15 |
| 14 | f | 1206 | CLA | C11-C10-C8-C7 |
| 14 | f | 1208 | CLA | C6-C7-C8-C10 |
| 14 | f | 1210 | CLA | C2-C3-C5-C6 |
| 14 | f | 1210 | CLA | C6-C7-C8-C10 |
| 14 | f | 1213 | CLA | C11-C12-C13-C15 |
| 14 | f | 1214 | CLA | C11-C12-C13-C15 |
| 14 | f | 1217 | CLA | C6-C7-C8-C10 |
| 14 | f | 1219 | CLA | C6-C7-C8-C10 |
| 14 | f | 1227 | CLA | C6-C7-C8-C10 |
| 18 | A | 5005 | LHG | O6-C4-C5-O7 |
| 18 | L | 5218 | LHG | C23-C24-C25-C26 |
| 18 | G | 5005 | LHG | O6-C4-C5-O7 |
| 18 | V | 5218 | LHG | C23-C24-C25-C26 |
| 18 | e | 5005 | LHG | O6-C4-C5-O7 |
| 17 | l | 4015 | BCR | C15-C16-C17-C18 |
| 14 | 3 | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1237 | CLA | C5-C6-C7-C8 |
| 14 | B | 1234 | CLA | C5-C6-C7-C8 |
| 14 | G | 1237 | CLA | C5-C6-C7-C8 |
| 14 | H | 1234 | CLA | C5-C6-C7-C8 |
| 14 | e | 1237 | CLA | C5-C6-C7-C8 |
| 14 | f | 1234 | CLA | C5-C6-C7-C8 |
| 14 | f | 1234 | CLA | C2C-C3C-CAC-CBC |
| 14 | B | 1208 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1234 | CLA | C2C-C3C-CAC-CBC |
| 14 | H | 1234 | CLA | C2C-C3C-CAC-CBC |
| 18 | B | 1842 | LHG | C4-C5-C6-O8 |
| 18 | H | 1842 | LHG | C4-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | f | 1842 | LHG | C4-C5-C6-O8 |
| 21 | l | 822 | SQD | O6-C44-C45-C46 |
| 21 | 4 | 822 | SQD | C44-C45-C46-O48 |
| 21 | Y | 822 | SQD | O6-C44-C45-C46 |
| 21 | b | 822 | SQD | C44-C45-C46-O48 |
| 21 | q | 822 | SQD | O6-C44-C45-C46 |
| 21 | t | 822 | SQD | C44-C45-C46-O48 |
| 14 | H | 1208 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1208 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5004 | LHG | O7-C5-C6-O8 |
| 18 | A | 5005 | LHG | O7-C5-C6-O8 |
| 18 | A | 5007 | LHG | O7-C5-C6-O8 |
| 18 | G | 5004 | LHG | O7-C5-C6-O8 |
| 18 | G | 5005 | LHG | O7-C5-C6-O8 |
| 18 | G | 5007 | LHG | O7-C5-C6-O8 |
| 18 | e | 5004 | LHG | O7-C5-C6-O8 |
| 18 | e | 5005 | LHG | O7-C5-C6-O8 |
| 18 | e | 5007 | LHG | O7-C5-C6-O8 |
| 21 | 6 | 822 | SQD | O47-C45-C46-O48 |
| 21 | d | 822 | SQD | O47-C45-C46-O48 |
| 21 | v | 822 | SQD | O47-C45-C46-O48 |
| 14 | 2 | 505 | CLA | C5-C6-C7-C8 |
| 14 | Z | 505 | CLA | C5-C6-C7-C8 |
| 14 | r | 505 | CLA | C5-C6-C7-C8 |
| 14 | l | 516 | CLA | C2C-C3C-CAC-CBC |
| 14 | Y | 516 | CLA | C2C-C3C-CAC-CBC |
| 14 | q | 516 | CLA | C2C-C3C-CAC-CBC |
| 14 | B | 1021 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1021 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1021 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1202 | CLA | C4-C3-C5-C6 |
| 14 | H | 1202 | CLA | C4-C3-C5-C6 |
| 14 | A | 1128 | CLA | C10-C11-C12-C13 |
| 14 | G | 1128 | CLA | C10-C11-C12-C13 |
| 14 | e | 1128 | CLA | C10-C11-C12-C13 |
| 14 | A | 1013 | CLA | C14-C13-C15-C16 |
| 14 | A | 1104 | CLA | C14-C13-C15-C16 |
| 14 | A | 1106 | CLA | C14-C13-C15-C16 |
| 14 | A | 1131 | CLA | C14-C13-C15-C16 |
| 14 | B | 1012 | CLA | C11-C10-C8-C9 |
| 14 | B | 1208 | CLA | C14-C13-C15-C16 |
| 14 | B | 1214 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1225 | CLA | C14-C13-C15-C16 |
| 14 | B | 1239 | CLA | C14-C13-C15-C16 |
| 14 | B | 1240 | CLA | C11-C12-C13-C14 |
| 14 | B | 1230 | CLA | C6-C7-C8-C9 |
| 14 | 5 | 509 | CLA | C6-C7-C8-C9 |
| 14 | G | 1013 | CLA | C14-C13-C15-C16 |
| 14 | G | 1104 | CLA | C14-C13-C15-C16 |
| 14 | G | 1106 | CLA | C14-C13-C15-C16 |
| 14 | G | 1131 | CLA | C14-C13-C15-C16 |
| 14 | H | 1012 | CLA | C11-C10-C8-C9 |
| 14 | H | 1208 | CLA | C14-C13-C15-C16 |
| 14 | H | 1214 | CLA | C11-C12-C13-C14 |
| 14 | H | 1225 | CLA | C14-C13-C15-C16 |
| 14 | H | 1239 | CLA | C14-C13-C15-C16 |
| 14 | H | 1240 | CLA | C11-C12-C13-C14 |
| 14 | H | 1230 | CLA | C6-C7-C8-C9 |
| 14 | c | 509 | CLA | C6-C7-C8-C9 |
| 14 | e | 1013 | CLA | C14-C13-C15-C16 |
| 14 | e | 1104 | CLA | C14-C13-C15-C16 |
| 14 | e | 1106 | CLA | C14-C13-C15-C16 |
| 14 | e | 1131 | CLA | C14-C13-C15-C16 |
| 14 | f | 1012 | CLA | C11-C10-C8-C9 |
| 14 | f | 1208 | CLA | C6-C7-C8-C9 |
| 14 | f | 1208 | CLA | C14-C13-C15-C16 |
| 14 | f | 1214 | CLA | C11-C12-C13-C14 |
| 14 | f | 1225 | CLA | C14-C13-C15-C16 |
| 14 | f | 1239 | CLA | C14-C13-C15-C16 |
| 14 | f | 1240 | CLA | C11-C12-C13-C14 |
| 14 | f | 1230 | CLA | C6-C7-C8-C9 |
| 14 | u | 509 | CLA | C6-C7-C8-C9 |
| 21 | 1 | 822 | SQD | O48-C23-C24-C25 |
| 21 | Y | 822 | SQD | O48-C23-C24-C25 |
| 21 | q | 822 | SQD | O48-C23-C24-C25 |
| 17 | B | 4010 | BCR | C11-C12-C13-C35 |
| 17 | 6 | 521 | BCR | C7-C8-C9-C34 |
| 17 | H | 4010 | BCR | C11-C12-C13-C35 |
| 17 | d | 521 | BCR | C7-C8-C9-C34 |
| 17 | f | 4010 | BCR | C11-C12-C13-C35 |
| 18 | n | 5221 | LHG | C29-C30-C31-C32 |
| 18 | L | 5221 | LHG | C29-C30-C31-C32 |
| 18 | V | 5221 | LHG | C29-C30-C31-C32 |
| 14 | B | 1229 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1229 | CLA | CAA-CBA-CGA-O2A |
| 18 | e | 5006 | LHG | C29-C30-C31-C32 |
| 14 | A | 1132 | CLA | C8-C10-C11-C12 |
| 14 | e | 1132 | CLA | C8-C10-C11-C12 |
| 18 | A | 5006 | LHG | C29-C30-C31-C32 |
| 14 | A | 1107 | CLA | C4-C3-C5-C6 |
| 14 | 3 | 505 | CLA | C4-C3-C5-C6 |
| 14 | G | 1107 | CLA | C4-C3-C5-C6 |
| 14 | e | 1107 | CLA | C4-C3-C5-C6 |
| 14 | f | 1202 | CLA | C4-C3-C5-C6 |
| 14 | f | 1229 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1204 | CLA | C2-C3-C5-C6 |
| 14 | H | 1204 | CLA | C2-C3-C5-C6 |
| 14 | f | 1204 | CLA | C2-C3-C5-C6 |
| 18 | G | 5006 | LHG | C29-C30-C31-C32 |
| 14 | G | 1132 | CLA | C8-C10-C11-C12 |
| 14 | 2 | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | 5 | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 518 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 501 | CLA | C2A-CAA-CBA-CGA |
| 18 | L | 5221 | LHG | O9-C7-O7-C5 |
| 18 | V | 5221 | LHG | O9-C7-O7-C5 |
| 18 | n | 5221 | LHG | O9-C7-O7-C5 |
| 20 | J | 5104 | LMG | O9-C10-O7-C8 |
| 20 | T | 5104 | LMG | O9-C10-O7-C8 |
| 20 | l | 5104 | LMG | O9-C10-O7-C8 |
| 14 | A | 1106 | CLA | C2-C1-O2A-CGA |
| 14 | A | 1107 | CLA | C2-C1-O2A-CGA |
| 14 | A | 1138 | CLA | C2-C1-O2A-CGA |
| 14 | A | 1237 | CLA | C2-C1-O2A-CGA |
| 14 | B | 1212 | CLA | C2-C1-O2A-CGA |
| 14 | 3 | 505 | CLA | C2-C1-O2A-CGA |
| 14 | 6 | 505 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1106 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1107 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1138 | CLA | C2-C1-O2A-CGA |
| 14 | G | 1237 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1212 | CLA | C2-C1-O2A-CGA |
| 14 | a | 505 | CLA | C2-C1-O2A-CGA |
| 14 | d | 505 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1106 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1107 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1138 | CLA | C2-C1-O2A-CGA |
| 14 | e | 1237 | CLA | C2-C1-O2A-CGA |
| 14 | f | 1212 | CLA | C2-C1-O2A-CGA |
| 14 | s | 505 | CLA | C2-C1-O2A-CGA |
| 14 | v | 505 | CLA | C2-C1-O2A-CGA |
| 21 | B | 1852 | SQD | O10-C23-O48-C46 |
| 21 | H | 1852 | SQD | O10-C23-O48-C46 |
| 21 | n | 5216 | SQD | C16-C17-C18-C19 |
| 21 | L | 5216 | SQD | C16-C17-C18-C19 |
| 14 | H | 1212 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1220 | CLA | O1A-CGA-O2A-C1 |
| 21 | f | 1852 | SQD | O10-C23-O48-C46 |
| 18 | A | 5007 | LHG | O6-C4-C5-O7 |
| 18 | G | 5007 | LHG | O6-C4-C5-O7 |
| 18 | e | 5007 | LHG | O6-C4-C5-O7 |
| 21 | V | 5216 | SQD | C16-C17-C18-C19 |
| 14 | a | 505 | CLA | C4-C3-C5-C6 |
| 14 | s | 505 | CLA | C4-C3-C5-C6 |
| 14 | f | 1212 | CLA | O1D-CGD-O2D-CED |
| 17 | 3 | 522 | BCR | C1-C6-C7-C8 |
| 17 | a | 522 | BCR | C1-C6-C7-C8 |
| 17 | s | 522 | BCR | C1-C6-C7-C8 |
| 14 | B | 1220 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1212 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1124 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1124 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1124 | CLA | CBA-CGA-O2A-C1 |
| 14 | 5 | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | c | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | u | 503 | CLA | C2A-CAA-CBA-CGA |
| 17 | L | 4020 | BCR | C20-C21-C22-C23 |
| 17 | V | 4020 | BCR | C20-C21-C22-C23 |
| 17 | n | 4020 | BCR | C20-C21-C22-C23 |
| 14 | H | 1220 | CLA | O1A-CGA-O2A-C1 |
| 18 | A | 5002 | LHG | O7-C5-C6-O8 |
| 18 | G | 5002 | LHG | O7-C5-C6-O8 |
| 18 | e | 5002 | LHG | O7-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1207 | CLA | C15-C16-C17-C18 |
| 14 | H | 1207 | CLA | C15-C16-C17-C18 |
| 14 | f | 1207 | CLA | C15-C16-C17-C18 |
| 18 | A | 5002 | LHG | C3-O3-P-O6 |
| 18 | A | 5007 | LHG | C3-O3-P-O6 |
| 18 | A | 5001 | LHG | C3-O3-P-O6 |
| 18 | A | 5003 | LHG | C3-O3-P-O6 |
| 18 | A | 5003 | LHG | C4-O6-P-O3 |
| 18 | I | 5001 | LHG | C4-O6-P-O3 |
| 18 | G | 5002 | LHG | C3-O3-P-O6 |
| 18 | G | 5007 | LHG | C3-O3-P-O6 |
| 18 | G | 5001 | LHG | C3-O3-P-O6 |
| 18 | G | 5003 | LHG | C3-O3-P-O6 |
| 18 | G | 5003 | LHG | C4-O6-P-O3 |
| 18 | S | 5001 | LHG | C4-O6-P-O3 |
| 18 | e | 5002 | LHG | C3-O3-P-O6 |
| 18 | e | 5007 | LHG | C3-O3-P-O6 |
| 18 | e | 5001 | LHG | C3-O3-P-O6 |
| 18 | e | 5003 | LHG | C3-O3-P-O6 |
| 18 | e | 5003 | LHG | C4-O6-P-O3 |
| 18 | k | 5001 | LHG | C4-O6-P-O3 |
| 20 | B | 5002 | LMG | C7-C8-C9-O8 |
| 20 | H | 5002 | LMG | C7-C8-C9-O8 |
| 20 | f | 5002 | LMG | C7-C8-C9-O8 |
| 14 | A | 1022 | CLA | C4-C3-C5-C6 |
| 14 | G | 1022 | CLA | C4-C3-C5-C6 |
| 14 | e | 1022 | CLA | C4-C3-C5-C6 |
| 14 | A | 1103 | CLA | C12-C13-C15-C16 |
| 14 | A | 1101 | CLA | C6-C7-C8-C10 |
| 14 | B | 1023 | CLA | C11-C10-C8-C7 |
| 14 | B | 1208 | CLA | C12-C13-C15-C16 |
| 14 | 2 | 505 | CLA | C12-C13-C15-C16 |
| 14 | G | 1103 | CLA | C12-C13-C15-C16 |
| 14 | G | 1101 | CLA | C6-C7-C8-C10 |
| 14 | H | 1023 | CLA | C11-C10-C8-C7 |
| 14 | H | 1208 | CLA | C12-C13-C15-C16 |
| 14 | Z | 505 | CLA | C12-C13-C15-C16 |
| 14 | e | 1103 | CLA | C12-C13-C15-C16 |
| 14 | e | 1101 | CLA | C6-C7-C8-C10 |
| 14 | f | 1023 | CLA | C11-C10-C8-C7 |
| 14 | f | 1208 | CLA | C12-C13-C15-C16 |
| 14 | r | 505 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1107 | CLA | C11-C10-C8-C9 |
| 14 | A | 1139 | CLA | C14-C13-C15-C16 |
| 14 | A | 1101 | CLA | C11-C10-C8-C9 |
| 14 | B | 1208 | CLA | C6-C7-C8-C9 |
| 14 | B | 1210 | CLA | C11-C12-C13-C14 |
| 14 | B | 1217 | CLA | C6-C7-C8-C9 |
| 14 | B | 1219 | CLA | C11-C10-C8-C9 |
| 14 | B | 1229 | CLA | C6-C7-C8-C9 |
| 14 | G | 1107 | CLA | C11-C10-C8-C9 |
| 14 | G | 1139 | CLA | C14-C13-C15-C16 |
| 14 | G | 1101 | CLA | C11-C10-C8-C9 |
| 14 | H | 1208 | CLA | C6-C7-C8-C9 |
| 14 | H | 1210 | CLA | C11-C12-C13-C14 |
| 14 | H | 1217 | CLA | C6-C7-C8-C9 |
| 14 | H | 1219 | CLA | C11-C10-C8-C9 |
| 14 | H | 1229 | CLA | C6-C7-C8-C9 |
| 14 | e | 1107 | CLA | C11-C10-C8-C9 |
| 14 | e | 1139 | CLA | C14-C13-C15-C16 |
| 14 | e | 1101 | CLA | C11-C10-C8-C9 |
| 14 | f | 1210 | CLA | C11-C12-C13-C14 |
| 14 | f | 1217 | CLA | C6-C7-C8-C9 |
| 14 | f | 1219 | CLA | C11-C10-C8-C9 |
| 14 | f | 1229 | CLA | C6-C7-C8-C9 |
| 17 | J | 4012 | BCR | C9-C10-C11-C12 |
| 17 | T | 4012 | BCR | C9-C10-C11-C12 |
| 17 | l | 4012 | BCR | C9-C10-C11-C12 |
| 14 | B | 1021 | CLA | C16-C17-C18-C20 |
| 14 | H | 1021 | CLA | C16-C17-C18-C20 |
| 14 | f | 1021 | CLA | C16-C17-C18-C20 |
| 14 | A | 1128 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1128 | CLA | CBA-CGA-O2A-C1 |
| 14 | 2 | 503 | CLA | C13-C15-C16-C17 |
| 14 | Z | 503 | CLA | C13-C15-C16-C17 |
| 14 | r | 503 | CLA | C13-C15-C16-C17 |
| 14 | A | 1128 | CLA | O1A-CGA-O2A-C1 |
| 14 | G | 1128 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1128 | CLA | O1A-CGA-O2A-C1 |
| 17 | l | 524 | BCR | C11-C12-C13-C35 |
| 17 | Y | 524 | BCR | C11-C12-C13-C35 |
| 17 | q | 524 | BCR | C11-C12-C13-C35 |
| 14 | B | 1210 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1210 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1128 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1210 | CLA | CBA-CGA-O2A-C1 |
| 18 | L | 5220 | LHG | C2-C3-O3-P |
| 18 | V | 5220 | LHG | C2-C3-O3-P |
| 18 | n | 5220 | LHG | C2-C3-O3-P |
| 18 | V | 5220 | LHG | C25-C26-C27-C28 |
| 18 | L | 5220 | LHG | C25-C26-C27-C28 |
| 14 | B | 1213 | CLA | C12-C13-C15-C16 |
| 14 | H | 1213 | CLA | C12-C13-C15-C16 |
| 14 | f | 1213 | CLA | C12-C13-C15-C16 |
| 18 | n | 5220 | LHG | C25-C26-C27-C28 |
| 14 | B | 1021 | CLA | C16-C17-C18-C19 |
| 14 | H | 1021 | CLA | C16-C17-C18-C19 |
| 14 | f | 1021 | CLA | C16-C17-C18-C19 |
| 14 | A | 1011 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1011 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1011 | CLA | CBA-CGA-O2A-C1 |
| 14 | e | 1130 | CLA | C3-C5-C6-C7 |
| 14 | A | 1126 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1126 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1126 | CLA | CAA-CBA-CGA-O2A |
| 18 | G | 5003 | LHG | C11-C12-C13-C14 |
| 18 | e | 5003 | LHG | C11-C12-C13-C14 |
| 14 | A | 1109 | CLA | C15-C16-C17-C18 |
| 14 | G | 1109 | CLA | C15-C16-C17-C18 |
| 14 | G | 1135 | CLA | C5-C6-C7-C8 |
| 18 | A | 5003 | LHG | C11-C12-C13-C14 |
| 19 | A | 1848 | LMU | O1'-C1-C2-C3 |
| 19 | G | 1848 | LMU | O1'-C1-C2-C3 |
| 19 | e | 1848 | LMU | O1'-C1-C2-C3 |
| 14 | 4 | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | b | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | t | 513 | CLA | C2A-CAA-CBA-CGA |
| 17 | A | 4001 | BCR | C13-C14-C15-C16 |
| 17 | 3 | 524 | BCR | C9-C10-C11-C12 |
| 17 | G | 4001 | BCR | C13-C14-C15-C16 |
| 17 | a | 524 | BCR | C9-C10-C11-C12 |
| 17 | e | 4001 | BCR | C13-C14-C15-C16 |
| 17 | s | 524 | BCR | C9-C10-C11-C12 |
| 18 | A | 5009 | LHG | O6-C4-C5-C6 |
| 18 | G | 5009 | LHG | O6-C4-C5-C6 |
| 18 | e | 5009 | LHG | O6-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1130 | CLA | C3-C5-C6-C7 |
| 14 | G | 1130 | CLA | C3-C5-C6-C7 |
| 14 | A | 1135 | CLA | C5-C6-C7-C8 |
| 14 | e | 1109 | CLA | C15-C16-C17-C18 |
| 14 | e | 1135 | CLA | C5-C6-C7-C8 |
| 18 | A | 5009 | LHG | O6-C4-C5-O7 |
| 18 | G | 5009 | LHG | O6-C4-C5-O7 |
| 18 | e | 5009 | LHG | O6-C4-C5-O7 |
| 14 | B | 1205 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1205 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1205 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1210 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1210 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1210 | CLA | O1A-CGA-O2A-C1 |
| 14 | a | 510 | CLA | O1D-CGD-O2D-CED |
| 18 | L | 5220 | LHG | C26-C27-C28-C29 |
| 18 | n | 5220 | LHG | C26-C27-C28-C29 |
| 14 | A | 1801 | CLA | CAA-CBA-CGA-O1A |
| 14 | l | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1801 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1801 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1132 | CLA | C2C-C3C-CAC-CBC |
| 14 | G | 1132 | CLA | C2C-C3C-CAC-CBC |
| 14 | e | 1132 | CLA | C2C-C3C-CAC-CBC |
| 18 | V | 5220 | LHG | C26-C27-C28-C29 |
| 19 | l | 5105 | LMU | C5-C6-C7-C8 |
| 14 | Y | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1137 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1237 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1204 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1210 | CLA | C2A-CAA-CBA-CGA |
| 14 | 6 | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1137 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1237 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1204 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1210 | CLA | C2A-CAA-CBA-CGA |
| 14 | d | 501 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1137 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1237 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1204 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1210 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | v | 501 | CLA | C2A-CAA-CBA-CGA |
| 19 | J | 5105 | LMU | C5-C6-C7-C8 |
| 19 | T | 5105 | LMU | C5-C6-C7-C8 |
| 14 | G | 1011 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | B | 1206 | CLA | C3A-C2A-CAA-CBA |
| 14 | B | 1228 | CLA | C3A-C2A-CAA-CBA |
| 14 | 2 | 512 | CLA | C3A-C2A-CAA-CBA |
| 14 | 4 | 517 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1206 | CLA | C3A-C2A-CAA-CBA |
| 14 | H | 1228 | CLA | C3A-C2A-CAA-CBA |
| 14 | Z | 512 | CLA | C3A-C2A-CAA-CBA |
| 14 | b | 517 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1206 | CLA | C3A-C2A-CAA-CBA |
| 14 | f | 1228 | CLA | C3A-C2A-CAA-CBA |
| 14 | r | 512 | CLA | C3A-C2A-CAA-CBA |
| 14 | t | 517 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1124 | CLA | O1D-CGD-O2D-CED |
| 14 | Y | 504 | CLA | CBD-CGD-O2D-CED |
| 17 | 4 | 521 | BCR | C13-C14-C15-C16 |
| 17 | a | 521 | BCR | C9-C10-C11-C12 |
| 17 | b | 521 | BCR | C13-C14-C15-C16 |
| 17 | s | 521 | BCR | C9-C10-C11-C12 |
| 17 | t | 521 | BCR | C13-C14-C15-C16 |
| 14 | u | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1224 | CLA | C4-C3-C5-C6 |
| 14 | J | 1302 | CLA | C4-C3-C5-C6 |
| 14 | H | 1224 | CLA | C4-C3-C5-C6 |
| 14 | T | 1302 | CLA | C4-C3-C5-C6 |
| 14 | f | 1224 | CLA | C4-C3-C5-C6 |
| 14 | l | 1302 | CLA | C4-C3-C5-C6 |
| 14 | s | 510 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 504 | CLA | CBD-CGD-O2D-CED |
| 14 | J | 1302 | CLA | C2-C3-C5-C6 |
| 14 | T | 1302 | CLA | C2-C3-C5-C6 |
| 14 | l | 1302 | CLA | C2-C3-C5-C6 |
| 14 | A | 1011 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1011 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1106 | CLA | C11-C10-C8-C9 |
| 14 | A | 1126 | CLA | C14-C13-C15-C16 |
| 14 | A | 1139 | CLA | C11-C12-C13-C14 |
| 14 | A | 1237 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1106 | CLA | C11-C10-C8-C9 |
| 14 | G | 1126 | CLA | C14-C13-C15-C16 |
| 14 | G | 1139 | CLA | C11-C12-C13-C14 |
| 14 | G | 1237 | CLA | C14-C13-C15-C16 |
| 14 | e | 1106 | CLA | C11-C10-C8-C9 |
| 14 | e | 1126 | CLA | C14-C13-C15-C16 |
| 14 | e | 1139 | CLA | C11-C12-C13-C14 |
| 14 | e | 1237 | CLA | C14-C13-C15-C16 |
| 18 | k | 5001 | LHG | C24-C25-C26-C27 |
| 14 | A | 1801 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1801 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1801 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1129 | CLA | CBD-CGD-O2D-CED |
| 18 | I | 5001 | LHG | C24-C25-C26-C27 |
| 18 | L | 5220 | LHG | C31-C32-C33-C34 |
| 18 | S | 5001 | LHG | C24-C25-C26-C27 |
| 18 | V | 5220 | LHG | C31-C32-C33-C34 |
| 18 | n | 5220 | LHG | C31-C32-C33-C34 |
| 17 | A | 4011 | BCR | C11-C10-C9-C34 |
| 17 | A | 4011 | BCR | C16-C17-C18-C36 |
| 17 | B | 4006 | BCR | C11-C10-C9-C34 |
| 17 | B | 4006 | BCR | C20-C21-C22-C37 |
| 17 | F | 4016 | BCR | C35-C13-C14-C15 |
| 17 | L | 4020 | BCR | C20-C21-C22-C37 |
| 17 | G | 4011 | BCR | C11-C10-C9-C34 |
| 17 | G | 4011 | BCR | C16-C17-C18-C36 |
| 17 | H | 4006 | BCR | C11-C10-C9-C34 |
| 17 | H | 4006 | BCR | C20-C21-C22-C37 |
| 17 | R | 4016 | BCR | C35-C13-C14-C15 |
| 17 | V | 4020 | BCR | C20-C21-C22-C37 |
| 17 | e | 4011 | BCR | C11-C10-C9-C34 |
| 17 | e | 4011 | BCR | C16-C17-C18-C36 |
| 17 | f | 4006 | BCR | C11-C10-C9-C34 |
| 17 | f | 4006 | BCR | C20-C21-C22-C37 |
| 17 | j | 4016 | BCR | C35-C13-C14-C15 |
| 17 | n | 4020 | BCR | C20-C21-C22-C37 |
| 21 | B | 1852 | SQD | C44-C45-C46-O48 |
| 21 | L | 5216 | SQD | O6-C44-C45-C46 |
| 21 | 2 | 822 | SQD | C44-C45-C46-O48 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | 4 | 822 | SQD | O6-C44-C45-C46 |
| 21 | H | 1852 | SQD | C44-C45-C46-O48 |
| 21 | V | 5216 | SQD | O6-C44-C45-C46 |
| 21 | Z | 822 | SQD | C44-C45-C46-O48 |
| 21 | b | 822 | SQD | O6-C44-C45-C46 |
| 21 | f | 1852 | SQD | C44-C45-C46-O48 |
| 21 | n | 5216 | SQD | O6-C44-C45-C46 |
| 21 | r | 822 | SQD | C44-C45-C46-O48 |
| 21 | t | 822 | SQD | O6-C44-C45-C46 |
| 14 | 3 | 518 | CLA | C3-C5-C6-C7 |
| 14 | a | 518 | CLA | C3-C5-C6-C7 |
| 14 | s | 518 | CLA | C3-C5-C6-C7 |
| 14 | 1 | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1216 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | 4 | 502 | CLA | C2A-CAA-CBA-CGA |
| 14 | H | 1216 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | b | 502 | CLA | C2A-CAA-CBA-CGA |
| 14 | f | 1216 | CLA | C2A-CAA-CBA-CGA |
| 14 | t | 502 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1124 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 5002 | LMG | C40-C41-C42-C43 |
| 20 | H | 5002 | LMG | C40-C41-C42-C43 |
| 14 | A | 1117 | CLA | C16-C17-C18-C19 |
| 14 | B | 1229 | CLA | C16-C17-C18-C19 |
| 14 | G | 1117 | CLA | C16-C17-C18-C19 |
| 14 | H | 1229 | CLA | C16-C17-C18-C19 |
| 14 | e | 1117 | CLA | C16-C17-C18-C19 |
| 14 | f | 1229 | CLA | C16-C17-C18-C19 |
| 14 | A | 1126 | CLA | O2A-C1-C2-C3 |
| 14 | B | 1216 | CLA | O2A-C1-C2-C3 |
| 14 | G | 1126 | CLA | O2A-C1-C2-C3 |
| 14 | H | 1216 | CLA | O2A-C1-C2-C3 |
| 14 | e | 1126 | CLA | O2A-C1-C2-C3 |
| 14 | f | 1216 | CLA | O2A-C1-C2-C3 |
| 18 | A | 5004 | LHG | O2-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | G | 5004 | LHG | O2-C2-C3-O3 |
| 18 | e | 5004 | LHG | O2-C2-C3-O3 |
| 14 | B | 1236 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1236 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1236 | CLA | CBA-CGA-O2A-C1 |
| 14 | G | 1124 | CLA | O1D-CGD-O2D-CED |
| 20 | f | 5002 | LMG | C40-C41-C42-C43 |
| 14 | 5 | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 508 | CLA | CAA-CBA-CGA-O1A |
| 17 | A | 4011 | BCR | C7-C8-C9-C34 |
| 17 | G | 4011 | BCR | C7-C8-C9-C34 |
| 17 | e | 4011 | BCR | C7-C8-C9-C34 |
| 14 | A | 1123 | CLA | C13-C15-C16-C17 |
| 14 | G | 1123 | CLA | C13-C15-C16-C17 |
| 14 | q | 504 | CLA | CBD-CGD-O2D-CED |
| 18 | e | 5004 | LHG | C28-C29-C30-C31 |
| 18 | A | 5004 | LHG | C28-C29-C30-C31 |
| 18 | G | 5004 | LHG | C28-C29-C30-C31 |
| 14 | 4 | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | 5 | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 517 | CLA | CAA-CBA-CGA-O1A |
| 21 | 5 | 822 | SQD | C46-C45-O47-C7 |
| 21 | c | 822 | SQD | C46-C45-O47-C7 |
| 21 | u | 822 | SQD | C46-C45-O47-C7 |
| 14 | A | 1022 | CLA | C15-C16-C17-C18 |
| 14 | G | 1022 | CLA | C15-C16-C17-C18 |
| 14 | e | 1123 | CLA | C13-C15-C16-C17 |
| 14 | A | 1111 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1128 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1206 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1228 | CLA | C1A-C2A-CAA-CBA |
| 14 | L | 1502 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 508 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 4 | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1111 | CLA | C1A-C2A-CAA-CBA |
| 14 | G | 1128 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1206 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1228 | CLA | C1A-C2A-CAA-CBA |
| 14 | V | 1502 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | b | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1111 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1128 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1206 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1228 | CLA | C1A-C2A-CAA-CBA |
| 14 | n | 1502 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 508 | CLA | C1A-C2A-CAA-CBA |
| 14 | t | 516 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | A | 1137 | CLA | C11-C10-C8-C7 |
| 14 | A | 1101 | CLA | C12-C13-C15-C16 |
| 14 | B | 1215 | CLA | C6-C7-C8-C10 |
| 14 | B | 1235 | CLA | C6-C7-C8-C10 |
| 14 | G | 1137 | CLA | C11-C10-C8-C7 |
| 14 | G | 1101 | CLA | C12-C13-C15-C16 |
| 14 | H | 1215 | CLA | C6-C7-C8-C10 |
| 14 | H | 1235 | CLA | C6-C7-C8-C10 |
| 14 | e | 1137 | CLA | C11-C10-C8-C7 |
| 14 | e | 1101 | CLA | C12-C13-C15-C16 |
| 14 | f | 1215 | CLA | C6-C7-C8-C10 |
| 14 | f | 1235 | CLA | C6-C7-C8-C10 |
| 14 | A | 1237 | CLA | C8-C10-C11-C12 |
| 14 | G | 1237 | CLA | C8-C10-C11-C12 |
| 14 | e | 1237 | CLA | C8-C10-C11-C12 |
| 14 | 1 | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 519 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | Y | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 519 | CLA | CAA-CBA-CGA-O1A |
| 17 | 3 | 521 | BCR | C9-C10-C11-C12 |
| 14 | A | 1129 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1011 | CLA | O1A-CGA-O2A-C1 |
| 14 | Z | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1022 | CLA | C15-C16-C17-C18 |
| 14 | A | 1109 | CLA | C3-C5-C6-C7 |
| 14 | A | 1110 | CLA | C3-C5-C6-C7 |
| 14 | G | 1109 | CLA | C3-C5-C6-C7 |
| 14 | G | 1110 | CLA | C3-C5-C6-C7 |
| 14 | e | 1110 | CLA | C3-C5-C6-C7 |
| 14 | 2 | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 503 | CLA | C2A-CAA-CBA-CGA |
| 14 | A | 1116 | CLA | C8-C10-C11-C12 |
| 14 | G | 1116 | CLA | C8-C10-C11-C12 |
| 19 | J | 5105 | LMU | C2-C3-C4-C5 |
| 19 | T | 5105 | LMU | C2-C3-C4-C5 |
| 19 | l | 5105 | LMU | C2-C3-C4-C5 |
| 14 | G | 1011 | CLA | O1A-CGA-O2A-C1 |
| 14 | 5 | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | c | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1116 | CLA | C8-C10-C11-C12 |
| 18 | L | 5221 | LHG | C12-C13-C14-C15 |
| 18 | V | 5221 | LHG | C12-C13-C14-C15 |
| 18 | n | 5221 | LHG | C12-C13-C14-C15 |
| 15 | G | 2001 | PQN | C23-C25-C26-C27 |
| 15 | e | 2001 | PQN | C23-C25-C26-C27 |
| 14 | 1 | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | 5 | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | 5 | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 519 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 15 | A | 2001 | PQN | C23-C25-C26-C27 |
| 14 | e | 1129 | CLA | CBD-CGD-O2D-CED |
| 14 | G | 1022 | CLA | C2-C3-C5-C6 |
| 14 | 4 | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1124 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1011 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1124 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1109 | CLA | C3-C5-C6-C7 |
| 17 | A | 4011 | BCR | C11-C10-C9-C8 |
| 17 | A | 4011 | BCR | C16-C17-C18-C19 |
| 17 | B | 4006 | BCR | C11-C10-C9-C8 |
| 17 | B | 4006 | BCR | C20-C21-C22-C23 |
| 17 | F | 4016 | BCR | C12-C13-C14-C15 |
| 17 | G | 4011 | BCR | C11-C10-C9-C8 |
| 17 | G | 4011 | BCR | C16-C17-C18-C19 |
| 17 | H | 4006 | BCR | C11-C10-C9-C8 |
| 17 | H | 4006 | BCR | C20-C21-C22-C23 |
| 17 | R | 4016 | BCR | C12-C13-C14-C15 |
| 17 | e | 4011 | BCR | C11-C10-C9-C8 |
| 17 | e | 4011 | BCR | C16-C17-C18-C19 |
| 17 | f | 4006 | BCR | C11-C10-C9-C8 |
| 17 | f | 4006 | BCR | C20-C21-C22-C23 |
| 17 | j | 4016 | BCR | C12-C13-C14-C15 |
| 14 | 4 | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | 5 | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | c | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 510 | CLA | CAA-CBA-CGA-O2A |
| 21 | L | 5216 | SQD | O6-C44-C45-O47 |
| 21 | V | 5216 | SQD | O6-C44-C45-O47 |
| 21 | n | 5216 | SQD | O6-C44-C45-O47 |
| 18 | A | 5001 | LHG | C24-C25-C26-C27 |
| 17 | A | 4008 | BCR | C19-C20-C21-C22 |
| 17 | G | 4008 | BCR | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | e | 4008 | BCR | C19-C20-C21-C22 |
| 14 | 4 | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1101 | CLA | C15-C16-C17-C18 |
| 14 | G | 1101 | CLA | C15-C16-C17-C18 |
| 14 | e | 1101 | CLA | C15-C16-C17-C18 |
| 14 | A | 1124 | CLA | O1A-CGA-O2A-C1 |
| 18 | e | 5001 | LHG | C24-C25-C26-C27 |
| 14 | B | 1220 | CLA | C6-C7-C8-C10 |
| 14 | H | 1220 | CLA | C6-C7-C8-C10 |
| 18 | I | 5001 | LHG | C30-C31-C32-C33 |
| 18 | G | 5001 | LHG | C24-C25-C26-C27 |
| 18 | k | 5001 | LHG | C30-C31-C32-C33 |
| 18 | S | 5001 | LHG | C30-C31-C32-C33 |
| 14 | 1 | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | 4 | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | b | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 519 | CLA | CAA-CBA-CGA-O1A |
| 18 | B | 1842 | LHG | C24-C25-C26-C27 |
| 18 | H | 1842 | LHG | C24-C25-C26-C27 |
| 18 | f | 1842 | LHG | C24-C25-C26-C27 |
| 14 | B | 1207 | CLA | C2-C1-O2A-CGA |
| 14 | H | 1207 | CLA | C2-C1-O2A-CGA |
| 14 | f | 1207 | CLA | C2-C1-O2A-CGA |
| 14 | q | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1022 | CLA | C2-C3-C5-C6 |
| 14 | B | 1224 | CLA | C2-C3-C5-C6 |
| 14 | H | 1224 | CLA | C2-C3-C5-C6 |
| 14 | e | 1022 | CLA | C2-C3-C5-C6 |
| 14 | f | 1224 | CLA | C2-C3-C5-C6 |
| 19 | B | 1843 | LMU | C6-C7-C8-C9 |
| 19 | H | 1843 | LMU | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 19 | f | 1843 | LMU | C6-C7-C8-C9 |
| 14 | 4 | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1202 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1116 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1202 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1220 | CLA | C6-C7-C8-C10 |
| 14 | A | 1103 | CLA | C14-C13-C15-C16 |
| 14 | B | 1023 | CLA | C11-C10-C8-C9 |
| 14 | B | 1204 | CLA | C11-C10-C8-C9 |
| 14 | B | 1215 | CLA | C14-C13-C15-C16 |
| 14 | G | 1103 | CLA | C14-C13-C15-C16 |
| 14 | H | 1023 | CLA | C11-C10-C8-C9 |
| 14 | H | 1204 | CLA | C11-C10-C8-C9 |
| 14 | H | 1215 | CLA | C14-C13-C15-C16 |
| 14 | e | 1103 | CLA | C14-C13-C15-C16 |
| 14 | f | 1023 | CLA | C11-C10-C8-C9 |
| 14 | f | 1204 | CLA | C11-C10-C8-C9 |
| 14 | f | 1215 | CLA | C14-C13-C15-C16 |
| 14 | 2 | 509 | CLA | O1A-CGA-O2A-C1 |
| 14 | Z | 509 | CLA | O1A-CGA-O2A-C1 |
| 14 | r | 509 | CLA | O1A-CGA-O2A-C1 |
| 14 | 1 | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1116 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1202 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 518 | CLA | CAA-CBA-CGA-O2A |
| 18 | A | 5008 | LHG | C9-C10-C11-C12 |
| 18 | G | 5008 | LHG | C9-C10-C11-C12 |
| 18 | e | 5005 | LHG | C30-C31-C32-C33 |
| 14 | 1 | 504 | CLA | O1D-CGD-O2D-CED |
| 18 | A | 5005 | LHG | C30-C31-C32-C33 |
| 18 | G | 5005 | LHG | C30-C31-C32-C33 |
| 18 | e | 5008 | LHG | C9-C10-C11-C12 |
| 14 | A | 1013 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1013 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1013 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1202 | CLA | C16-C17-C18-C20 |
| 14 | 6 | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1236 | CLA | O1A-CGA-O2A-C1 |
| 14 | H | 1236 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1236 | CLA | O1A-CGA-O2A-C1 |
| 17 | A | 4001 | BCR | C1-C6-C7-C8 |
| 17 | A | 4008 | BCR | C1-C6-C7-C8 |
| 17 | B | 4014 | BCR | C1-C6-C7-C8 |
| 17 | B | 4014 | BCR | C5-C6-C7-C8 |
| 17 | L | 4022 | BCR | C23-C24-C25-C30 |
| 17 | L | 4020 | BCR | C23-C24-C25-C30 |
| 17 | 4 | 523 | BCR | C1-C6-C7-C8 |
| 17 | 5 | 521 | BCR | C1-C6-C7-C8 |
| 17 | 6 | 524 | BCR | C1-C6-C7-C8 |
| 17 | G | 4001 | BCR | C1-C6-C7-C8 |
| 17 | G | 4008 | BCR | C1-C6-C7-C8 |
| 17 | H | 4014 | BCR | C1-C6-C7-C8 |
| 17 | V | 4022 | BCR | C23-C24-C25-C30 |
| 17 | V | 4020 | BCR | C23-C24-C25-C30 |
| 17 | b | 523 | BCR | C1-C6-C7-C8 |
| 17 | c | 521 | BCR | C1-C6-C7-C8 |
| 17 | d | 524 | BCR | C1-C6-C7-C8 |
| 17 | d | 524 | BCR | C23-C24-C25-C30 |
| 17 | e | 4001 | BCR | C1-C6-C7-C8 |
| 17 | e | 4008 | BCR | C1-C6-C7-C8 |
| 17 | f | 4014 | BCR | C1-C6-C7-C8 |
| 17 | f | 4014 | BCR | C5-C6-C7-C8 |
| 17 | n | 4022 | BCR | C23-C24-C25-C30 |
| 17 | n | 4020 | BCR | C23-C24-C25-C30 |
| 17 | t | 523 | BCR | C1-C6-C7-C8 |
| 17 | u | 521 | BCR | C1-C6-C7-C8 |
| 17 | v | 524 | BCR | C1-C6-C7-C8 |
| 14 | Y | 504 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1116 | CLA | CAA-CBA-CGA-O2A |
| 21 | 3 | 822 | SQD | O6-C44-C45-C46 |
| 21 | a | 822 | SQD | O6-C44-C45-C46 |
| 21 | s | 822 | SQD | O6-C44-C45-C46 |
| 18 | A | 5007 | LHG | O1-C1-C2-C3 |
| 18 | G | 5007 | LHG | O1-C1-C2-C3 |
| 18 | e | 5007 | LHG | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | B | 1228 | CLA | O1A-CGA-O2A-C1 |
| 17 | A | 4011 | BCR | C19-C20-C21-C22 |
| 17 | 1 | 522 | BCR | C15-C16-C17-C18 |
| 17 | 4 | 521 | BCR | C15-C16-C17-C18 |
| 17 | G | 4011 | BCR | C19-C20-C21-C22 |
| 17 | Y | 522 | BCR | C15-C16-C17-C18 |
| 17 | b | 521 | BCR | C15-C16-C17-C18 |
| 17 | e | 4011 | BCR | C19-C20-C21-C22 |
| 17 | q | 522 | BCR | C15-C16-C17-C18 |
| 17 | t | 521 | BCR | C15-C16-C17-C18 |
| 14 | A | 1106 | CLA | C4-C3-C5-C6 |
| 14 | G | 1106 | CLA | C4-C3-C5-C6 |
| 14 | e | 1106 | CLA | C4-C3-C5-C6 |
| 17 | B | 4010 | BCR | C11-C12-C13-C14 |
| 17 | J | 4015 | BCR | C7-C8-C9-C10 |
| 17 | 2 | 523 | BCR | C7-C8-C9-C10 |
| 17 | H | 4010 | BCR | C11-C12-C13-C14 |
| 17 | T | 4015 | BCR | C7-C8-C9-C10 |
| 17 | Z | 523 | BCR | C7-C8-C9-C10 |
| 17 | f | 4010 | BCR | C11-C12-C13-C14 |
| 17 | l | 4015 | BCR | C7-C8-C9-C10 |
| 17 | r | 523 | BCR | C7-C8-C9-C10 |
| 14 | A | 1107 | CLA | C2-C3-C5-C6 |
| 14 | B | 1202 | CLA | C2-C3-C5-C6 |
| 14 | G | 1107 | CLA | C2-C3-C5-C6 |
| 14 | H | 1202 | CLA | C2-C3-C5-C6 |
| 14 | e | 1107 | CLA | C2-C3-C5-C6 |
| 14 | f | 1202 | CLA | C2-C3-C5-C6 |
| 14 | 1 | 505 | CLA | CAA-CBA-CGA-O2A |
| 14 | 4 | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | 5 | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | b | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | c | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 505 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1201 | CLA | C8-C10-C11-C12 |
| 18 | A | 5001 | LHG | C19-C20-C21-C22 |
| 18 | e | 5001 | LHG | C19-C20-C21-C22 |
| 14 | B | 1201 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 1 | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 505 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1228 | CLA | O1A-CGA-O2A-C1 |
| 14 | f | 1228 | CLA | O1A-CGA-O2A-C1 |
| 18 | G | 5001 | LHG | C19-C20-C21-C22 |
| 14 | B | 1202 | CLA | C16-C17-C18-C20 |
| 14 | f | 1202 | CLA | C16-C17-C18-C20 |
| 18 | A | 5005 | LHG | C26-C27-C28-C29 |
| 18 | G | 5005 | LHG | C26-C27-C28-C29 |
| 18 | e | 5005 | LHG | C26-C27-C28-C29 |
| 14 | e | 1129 | CLA | O1D-CGD-O2D-CED |
| 14 | f | 1201 | CLA | C8-C10-C11-C12 |
| 18 | L | 5221 | LHG | C23-C24-C25-C26 |
| 18 | V | 5221 | LHG | C23-C24-C25-C26 |
| 18 | n | 5221 | LHG | C23-C24-C25-C26 |
| 14 | 5 | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 512 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 5002 | LMG | C38-C39-C40-C41 |
| 14 | G | 1126 | CLA | O1A-CGA-O2A-C1 |
| 20 | H | 5002 | LMG | C38-C39-C40-C41 |
| 20 | f | 5002 | LMG | C38-C39-C40-C41 |
| 14 | 2 | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | c | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1129 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1126 | CLA | O1A-CGA-O2A-C1 |
| 14 | e | 1126 | CLA | O1A-CGA-O2A-C1 |
| 14 | B | 1240 | CLA | C4-C3-C5-C6 |
| 14 | H | 1240 | CLA | C4-C3-C5-C6 |
| 14 | f | 1240 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1129 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1101 | CLA | C11-C10-C8-C7 |
| 14 | B | 1203 | CLA | C11-C10-C8-C7 |
| 14 | B | 1205 | CLA | C12-C13-C15-C16 |
| 14 | B | 1213 | CLA | C6-C7-C8-C10 |
| 14 | B | 1229 | CLA | C6-C7-C8-C10 |
| 14 | L | 1501 | CLA | C11-C10-C8-C7 |
| 14 | G | 1101 | CLA | C11-C10-C8-C7 |
| 14 | H | 1203 | CLA | C11-C10-C8-C7 |
| 14 | H | 1205 | CLA | C12-C13-C15-C16 |
| 14 | H | 1213 | CLA | C6-C7-C8-C10 |
| 14 | H | 1229 | CLA | C6-C7-C8-C10 |
| 14 | V | 1501 | CLA | C11-C10-C8-C7 |
| 14 | e | 1101 | CLA | C11-C10-C8-C7 |
| 14 | f | 1203 | CLA | C11-C10-C8-C7 |
| 14 | f | 1205 | CLA | C12-C13-C15-C16 |
| 14 | f | 1213 | CLA | C6-C7-C8-C10 |
| 14 | f | 1229 | CLA | C6-C7-C8-C10 |
| 14 | n | 1501 | CLA | C11-C10-C8-C7 |
| 14 | 2 | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 511 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 511 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | r | 510 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 511 | CLA | CAA-CBA-CGA-O2A |
| 21 | H | 1852 | SQD | C26-C27-C28-C29 |
| 21 | B | 1852 | SQD | C26-C27-C28-C29 |
| 17 | 6 | 521 | BCR | C9-C10-C11-C12 |
| 17 | d | 521 | BCR | C9-C10-C11-C12 |
| 17 | v | 521 | BCR | C9-C10-C11-C12 |
| 14 | 3 | 519 | CLA | CAA-CBA-CGA-O1A |
| 21 | f | 1852 | SQD | C26-C27-C28-C29 |
| 14 | 6 | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1203 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1203 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1203 | CLA | CAA-CBA-CGA-O2A |
| 14 | 1 | 508 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 508 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | q | 508 | CLA | C2A-CAA-CBA-CGA |
| 14 | 4 | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | b | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 509 | CLA | O1D-CGD-O2D-CED |
| 14 | A | 1013 | CLA | C4-C3-C5-C6 |
| 14 | A | 1126 | CLA | C4-C3-C5-C6 |
| 14 | A | 1127 | CLA | C4-C3-C5-C6 |
| 14 | G | 1013 | CLA | C4-C3-C5-C6 |
| 14 | G | 1126 | CLA | C4-C3-C5-C6 |
| 14 | G | 1127 | CLA | C4-C3-C5-C6 |
| 14 | e | 1013 | CLA | C4-C3-C5-C6 |
| 14 | e | 1126 | CLA | C4-C3-C5-C6 |
| 14 | e | 1127 | CLA | C4-C3-C5-C6 |
| 14 | 6 | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 505 | CLA | C2-C3-C5-C6 |
| 14 | a | 505 | CLA | C2-C3-C5-C6 |
| 14 | s | 505 | CLA | C2-C3-C5-C6 |
| 14 | H | 1228 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1123 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1138 | CLA | C11-C12-C13-C14 |
| 14 | B | 1227 | CLA | C6-C7-C8-C9 |
| 14 | B | 1235 | CLA | C6-C7-C8-C9 |
| 14 | 2 | 505 | CLA | C6-C7-C8-C9 |
| 14 | 2 | 505 | CLA | C14-C13-C15-C16 |
| 14 | G | 1138 | CLA | C11-C12-C13-C14 |
| 14 | H | 1227 | CLA | C6-C7-C8-C9 |
| 14 | H | 1235 | CLA | C6-C7-C8-C9 |
| 14 | Z | 505 | CLA | C6-C7-C8-C9 |
| 14 | Z | 505 | CLA | C14-C13-C15-C16 |
| 14 | e | 1138 | CLA | C11-C12-C13-C14 |
| 14 | f | 1227 | CLA | C6-C7-C8-C9 |
| 14 | f | 1235 | CLA | C6-C7-C8-C9 |
| 14 | r | 505 | CLA | C6-C7-C8-C9 |
| 14 | r | 505 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | L | 5218 | LHG | C9-C10-C11-C12 |
| 18 | V | 5218 | LHG | C9-C10-C11-C12 |
| 14 | 1 | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | 4 | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | b | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 519 | CLA | CAA-CBA-CGA-O2A |
| 18 | n | 5218 | LHG | C9-C10-C11-C12 |
| 14 | A | 1111 | CLA | C3A-C2A-CAA-CBA |
| 14 | 4 | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1111 | CLA | C3A-C2A-CAA-CBA |
| 14 | b | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1111 | CLA | C3A-C2A-CAA-CBA |
| 14 | t | 516 | CLA | C3A-C2A-CAA-CBA |
| 14 | 3 | 509 | CLA | O1D-CGD-O2D-CED |
| 20 | J | 5104 | LMG | O10-C28-O8-C9 |
| 20 | T | 5104 | LMG | O10-C28-O8-C9 |
| 20 | l | 5104 | LMG | O10-C28-O8-C9 |
| 14 | G | 1123 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1123 | CLA | CAA-CBA-CGA-O2A |
| 14 | 1 | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | 1 | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | 1 | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | 1 | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 504 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 512 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 507 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 504 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1109 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1114 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1129 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1138 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1210 | CLA | CAD-CBD-CGD-O2D |
| 14 | B | 1229 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 507 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | 1 | 519 | CLA | CAD-CBD-CGD-O2D |
| 14 | 2 | 501 | CLA | CAD-CBD-CGD-O2D |
| 14 | 2 | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | 2 | 508 | CLA | CAD-CBD-CGD-O2D |
| 14 | 3 | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | 4 | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | 4 | 510 | CLA | CAD-CBD-CGD-O2D |
| 14 | 5 | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | 5 | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | 5 | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | 6 | 501 | CLA | CAD-CBD-CGD-O2D |
| 14 | 6 | 504 | CLA | CAD-CBD-CGD-O2D |
| 14 | 6 | 507 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1109 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1114 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1129 | CLA | CAD-CBD-CGD-O2D |
| 14 | G | 1138 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1210 | CLA | CAD-CBD-CGD-O2D |
| 14 | H | 1229 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 507 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | Y | 519 | CLA | CAD-CBD-CGD-O2D |
| 14 | Z | 501 | CLA | CAD-CBD-CGD-O2D |
| 14 | Z | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | Z | 508 | CLA | CAD-CBD-CGD-O2D |
| 14 | a | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | b | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | b | 510 | CLA | CAD-CBD-CGD-O2D |
| 14 | c | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | c | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | c | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | d | 501 | CLA | CAD-CBD-CGD-O2D |
| 14 | d | 504 | CLA | CAD-CBD-CGD-O2D |
| 14 | d | 507 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1109 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1114 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1129 | CLA | CAD-CBD-CGD-O2D |
| 14 | e | 1138 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1210 | CLA | CAD-CBD-CGD-O2D |
| 14 | f | 1229 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 507 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | q | 519 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 501 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 508 | CLA | CAD-CBD-CGD-O2D |
| 14 | r | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | s | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | t | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | t | 510 | CLA | CAD-CBD-CGD-O2D |
| 14 | u | 502 | CLA | CAD-CBD-CGD-O2D |
| 14 | u | 505 | CLA | CAD-CBD-CGD-O2D |
| 14 | u | 509 | CLA | CAD-CBD-CGD-O2D |
| 14 | v | 501 | CLA | CAD-CBD-CGD-O2D |
| 14 | v | 504 | CLA | CAD-CBD-CGD-O2D |
| 14 | v | 507 | CLA | CAD-CBD-CGD-O2D |
| 14 | A | 1022 | CLA | C16-C17-C18-C19 |
| 14 | G | 1022 | CLA | C16-C17-C18-C19 |
| 14 | e | 1022 | CLA | C16-C17-C18-C19 |
| 14 | f | 1215 | CLA | C15-C16-C17-C18 |
| 14 | A | 1114 | CLA | CAA-CBA-CGA-O2A |
| 14 | 5 | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | c | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 504 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1114 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 513 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1206 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1206 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1206 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1228 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1228 | CLA | CBA-CGA-O2A-C1 |
| 14 | a | 509 | CLA | O1D-CGD-O2D-CED |
| 14 | 1 | 505 | CLA | CAA-CBA-CGA-O1A |
| 14 | 1 | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | 5 | 512 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1114 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 505 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 505 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1215 | CLA | C15-C16-C17-C18 |
| 14 | A | 1126 | CLA | C2-C3-C5-C6 |
| 14 | G | 1126 | CLA | C2-C3-C5-C6 |
| 14 | e | 1126 | CLA | C2-C3-C5-C6 |
| 18 | A | 5002 | LHG | O7-C7-C8-C9 |
| 18 | L | 5220 | LHG | O8-C23-C24-C25 |
| 18 | G | 5002 | LHG | O7-C7-C8-C9 |
| 18 | V | 5220 | LHG | O8-C23-C24-C25 |
| 18 | e | 5002 | LHG | O7-C7-C8-C9 |
| 17 | 1 | 524 | BCR | C11-C12-C13-C14 |
| 17 | 6 | 521 | BCR | C7-C8-C9-C10 |
| 17 | Y | 524 | BCR | C11-C12-C13-C14 |
| 17 | d | 521 | BCR | C7-C8-C9-C10 |
| 17 | v | 521 | BCR | C7-C8-C9-C10 |
| 18 | A | 5009 | LHG | C4-C5-C6-O8 |
| 18 | G | 5009 | LHG | C4-C5-C6-O8 |
| 18 | e | 5009 | LHG | C4-C5-C6-O8 |
| 14 | F | 1302 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | R | 1302 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | Z | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 511 | CLA | CAA-CBA-CGA-O1A |
| 14 | j | 1302 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | r | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | r | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 511 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5001 | LHG | O6-C4-C5-O7 |
| 18 | G | 5001 | LHG | O6-C4-C5-O7 |
| 18 | e | 5001 | LHG | O6-C4-C5-O7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1123 | CLA | C8-C10-C11-C12 |
| 14 | G | 1123 | CLA | C8-C10-C11-C12 |
| 14 | H | 1215 | CLA | C15-C16-C17-C18 |
| 18 | n | 5220 | LHG | O8-C23-C24-C25 |
| 20 | B | 5002 | LMG | O7-C10-C11-C12 |
| 20 | H | 5002 | LMG | O7-C10-C11-C12 |
| 20 | f | 5002 | LMG | O7-C10-C11-C12 |
| 21 | B | 1852 | SQD | O47-C7-C8-C9 |
| 21 | H | 1852 | SQD | O47-C7-C8-C9 |
| 21 | f | 1852 | SQD | O47-C7-C8-C9 |
| 14 | 1 | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | 2 | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | 5 | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | 5 | 517 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 511 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | Z | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | c | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | s | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | H | 1216 | CLA | C8-C10-C11-C12 |
| 14 | e | 1123 | CLA | C8-C10-C11-C12 |
| 14 | f | 1216 | CLA | C8-C10-C11-C12 |
| 14 | A | 1125 | CLA | O2A-C1-C2-C3 |
| 14 | G | 1125 | CLA | O2A-C1-C2-C3 |
| 14 | e | 1125 | CLA | O2A-C1-C2-C3 |
| 14 | J | 1302 | CLA | C2A-CAA-CBA-CGA |
| 14 | T | 1302 | CLA | C2A-CAA-CBA-CGA |
| 14 | l | 1302 | CLA | C2A-CAA-CBA-CGA |
| 14 | B | 1216 | CLA | C8-C10-C11-C12 |
| 14 | K | 1401 | CLA | CAA-CBA-CGA-O2A |
| 14 | U | 1401 | CLA | CAA-CBA-CGA-O2A |
| 14 | m | 1401 | CLA | CAA-CBA-CGA-O2A |
| 18 | A | 5001 | LHG | O8-C23-C24-C25 |
| 18 | G | 5001 | LHG | O8-C23-C24-C25 |
| 18 | e | 5001 | LHG | O8-C23-C24-C25 |
| 14 | 1 | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | 1 | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | 2 | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | 3 | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 506 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | 3 | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | Z | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | a | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | a | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 506 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | r | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | s | 501 | CLA | CAA-CBA-CGA-O1A |
| 14 | s | 506 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 507 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5006 | LHG | C10-C11-C12-C13 |
| 18 | e | 5006 | LHG | C10-C11-C12-C13 |
| 14 | A | 1011 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1106 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1106 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1111 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1112 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1112 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1123 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1127 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1127 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1128 | CLA | CHA-CBD-CGD-O1D |
| 14 | A | 1128 | CLA | CHA-CBD-CGD-O2D |
| 14 | A | 1134 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1201 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1212 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1222 | CLA | CHA-CBD-CGD-O1D |
| 14 | B | 1222 | CLA | CHA-CBD-CGD-O2D |
| 14 | B | 1235 | CLA | CHA-CBD-CGD-O2D |
| 14 | K | 1103 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | L | 1501 | CLA | CHA-CBD-CGD-O1D |
| 14 | L | 1501 | CLA | CHA-CBD-CGD-O2D |
| 14 | 1 | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | 1 | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | 2 | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | 2 | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | 3 | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | 3 | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | 4 | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 512 | CLA | CHA-CBD-CGD-O1D |
| 14 | 4 | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | 5 | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | 5 | 512 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 502 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 511 | CLA | CHA-CBD-CGD-O2D |
| 14 | 6 | 512 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | 6 | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1011 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1106 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1106 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1111 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1112 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1112 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1123 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1127 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1127 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1128 | CLA | CHA-CBD-CGD-O1D |
| 14 | G | 1128 | CLA | CHA-CBD-CGD-O2D |
| 14 | G | 1134 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1201 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1212 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | H | 1222 | CLA | CHA-CBD-CGD-O1D |
| 14 | H | 1222 | CLA | CHA-CBD-CGD-O2D |
| 14 | H | 1235 | CLA | CHA-CBD-CGD-O2D |
| 14 | U | 1103 | CLA | CHA-CBD-CGD-O2D |
| 14 | V | 1501 | CLA | CHA-CBD-CGD-O1D |
| 14 | V | 1501 | CLA | CHA-CBD-CGD-O2D |
| 14 | Y | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | Y | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | Z | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | Z | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | a | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | a | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | b | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 512 | CLA | CHA-CBD-CGD-O1D |
| 14 | b | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | c | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | c | 512 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 502 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 511 | CLA | CHA-CBD-CGD-O2D |
| 14 | d | 512 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | d | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1011 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1106 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1106 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1111 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1112 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1112 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1123 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1127 | CLA | CHA-CBD-CGD-O1D |
| 14 | e | 1127 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1128 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1128 | CLA | CHA-CBD-CGD-O2D |
| 14 | e | 1134 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1201 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1212 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1222 | CLA | CHA-CBD-CGD-O1D |
| 14 | f | 1222 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1223 | CLA | CHA-CBD-CGD-O2D |
| 14 | f | 1235 | CLA | CHA-CBD-CGD-O2D |
| 14 | m | 1103 | CLA | CHA-CBD-CGD-O2D |
| 14 | n | 1501 | CLA | CHA-CBD-CGD-O1D |
| 14 | n | 1501 | CLA | CHA-CBD-CGD-O2D |
| 14 | q | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 518 | CLA | CHA-CBD-CGD-O1D |
| 14 | q | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 504 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | r | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | r | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 506 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 517 | CLA | CHA-CBD-CGD-O1D |
| 14 | s | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 518 | CLA | CHA-CBD-CGD-O2D |
| 14 | s | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 503 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 503 | CLA | CHA-CBD-CGD-O2D |
| 14 | t | 506 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 512 | CLA | CHA-CBD-CGD-O1D |
| 14 | t | 517 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 507 | CLA | CHA-CBD-CGD-O1D |
| 14 | u | 507 | CLA | CHA-CBD-CGD-O2D |
| 14 | u | 512 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 502 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 511 | CLA | CHA-CBD-CGD-O2D |
| 14 | v | 512 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 516 | CLA | CHA-CBD-CGD-O1D |
| 14 | v | 519 | CLA | CHA-CBD-CGD-O1D |
| 14 | F | 1302 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | 5 | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | R | 1302 | CLA | CAA-CBA-CGA-O1A |
| 14 | Z | 516 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | b | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 504 | CLA | CAA-CBA-CGA-O1A |
| 14 | j | 1302 | CLA | CAA-CBA-CGA-O1A |
| 14 | r | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | s | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 507 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 504 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1106 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1108 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1120 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1137 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1106 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1120 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1106 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1108 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1120 | CLA | CAA-CBA-CGA-O2A |
| 18 | G | 5006 | LHG | C10-C11-C12-C13 |
| 18 | A | 5003 | LHG | O6-C4-C5-C6 |
| 18 | G | 5003 | LHG | O6-C4-C5-C6 |
| 18 | e | 5003 | LHG | O6-C4-C5-C6 |
| 14 | 2 | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | 5 | 513 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 504 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | t | 509 | CLA | CAA-CBA-CGA-O2A |
| 14 | u | 513 | CLA | CAA-CBA-CGA-O1A |
| 19 | G | 1848 | LMU | C7-C8-C9-C10 |
| 14 | G | 1108 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1137 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1221 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1137 | CLA | CAA-CBA-CGA-O2A |
| 18 | A | 5006 | LHG | O8-C23-C24-C25 |
| 18 | G | 5006 | LHG | O8-C23-C24-C25 |
| 18 | e | 5006 | LHG | O8-C23-C24-C25 |
| 19 | e | 1848 | LMU | C7-C8-C9-C10 |
| 20 | J | 5104 | LMG | O1-C7-C8-O7 |
| 20 | T | 5104 | LMG | O1-C7-C8-O7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 20 | l | 5104 | LMG | O1-C7-C8-O7 |
| 21 | 4 | 822 | SQD | O6-C44-C45-O47 |
| 21 | b | 822 | SQD | O6-C44-C45-O47 |
| 21 | t | 822 | SQD | O6-C44-C45-O47 |
| 19 | A | 1848 | LMU | C7-C8-C9-C10 |
| 14 | 5 | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | 6 | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 508 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1107 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1135 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1237 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1221 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1107 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1135 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1237 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1107 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1135 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1237 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1221 | CLA | CAA-CBA-CGA-O2A |
| 14 | l | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | l | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | d | 512 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 519 | CLA | CAA-CBA-CGA-O2A |
| 14 | v | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | 4 | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 516 | CLA | CAA-CBA-CGA-O1A |
| 18 | B | 1855 | LHG | C16-C17-C18-C19 |
| 18 | f | 1855 | LHG | C16-C17-C18-C19 |
| 14 | A | 1013 | CLA | C12-C13-C15-C16 |
| 14 | A | 1126 | CLA | C12-C13-C15-C16 |
| 14 | A | 1136 | CLA | C12-C13-C15-C16 |
| 14 | A | 1137 | CLA | C6-C7-C8-C10 |
| 14 | A | 1237 | CLA | C6-C7-C8-C10 |
| 14 | B | 1204 | CLA | C11-C10-C8-C7 |
| 14 | 6 | 505 | CLA | C11-C12-C13-C15 |
| 14 | G | 1013 | CLA | C12-C13-C15-C16 |
| 14 | G | 1126 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1136 | CLA | C12-C13-C15-C16 |
| 14 | G | 1137 | CLA | C6-C7-C8-C10 |
| 14 | G | 1237 | CLA | C6-C7-C8-C10 |
| 14 | H | 1204 | CLA | C11-C10-C8-C7 |
| 14 | d | 505 | CLA | C11-C12-C13-C15 |
| 14 | e | 1013 | CLA | C12-C13-C15-C16 |
| 14 | e | 1126 | CLA | C12-C13-C15-C16 |
| 14 | e | 1136 | CLA | C12-C13-C15-C16 |
| 14 | e | 1137 | CLA | C6-C7-C8-C10 |
| 14 | e | 1237 | CLA | C6-C7-C8-C10 |
| 14 | f | 1204 | CLA | C11-C10-C8-C7 |
| 14 | v | 505 | CLA | C11-C12-C13-C15 |
| 18 | H | 1855 | LHG | C16-C17-C18-C19 |
| 14 | r | 505 | CLA | C13-C15-C16-C17 |
| 18 | B | 1842 | LHG | O8-C23-C24-C25 |
| 18 | H | 1842 | LHG | O8-C23-C24-C25 |
| 18 | f | 1842 | LHG | O8-C23-C24-C25 |
| 14 | b | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | d | 516 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1109 | CLA | C6-C7-C8-C9 |
| 14 | B | 1207 | CLA | C11-C12-C13-C14 |
| 14 | 6 | 505 | CLA | C11-C12-C13-C14 |
| 14 | H | 1207 | CLA | C11-C12-C13-C14 |
| 14 | d | 505 | CLA | C11-C12-C13-C14 |
| 14 | e | 1109 | CLA | C6-C7-C8-C9 |
| 14 | f | 1207 | CLA | C11-C12-C13-C14 |
| 14 | v | 505 | CLA | C11-C12-C13-C14 |
| 21 | 3 | 822 | SQD | O48-C23-C24-C25 |
| 21 | a | 822 | SQD | O48-C23-C24-C25 |
| 21 | s | 822 | SQD | O48-C23-C24-C25 |
| 14 | 2 | 505 | CLA | C13-C15-C16-C17 |
| 14 | Z | 505 | CLA | C13-C15-C16-C17 |
| 18 | G | 5007 | LHG | O9-C7-C8-C9 |
| 18 | A | 5006 | LHG | C31-C32-C33-C34 |
| 18 | L | 5218 | LHG | C33-C34-C35-C36 |
| 18 | V | 5218 | LHG | C33-C34-C35-C36 |
| 18 | e | 5006 | LHG | C31-C32-C33-C34 |
| 18 | n | 5218 | LHG | C33-C34-C35-C36 |
| 14 | 1 | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1117 | CLA | C2A-CAA-CBA-CGA |
| 14 | 1 | 502 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1117 | CLA | C2A-CAA-CBA-CGA |
| 14 | Y | 502 | CLA | C2A-CAA-CBA-CGA |
| 14 | e | 1117 | CLA | C2A-CAA-CBA-CGA |
| 14 | q | 502 | CLA | C2A-CAA-CBA-CGA |
| 18 | A | 5007 | LHG | O9-C7-C8-C9 |
| 18 | e | 5007 | LHG | O9-C7-C8-C9 |
| 18 | G | 5006 | LHG | C31-C32-C33-C34 |
| 14 | Y | 517 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1206 | CLA | CAA-CBA-CGA-O1A |
| 14 | H | 1206 | CLA | CAA-CBA-CGA-O1A |
| 14 | f | 1206 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1220 | CLA | C6-C7-C8-C9 |
| 14 | H | 1220 | CLA | C6-C7-C8-C9 |
| 14 | f | 1220 | CLA | C6-C7-C8-C9 |
| 21 | B | 1852 | SQD | O48-C23-C24-C25 |
| 21 | H | 1852 | SQD | O48-C23-C24-C25 |
| 21 | f | 1852 | SQD | O48-C23-C24-C25 |
| 14 | 3 | 506 | CLA | CAA-CBA-CGA-O1A |
| 14 | a | 506 | CLA | CAA-CBA-CGA-O1A |
| 14 | s | 506 | CLA | CAA-CBA-CGA-O1A |
| 17 | q | 524 | BCR | C11-C12-C13-C14 |
| 18 | A | 5001 | LHG | C28-C29-C30-C31 |
| 18 | G | 5001 | LHG | C28-C29-C30-C31 |
| 14 | B | 1204 | CLA | CBA-CGA-O2A-C1 |
| 14 | H | 1204 | CLA | CBA-CGA-O2A-C1 |
| 14 | f | 1204 | CLA | CBA-CGA-O2A-C1 |
| 14 | A | 1107 | CLA | C8-C10-C11-C12 |
| 14 | G | 1107 | CLA | C8-C10-C11-C12 |
| 14 | e | 1107 | CLA | C8-C10-C11-C12 |
| 14 | A | 1105 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1012 | CLA | C1A-C2A-CAA-CBA |
| 14 | B | 1223 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 507 | CLA | C1A-C2A-CAA-CBA |
| 14 | 2 | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | 3 | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | 4 | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | 5 | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | 6 | 519 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | G | 1105 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1012 | CLA | C1A-C2A-CAA-CBA |
| 14 | H | 1223 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 507 | CLA | C1A-C2A-CAA-CBA |
| 14 | Z | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | a | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | b | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | c | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | d | 519 | CLA | C1A-C2A-CAA-CBA |
| 14 | e | 1105 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1012 | CLA | C1A-C2A-CAA-CBA |
| 14 | f | 1223 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 507 | CLA | C1A-C2A-CAA-CBA |
| 14 | r | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 504 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 512 | CLA | C1A-C2A-CAA-CBA |
| 14 | s | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | t | 506 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 511 | CLA | C1A-C2A-CAA-CBA |
| 14 | u | 517 | CLA | C1A-C2A-CAA-CBA |
| 14 | v | 519 | CLA | C1A-C2A-CAA-CBA |
| 18 | e | 5001 | LHG | C28-C29-C30-C31 |
| 14 | G | 1123 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1123 | CLA | CAA-CBA-CGA-O1A |
| 14 | f | 1023 | CLA | C8-C10-C11-C12 |
| 14 | n | 1502 | CLA | C8-C10-C11-C12 |
| 14 | 2 | 518 | CLA | C2-C1-O2A-CGA |
| 14 | Z | 518 | CLA | C2-C1-O2A-CGA |
| 14 | r | 518 | CLA | C2-C1-O2A-CGA |
| 14 | B | 1023 | CLA | C8-C10-C11-C12 |
| 14 | L | 1502 | CLA | C8-C10-C11-C12 |
| 14 | A | 1123 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5007 | LHG | C17-C18-C19-C20 |
| 17 | B | 4009 | BCR | C19-C20-C21-C22 |
| 21 | 6 | 822 | SQD | O6-C44-C45-C46 |
| 21 | d | 822 | SQD | O6-C44-C45-C46 |
| 21 | v | 822 | SQD | O6-C44-C45-C46 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | G | 5007 | LHG | C17-C18-C19-C20 |
| 14 | H | 1023 | CLA | C8-C10-C11-C12 |
| 14 | V | 1502 | CLA | C8-C10-C11-C12 |
| 14 | f | 1023 | CLA | C13-C15-C16-C17 |
| 18 | e | 5007 | LHG | C17-C18-C19-C20 |
| 14 | H | 1203 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5003 | LHG | O9-C7-C8-C9 |
| 18 | G | 5003 | LHG | O9-C7-C8-C9 |
| 18 | e | 5006 | LHG | O10-C23-C24-C25 |
| 18 | e | 5003 | LHG | O9-C7-C8-C9 |
| 14 | H | 1023 | CLA | C13-C15-C16-C17 |
| 14 | 1 | 519 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5008 | LHG | O7-C7-C8-C9 |
| 18 | G | 5008 | LHG | O7-C7-C8-C9 |
| 18 | e | 5008 | LHG | O7-C7-C8-C9 |
| 14 | A | 1011 | CLA | C8-C10-C11-C12 |
| 14 | B | 1023 | CLA | C13-C15-C16-C17 |
| 14 | e | 1138 | CLA | C15-C16-C17-C18 |
| 14 | B | 1203 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1221 | CLA | CAA-CBA-CGA-O1A |
| 14 | H | 1221 | CLA | CAA-CBA-CGA-O1A |
| 14 | f | 1203 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5006 | LHG | O10-C23-C24-C25 |
| 18 | G | 5006 | LHG | O10-C23-C24-C25 |
| 14 | H | 1204 | CLA | O1A-CGA-O2A-C1 |
| 14 | 5 | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | Y | 519 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | c | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | t | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | u | 508 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1011 | CLA | C8-C10-C11-C12 |
| 14 | e | 1011 | CLA | C8-C10-C11-C12 |
| 18 | A | 5002 | LHG | C3-O3-P-O5 |
| 18 | A | 5006 | LHG | C3-O3-P-O5 |
| 18 | A | 5007 | LHG | C3-O3-P-O5 |
| 18 | A | 5009 | LHG | C4-O6-P-O5 |
| 18 | A | 5001 | LHG | C3-O3-P-O5 |
| 18 | A | 5003 | LHG | C3-O3-P-O5 |
| 18 | B | 1842 | LHG | C4-O6-P-O5 |
| 18 | I | 5001 | LHG | C4-O6-P-O4 |
| 18 | I | 5001 | LHG | C4-O6-P-O5 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | G | 5002 | LHG | C3-O3-P-O5 |
| 18 | G | 5006 | LHG | C3-O3-P-O5 |
| 18 | G | 5007 | LHG | C3-O3-P-O5 |
| 18 | G | 5009 | LHG | C4-O6-P-O5 |
| 18 | G | 5001 | LHG | C3-O3-P-O5 |
| 18 | G | 5003 | LHG | C3-O3-P-O5 |
| 18 | H | 1842 | LHG | C4-O6-P-O5 |
| 18 | S | 5001 | LHG | C4-O6-P-O4 |
| 18 | S | 5001 | LHG | C4-O6-P-O5 |
| 18 | e | 5002 | LHG | C3-O3-P-O5 |
| 18 | e | 5006 | LHG | C3-O3-P-O5 |
| 18 | e | 5007 | LHG | C3-O3-P-O5 |
| 18 | e | 5009 | LHG | C4-O6-P-O5 |
| 18 | e | 5001 | LHG | C3-O3-P-O5 |
| 18 | e | 5003 | LHG | C3-O3-P-O5 |
| 18 | f | 1842 | LHG | C4-O6-P-O5 |
| 18 | k | 5001 | LHG | C4-O6-P-O4 |
| 18 | k | 5001 | LHG | C4-O6-P-O5 |
| 14 | A | 1108 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1120 | CLA | CAA-CBA-CGA-O1A |
| 14 | K | 1401 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1120 | CLA | CAA-CBA-CGA-O1A |
| 14 | U | 1401 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1108 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1120 | CLA | CAA-CBA-CGA-O1A |
| 14 | f | 1221 | CLA | CAA-CBA-CGA-O1A |
| 14 | m | 1401 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5007 | LHG | O7-C7-C8-C9 |
| 18 | G | 5007 | LHG | O7-C7-C8-C9 |
| 18 | e | 5007 | LHG | O7-C7-C8-C9 |
| 20 | J | 5104 | LMG | O6-C1-O1-C7 |
| 20 | T | 5104 | LMG | O6-C1-O1-C7 |
| 20 | l | 5104 | LMG | O6-C1-O1-C7 |
| 14 | A | 1138 | CLA | C15-C16-C17-C18 |
| 14 | f | 1204 | CLA | O1A-CGA-O2A-C1 |
| 14 | 4 | 509 | CLA | CAA-CBA-CGA-O1A |
| 14 | q | 519 | CLA | CAA-CBA-CGA-O1A |
| 17 | A | 4008 | BCR | C5-C6-C7-C8 |
| 17 | 6 | 524 | BCR | C23-C24-C25-C30 |
| 17 | G | 4008 | BCR | C5-C6-C7-C8 |
| 17 | H | 4014 | BCR | C5-C6-C7-C8 |
| 17 | e | 4008 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | v | 524 | BCR | C23-C24-C25-C30 |
| 14 | A | 1123 | CLA | C10-C11-C12-C13 |
| 14 | B | 1021 | CLA | C13-C15-C16-C17 |
| 14 | G | 1123 | CLA | C10-C11-C12-C13 |
| 14 | G | 1138 | CLA | C15-C16-C17-C18 |
| 14 | H | 1021 | CLA | C13-C15-C16-C17 |
| 14 | e | 1123 | CLA | C10-C11-C12-C13 |
| 14 | f | 1021 | CLA | C13-C15-C16-C17 |
| 14 | G | 1108 | CLA | CAA-CBA-CGA-O1A |
| 14 | B | 1204 | CLA | O1A-CGA-O2A-C1 |
| 14 | v | 508 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 5002 | LMG | O8-C28-C29-C30 |
| 20 | H | 5002 | LMG | O8-C28-C29-C30 |
| 21 | L | 5216 | SQD | O47-C7-C8-C9 |
| 21 | V | 5216 | SQD | O47-C7-C8-C9 |
| 21 | n | 5216 | SQD | O47-C7-C8-C9 |
| 14 | d | 518 | CLA | CAA-CBA-CGA-O1A |
| 14 | v | 518 | CLA | CAA-CBA-CGA-O1A |
| 14 | L | 1501 | CLA | C11-C12-C13-C14 |
| 14 | V | 1501 | CLA | C11-C12-C13-C14 |
| 14 | n | 1501 | CLA | C11-C12-C13-C14 |
| 18 | I | 5001 | LHG | C26-C27-C28-C29 |
| 18 | e | 5006 | LHG | C33-C34-C35-C36 |
| 14 | A | 1106 | CLA | CAA-CBA-CGA-O1A |
| 14 | A | 1237 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1237 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1237 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 5002 | LMG | O10-C28-C29-C30 |
| 20 | H | 5002 | LMG | O10-C28-C29-C30 |
| 20 | f | 5002 | LMG | O10-C28-C29-C30 |
| 18 | A | 5006 | LHG | C33-C34-C35-C36 |
| 18 | k | 5001 | LHG | C26-C27-C28-C29 |
| 18 | G | 5006 | LHG | C33-C34-C35-C36 |
| 18 | S | 5001 | LHG | C26-C27-C28-C29 |
| 14 | A | 1114 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1114 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1114 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5006 | LHG | O7-C7-C8-C9 |
| 18 | G | 5006 | LHG | O7-C7-C8-C9 |
| 20 | f | 5002 | LMG | O8-C28-C29-C30 |
| 14 | 6 | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | G | 1106 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1106 | CLA | CAA-CBA-CGA-O1A |
| 17 | H | 4009 | BCR | C19-C20-C21-C22 |
| 17 | f | 4009 | BCR | C19-C20-C21-C22 |
| 14 | d | 508 | CLA | O1D-CGD-O2D-CED |
| 14 | 4 | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | 6 | 518 | CLA | CAA-CBA-CGA-O1A |
| 14 | b | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1011 | CLA | CAD-CBD-CGD-O1D |
| 14 | A | 1132 | CLA | CAD-CBD-CGD-O1D |
| 14 | A | 1135 | CLA | CAD-CBD-CGD-O1D |
| 14 | B | 1210 | CLA | CAD-CBD-CGD-O1D |
| 14 | B | 1212 | CLA | CAD-CBD-CGD-O1D |
| 14 | L | 1501 | CLA | CAD-CBD-CGD-O1D |
| 14 | 1 | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | 4 | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | 6 | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | 6 | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1011 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1132 | CLA | CAD-CBD-CGD-O1D |
| 14 | G | 1135 | CLA | CAD-CBD-CGD-O1D |
| 14 | H | 1210 | CLA | CAD-CBD-CGD-O1D |
| 14 | H | 1212 | CLA | CAD-CBD-CGD-O1D |
| 14 | V | 1501 | CLA | CAD-CBD-CGD-O1D |
| 14 | Y | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | b | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 511 | CLA | CAD-CBD-CGD-O1D |
| 14 | d | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1011 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1132 | CLA | CAD-CBD-CGD-O1D |
| 14 | e | 1135 | CLA | CAD-CBD-CGD-O1D |
| 14 | f | 1210 | CLA | CAD-CBD-CGD-O1D |
| 14 | f | 1212 | CLA | CAD-CBD-CGD-O1D |
| 14 | n | 1501 | CLA | CAD-CBD-CGD-O1D |
| 14 | q | 517 | CLA | CAD-CBD-CGD-O1D |
| 14 | t | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | v | 504 | CLA | CAD-CBD-CGD-O1D |
| 14 | v | 516 | CLA | CAD-CBD-CGD-O1D |
| 14 | A | 1103 | CLA | CAA-CBA-CGA-O2A |
| 14 | 2 | 501 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1103 | CLA | CAA-CBA-CGA-O2A |
| 14 | Z | 501 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1103 | CLA | CAA-CBA-CGA-O2A |
| 14 | r | 501 | CLA | CAA-CBA-CGA-O2A |
| 18 | e | 5006 | LHG | O7-C7-C8-C9 |
| 18 | f | 1855 | LHG | O7-C7-C8-C9 |
| 14 | B | 1229 | CLA | C10-C11-C12-C13 |
| 14 | H | 1229 | CLA | C10-C11-C12-C13 |
| 14 | f | 1229 | CLA | C10-C11-C12-C13 |
| 14 | A | 1013 | CLA | C11-C12-C13-C14 |
| 14 | A | 1111 | CLA | C14-C13-C15-C16 |
| 14 | A | 1119 | CLA | C14-C13-C15-C16 |
| 14 | A | 1136 | CLA | C11-C10-C8-C9 |
| 14 | A | 1136 | CLA | C14-C13-C15-C16 |
| 14 | G | 1013 | CLA | C11-C12-C13-C14 |
| 14 | G | 1109 | CLA | C6-C7-C8-C9 |
| 14 | G | 1111 | CLA | C14-C13-C15-C16 |
| 14 | G | 1136 | CLA | C11-C10-C8-C9 |
| 14 | G | 1136 | CLA | C14-C13-C15-C16 |
| 14 | e | 1013 | CLA | C11-C12-C13-C14 |
| 14 | e | 1111 | CLA | C14-C13-C15-C16 |
| 14 | e | 1119 | CLA | C14-C13-C15-C16 |
| 14 | e | 1136 | CLA | C11-C10-C8-C9 |
| 14 | e | 1136 | CLA | C14-C13-C15-C16 |
| 14 | t | 516 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1135 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1135 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1135 | CLA | CAA-CBA-CGA-O1A |
| 18 | B | 1855 | LHG | O7-C7-C8-C9 |
| 18 | H | 1855 | LHG | O7-C7-C8-C9 |
| 14 | A | 1110 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1111 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1115 | CLA | CAA-CBA-CGA-O2A |
| 14 | B | 1213 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1110 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1111 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1115 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1110 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1111 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1115 | CLA | CAA-CBA-CGA-O2A |
| 14 | f | 1213 | CLA | CAA-CBA-CGA-O2A |
| 14 | l | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | Y | 518 | CLA | CAA-CBA-CGA-O2A |
| 14 | q | 518 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | A | 1118 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1119 | CLA | C12-C13-C15-C16 |
| 14 | A | 1125 | CLA | C11-C12-C13-C15 |
| 14 | B | 1201 | CLA | C6-C7-C8-C10 |
| 14 | B | 1215 | CLA | C11-C12-C13-C15 |
| 14 | B | 1215 | CLA | C12-C13-C15-C16 |
| 14 | B | 1229 | CLA | C11-C10-C8-C7 |
| 14 | B | 1207 | CLA | C11-C12-C13-C15 |
| 14 | B | 1230 | CLA | C11-C10-C8-C7 |
| 14 | 5 | 518 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1118 | CLA | C3A-C2A-CAA-CBA |
| 14 | G | 1119 | CLA | C12-C13-C15-C16 |
| 14 | G | 1125 | CLA | C11-C12-C13-C15 |
| 14 | H | 1201 | CLA | C6-C7-C8-C10 |
| 14 | H | 1215 | CLA | C11-C12-C13-C15 |
| 14 | H | 1215 | CLA | C12-C13-C15-C16 |
| 14 | H | 1207 | CLA | C11-C12-C13-C15 |
| 14 | H | 1230 | CLA | C11-C10-C8-C7 |
| 14 | c | 518 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1118 | CLA | C3A-C2A-CAA-CBA |
| 14 | e | 1119 | CLA | C12-C13-C15-C16 |
| 14 | e | 1125 | CLA | C11-C12-C13-C15 |
| 14 | f | 1201 | CLA | C6-C7-C8-C10 |
| 14 | f | 1215 | CLA | C11-C12-C13-C15 |
| 14 | f | 1215 | CLA | C12-C13-C15-C16 |
| 14 | f | 1207 | CLA | C11-C12-C13-C15 |
| 14 | f | 1230 | CLA | C11-C10-C8-C7 |
| 14 | u | 518 | CLA | C3A-C2A-CAA-CBA |
| 14 | A | 1107 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1107 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1137 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1137 | CLA | CAA-CBA-CGA-O1A |
| 18 | A | 5007 | LHG | O10-C23-C24-C25 |
| 18 | G | 5007 | LHG | O10-C23-C24-C25 |
| 18 | e | 5007 | LHG | O10-C23-C24-C25 |
| 14 | A | 1013 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1013 | CLA | CAA-CBA-CGA-O2A |
| 14 | H | 1213 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 509 | CLA | CBD-CGD-O2D-CED |
| 18 | e | 5009 | LHG | C12-C13-C14-C15 |
| 17 | A | 4011 | BCR | C7-C8-C9-C10 |
| 17 | 1 | 521 | BCR | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 17 | G | 4011 | BCR | C7-C8-C9-C10 |
| 17 | Y | 521 | BCR | C17-C18-C19-C20 |
| 17 | e | 4011 | BCR | C7-C8-C9-C10 |
| 17 | q | 521 | BCR | C17-C18-C19-C20 |
| 14 | A | 1137 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1107 | CLA | CAA-CBA-CGA-O1A |
| 17 | 2 | 522 | BCR | C15-C16-C17-C18 |
| 17 | 2 | 524 | BCR | C9-C10-C11-C12 |
| 17 | 5 | 521 | BCR | C9-C10-C11-C12 |
| 17 | Z | 522 | BCR | C15-C16-C17-C18 |
| 17 | Z | 524 | BCR | C9-C10-C11-C12 |
| 17 | c | 521 | BCR | C9-C10-C11-C12 |
| 17 | r | 522 | BCR | C15-C16-C17-C18 |
| 17 | r | 524 | BCR | C9-C10-C11-C12 |
| 17 | u | 521 | BCR | C9-C10-C11-C12 |
| 18 | A | 5009 | LHG | C12-C13-C14-C15 |
| 18 | G | 5009 | LHG | C12-C13-C14-C15 |
| 19 | A | 1849 | LMU | C2-C1-O1'-C1' |
| 19 | G | 1849 | LMU | C2-C1-O1'-C1' |
| 19 | e | 1849 | LMU | C2-C1-O1'-C1' |
| 14 | A | 1111 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1111 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1111 | CLA | CAA-CBA-CGA-O1A |
| 14 | e | 1125 | CLA | CAA-CBA-CGA-O1A |
| 20 | J | 5104 | LMG | O10-C28-C29-C30 |
| 20 | l | 5104 | LMG | O10-C28-C29-C30 |
| 14 | 3 | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | a | 509 | CLA | CBD-CGD-O2D-CED |
| 14 | A | 1125 | CLA | CAA-CBA-CGA-O2A |
| 14 | G | 1125 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1013 | CLA | CAA-CBA-CGA-O2A |
| 14 | e | 1125 | CLA | CAA-CBA-CGA-O2A |
| 14 | A | 1125 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1125 | CLA | CAA-CBA-CGA-O1A |
| 14 | 2 | 504 | CLA | C2A-CAA-CBA-CGA |
| 14 | 3 | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | Z | 504 | CLA | C2A-CAA-CBA-CGA |
| 14 | a | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | r | 504 | CLA | C2A-CAA-CBA-CGA |
| 14 | s | 513 | CLA | C2A-CAA-CBA-CGA |
| 14 | G | 1105 | CLA | C5-C6-C7-C8 |
| 14 | G | 1237 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 14 | e | 1237 | CLA | C13-C15-C16-C17 |
| 14 | A | 1115 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1013 | CLA | CAA-CBA-CGA-O1A |
| 14 | G | 1115 | CLA | CAA-CBA-CGA-O1A |
| 20 | T | 5104 | LMG | O10-C28-C29-C30 |
| 14 | A | 1131 | CLA | C4-C3-C5-C6 |
| 14 | G | 1131 | CLA | C4-C3-C5-C6 |
| 14 | e | 1131 | CLA | C4-C3-C5-C6 |
| 14 | K | 1105 | CLA | CAA-CBA-CGA-O2A |
| 14 | 3 | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | U | 1105 | CLA | CAA-CBA-CGA-O2A |
| 14 | a | 510 | CLA | CAA-CBA-CGA-O1A |
| 14 | m | 1105 | CLA | CAA-CBA-CGA-O2A |
| 14 | s | 510 | CLA | CAA-CBA-CGA-O1A |

There are no ring outliers.

402 monomers are involved in 1033 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | B | 1203 | CLA | 2 | 0 |
| 14 | B | 1219 | CLA | 3 | 0 |
| 14 | A | 1011 | CLA | 4 | 0 |
| 14 | 6 | 502 | CLA | 2 | 0 |
| 14 | G | 1136 | CLA | 4 | 0 |
| 14 | Z | 501 | CLA | 2 | 0 |
| 17 | 3 | 522 | BCR | 1 | 0 |
| 14 | H | 1206 | CLA | 5 | 0 |
| 17 | 2 | 522 | BCR | 2 | 0 |
| 14 | B | 1225 | CLA | 4 | 0 |
| 14 | A | 1126 | CLA | 9 | 0 |
| 14 | 6 | 513 | CLA | 3 | 0 |
| 14 | 3 | 511 | CLA | 1 | 0 |
| 14 | Y | 511 | CLA | 1 | 0 |
| 14 | G | 1140 | CLA | 3 | 0 |
| 14 | B | 1216 | CLA | 5 | 0 |
| 14 | 4 | 512 | CLA | 2 | 0 |
| 17 | Z | 522 | BCR | 2 | 0 |
| 14 | A | 1108 | CLA | 2 | 0 |
| 14 | G | 1137 | CLA | 5 | 0 |
| 14 | 3 | 517 | CLA | 1 | 0 |
| 14 | H | 1219 | CLA | 3 | 0 |
| 14 | G | 1118 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | G | 1122 | CLA | 3 | 0 |
| 14 | Z | 503 | CLA | 3 | 0 |
| 22 | X | 170 | FMN | 1 | 0 |
| 14 | H | 1214 | CLA | 3 | 0 |
| 14 | 3 | 505 | CLA | 2 | 0 |
| 14 | 1 | 511 | CLA | 1 | 0 |
| 17 | 3 | 521 | BCR | 1 | 0 |
| 14 | 2 | 506 | CLA | 2 | 0 |
| 14 | 1 | 510 | CLA | 1 | 0 |
| 17 | H | 4004 | BCR | 5 | 0 |
| 14 | 2 | 512 | CLA | 5 | 0 |
| 14 | A | 1134 | CLA | 3 | 0 |
| 14 | A | 1131 | CLA | 3 | 0 |
| 14 | 4 | 511 | CLA | 3 | 0 |
| 17 | 6 | 524 | BCR | 4 | 0 |
| 14 | G | 1237 | CLA | 8 | 0 |
| 17 | B | 4004 | BCR | 3 | 0 |
| 14 | 2 | 502 | CLA | 3 | 0 |
| 17 | Z | 523 | BCR | 2 | 0 |
| 15 | A | 2001 | PQN | 4 | 0 |
| 14 | 4 | 508 | CLA | 1 | 0 |
| 14 | B | 1230 | CLA | 2 | 0 |
| 14 | 6 | 510 | CLA | 2 | 0 |
| 14 | G | 1128 | CLA | 7 | 0 |
| 14 | B | 1012 | CLA | 5 | 0 |
| 14 | G | 1123 | CLA | 3 | 0 |
| 15 | H | 2002 | PQN | 5 | 0 |
| 14 | H | 1215 | CLA | 4 | 0 |
| 14 | B | 1220 | CLA | 3 | 0 |
| 18 | V | 5220 | LHG | 4 | 0 |
| 14 | A | 1109 | CLA | 2 | 0 |
| 14 | 2 | 513 | CLA | 2 | 0 |
| 14 | 5 | 506 | CLA | 4 | 0 |
| 17 | 3 | 523 | BCR | 2 | 0 |
| 14 | H | 1225 | CLA | 4 | 0 |
| 18 | G | 5004 | LHG | 2 | 0 |
| 20 | T | 5104 | LMG | 1 | 0 |
| 14 | B | 1202 | CLA | 2 | 0 |
| 19 | G | 1849 | LMU | 1 | 0 |
| 17 | T | 4015 | BCR | 5 | 0 |
| 15 | B | 2002 | PQN | 4 | 0 |
| 14 | 2 | 511 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | 5 | 512 | CLA | 4 | 0 |
| 14 | H | 1222 | CLA | 2 | 0 |
| 14 | B | 1214 | CLA | 3 | 0 |
| 17 | A | 4002 | BCR | 5 | 0 |
| 14 | R | 1301 | CLA | 1 | 0 |
| 14 | B | 1023 | CLA | 2 | 0 |
| 19 | G | 1848 | LMU | 2 | 0 |
| 14 | 5 | 502 | CLA | 2 | 0 |
| 17 | Z | 521 | BCR | 7 | 0 |
| 14 | 4 | 509 | CLA | 4 | 0 |
| 17 | G | 4003 | BCR | 3 | 0 |
| 17 | R | 4016 | BCR | 6 | 0 |
| 14 | B | 1229 | CLA | 8 | 0 |
| 14 | B | 1226 | CLA | 5 | 0 |
| 15 | G | 2001 | PQN | 3 | 0 |
| 17 | G | 4008 | BCR | 4 | 0 |
| 14 | 5 | 513 | CLA | 2 | 0 |
| 14 | Y | 509 | CLA | 2 | 0 |
| 17 | K | 4104 | BCR | 3 | 0 |
| 18 | A | 5003 | LHG | 2 | 0 |
| 14 | K | 1401 | CLA | 1 | 0 |
| 18 | A | 5004 | LHG | 3 | 0 |
| 14 | 5 | 511 | CLA | 2 | 0 |
| 14 | 2 | 505 | CLA | 5 | 0 |
| 14 | B | 1215 | CLA | 3 | 0 |
| 21 | 1 | 822 | SQD | 1 | 0 |
| 14 | 2 | 510 | CLA | 2 | 0 |
| 14 | B | 1238 | CLA | 1 | 0 |
| 14 | G | 1139 | CLA | 1 | 0 |
| 17 | Y | 523 | BCR | 1 | 0 |
| 14 | H | 1210 | CLA | 9 | 0 |
| 17 | 2 | 523 | BCR | 2 | 0 |
| 17 | L | 4219 | BCR | 6 | 0 |
| 21 | B | 1852 | SQD | 8 | 0 |
| 14 | 4 | 517 | CLA | 1 | 0 |
| 14 | 2 | 519 | CLA | 1 | 0 |
| 14 | B | 1231 | CLA | 3 | 0 |
| 18 | H | 1855 | LHG | 3 | 0 |
| 14 | 3 | 504 | CLA | 1 | 0 |
| 17 | J | 4015 | BCR | 6 | 0 |
| 14 | G | 1106 | CLA | 6 | 0 |
| 17 | B | 4010 | BCR | 6 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | A | 1127 | CLA | 1 | 0 |
| 14 | V | 1501 | CLA | 8 | 0 |
| 14 | H | 1205 | CLA | 3 | 0 |
| 17 | 1 | 524 | BCR | 6 | 0 |
| 14 | Y | 518 | CLA | 1 | 0 |
| 18 | G | 5008 | LHG | 8 | 0 |
| 21 | 3 | 822 | SQD | 2 | 0 |
| 14 | Y | 519 | CLA | 1 | 0 |
| 14 | A | 1111 | CLA | 2 | 0 |
| 14 | B | 1234 | CLA | 6 | 0 |
| 14 | G | 1133 | CLA | 2 | 0 |
| 17 | 4 | 523 | BCR | 2 | 0 |
| 14 | H | 1227 | CLA | 4 | 0 |
| 14 | Z | 506 | CLA | 2 | 0 |
| 14 | 2 | 518 | CLA | 2 | 0 |
| 14 | 5 | 510 | CLA | 2 | 0 |
| 14 | H | 1230 | CLA | 3 | 0 |
| 17 | A | 4001 | BCR | 4 | 0 |
| 14 | H | 1229 | CLA | 6 | 0 |
| 14 | A | 1128 | CLA | 7 | 0 |
| 14 | H | 1203 | CLA | 2 | 0 |
| 14 | A | 1114 | CLA | 1 | 0 |
| 14 | 1 | 518 | CLA | 1 | 0 |
| 17 | S | 4018 | BCR | 3 | 0 |
| 14 | G | 1130 | CLA | 5 | 0 |
| 18 | A | 5007 | LHG | 2 | 0 |
| 14 | 1 | 513 | CLA | 2 | 0 |
| 14 | H | 1208 | CLA | 5 | 0 |
| 14 | A | 1105 | CLA | 2 | 0 |
| 18 | G | 5001 | LHG | 5 | 0 |
| 14 | Z | 512 | CLA | 6 | 0 |
| 14 | 1 | 507 | CLA | 1 | 0 |
| 17 | 4 | 522 | BCR | 1 | 0 |
| 14 | J | 1302 | CLA | 1 | 0 |
| 17 | T | 4012 | BCR | 4 | 0 |
| 14 | 3 | 512 | CLA | 5 | 0 |
| 14 | B | 1205 | CLA | 3 | 0 |
| 14 | G | 1111 | CLA | 2 | 0 |
| 14 | 4 | 516 | CLA | 2 | 0 |
| 14 | G | 1132 | CLA | 1 | 0 |
| 14 | A | 1140 | CLA | 3 | 0 |
| 18 | H | 1842 | LHG | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 17 | L | 4019 | BCR | 4 | 0 |
| 14 | Z | 513 | CLA | 2 | 0 |
| 14 | B | 1222 | CLA | 1 | 0 |
| 17 | L | 4020 | BCR | 2 | 0 |
| 14 | 3 | 502 | CLA | 5 | 0 |
| 14 | A | 1137 | CLA | 5 | 0 |
| 14 | B | 1223 | CLA | 4 | 0 |
| 18 | A | 5005 | LHG | 7 | 0 |
| 17 | H | 4017 | BCR | 3 | 0 |
| 14 | A | 1118 | CLA | 2 | 0 |
| 14 | H | 1231 | CLA | 3 | 0 |
| 17 | H | 4006 | BCR | 4 | 0 |
| 17 | H | 4009 | BCR | 2 | 0 |
| 14 | H | 1224 | CLA | 4 | 0 |
| 18 | B | 1855 | LHG | 3 | 0 |
| 14 | 3 | 513 | CLA | 2 | 0 |
| 14 | A | 1135 | CLA | 2 | 0 |
| 14 | H | 1023 | CLA | 4 | 0 |
| 14 | A | 1112 | CLA | 1 | 0 |
| 14 | A | 1013 | CLA | 9 | 0 |
| 17 | V | 4020 | BCR | 2 | 0 |
| 17 | Y | 521 | BCR | 6 | 0 |
| 17 | B | 4009 | BCR | 3 | 0 |
| 14 | B | 1224 | CLA | 4 | 0 |
| 14 | B | 1209 | CLA | 2 | 0 |
| 17 | G | 4011 | BCR | 5 | 0 |
| 14 | G | 1013 | CLA | 8 | 0 |
| 18 | L | 5220 | LHG | 4 | 0 |
| 14 | H | 1236 | CLA | 5 | 0 |
| 14 | V | 1502 | CLA | 4 | 0 |
| 18 | I | 5001 | LHG | 2 | 0 |
| 14 | G | 1112 | CLA | 1 | 0 |
| 14 | A | 1237 | CLA | 8 | 0 |
| 17 | 5 | 521 | BCR | 3 | 0 |
| 14 | B | 1236 | CLA | 4 | 0 |
| 14 | A | 1801 | CLA | 3 | 0 |
| 14 | A | 1122 | CLA | 2 | 0 |
| 14 | Y | 502 | CLA | 2 | 0 |
| 14 | U | 1401 | CLA | 1 | 0 |
| 14 | H | 1218 | CLA | 3 | 0 |
| 14 | H | 1228 | CLA | 1 | 0 |
| 14 | Z | 519 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | Y | 507 | CLA | 1 | 0 |
| 14 | H | 1226 | CLA | 5 | 0 |
| 14 | 1 | 509 | CLA | 2 | 0 |
| 14 | 6 | 518 | CLA | 1 | 0 |
| 17 | B | 4017 | BCR | 4 | 0 |
| 14 | B | 1206 | CLA | 4 | 0 |
| 14 | 2 | 503 | CLA | 3 | 0 |
| 14 | G | 1126 | CLA | 10 | 0 |
| 19 | A | 1849 | LMU | 1 | 0 |
| 14 | B | 1218 | CLA | 3 | 0 |
| 18 | A | 5002 | LHG | 1 | 0 |
| 17 | 2 | 521 | BCR | 7 | 0 |
| 14 | Y | 513 | CLA | 2 | 0 |
| 14 | 3 | 510 | CLA | 3 | 0 |
| 14 | A | 1120 | CLA | 2 | 0 |
| 14 | A | 1139 | CLA | 3 | 0 |
| 22 | P | 170 | FMN | 1 | 0 |
| 19 | A | 1848 | LMU | 2 | 0 |
| 14 | 6 | 517 | CLA | 2 | 0 |
| 17 | 1 | 522 | BCR | 2 | 0 |
| 17 | 1 | 523 | BCR | 2 | 0 |
| 14 | 6 | 509 | CLA | 1 | 0 |
| 14 | A | 1107 | CLA | 2 | 0 |
| 17 | V | 4019 | BCR | 4 | 0 |
| 17 | J | 4012 | BCR | 4 | 0 |
| 17 | Y | 524 | BCR | 6 | 0 |
| 18 | G | 5009 | LHG | 3 | 0 |
| 14 | A | 1117 | CLA | 5 | 0 |
| 14 | H | 1216 | CLA | 6 | 0 |
| 17 | 5 | 522 | BCR | 2 | 0 |
| 14 | Z | 517 | CLA | 1 | 0 |
| 14 | F | 1302 | CLA | 3 | 0 |
| 14 | U | 1105 | CLA | 2 | 0 |
| 14 | G | 1119 | CLA | 9 | 0 |
| 14 | Z | 509 | CLA | 3 | 0 |
| 17 | A | 4008 | BCR | 6 | 0 |
| 17 | 1 | 521 | BCR | 6 | 0 |
| 14 | H | 1221 | CLA | 9 | 0 |
| 21 | H | 1852 | SQD | 9 | 0 |
| 14 | G | 1102 | CLA | 1 | 0 |
| 17 | 2 | 524 | BCR | 5 | 0 |
| 14 | B | 1240 | CLA | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | 5 | 509 | CLA | 2 | 0 |
| 14 | 5 | 507 | CLA | 1 | 0 |
| 14 | 4 | 502 | CLA | 4 | 0 |
| 17 | H | 4010 | BCR | 7 | 0 |
| 14 | Y | 510 | CLA | 1 | 0 |
| 14 | G | 1127 | CLA | 1 | 0 |
| 17 | H | 4014 | BCR | 5 | 0 |
| 14 | H | 1204 | CLA | 4 | 0 |
| 14 | H | 1217 | CLA | 1 | 0 |
| 14 | H | 1201 | CLA | 3 | 0 |
| 14 | K | 1105 | CLA | 2 | 0 |
| 17 | T | 4013 | BCR | 6 | 0 |
| 17 | M | 4021 | BCR | 2 | 0 |
| 14 | G | 1107 | CLA | 2 | 0 |
| 18 | B | 1842 | LHG | 3 | 0 |
| 17 | B | 4014 | BCR | 7 | 0 |
| 14 | B | 1204 | CLA | 5 | 0 |
| 14 | B | 1217 | CLA | 2 | 0 |
| 14 | H | 1239 | CLA | 5 | 0 |
| 14 | H | 1234 | CLA | 7 | 0 |
| 17 | 5 | 523 | BCR | 2 | 0 |
| 14 | G | 1131 | CLA | 3 | 0 |
| 14 | Z | 518 | CLA | 2 | 0 |
| 14 | A | 1133 | CLA | 2 | 0 |
| 14 | A | 1136 | CLA | 3 | 0 |
| 17 | V | 4022 | BCR | 8 | 0 |
| 18 | L | 5218 | LHG | 2 | 0 |
| 21 | V | 5216 | SQD | 6 | 0 |
| 14 | B | 1221 | CLA | 9 | 0 |
| 14 | A | 1116 | CLA | 5 | 0 |
| 14 | G | 1011 | CLA | 5 | 0 |
| 14 | G | 1801 | CLA | 3 | 0 |
| 17 | B | 4005 | BCR | 4 | 0 |
| 14 | G | 1108 | CLA | 2 | 0 |
| 18 | G | 5005 | LHG | 6 | 0 |
| 14 | Y | 504 | CLA | 1 | 0 |
| 14 | A | 1022 | CLA | 2 | 0 |
| 17 | V | 4219 | BCR | 8 | 0 |
| 21 | L | 5216 | SQD | 4 | 0 |
| 14 | G | 1134 | CLA | 2 | 0 |
| 14 | B | 1201 | CLA | 3 | 0 |
| 14 | G | 1114 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | G | 1101 | CLA | 5 | 0 |
| 14 | 3 | 503 | CLA | 1 | 0 |
| 18 | G | 5006 | LHG | 4 | 0 |
| 14 | Y | 516 | CLA | 6 | 0 |
| 14 | G | 1022 | CLA | 2 | 0 |
| 14 | G | 1113 | CLA | 1 | 0 |
| 14 | 6 | 505 | CLA | 5 | 0 |
| 14 | A | 1124 | CLA | 3 | 0 |
| 14 | 1 | 504 | CLA | 1 | 0 |
| 17 | J | 4013 | BCR | 6 | 0 |
| 14 | Y | 512 | CLA | 4 | 0 |
| 14 | B | 1239 | CLA | 5 | 0 |
| 18 | V | 5221 | LHG | 8 | 0 |
| 19 | H | 1843 | LMU | 1 | 0 |
| 14 | 3 | 509 | CLA | 1 | 0 |
| 14 | A | 1101 | CLA | 5 | 0 |
| 14 | H | 1202 | CLA | 3 | 0 |
| 14 | H | 1209 | CLA | 2 | 0 |
| 14 | 2 | 501 | CLA | 2 | 0 |
| 14 | A | 1113 | CLA | 1 | 0 |
| 17 | Z | 524 | BCR | 5 | 0 |
| 14 | 1 | 516 | CLA | 6 | 0 |
| 18 | G | 5002 | LHG | 1 | 0 |
| 14 | 1 | 512 | CLA | 4 | 0 |
| 18 | A | 5008 | LHG | 7 | 0 |
| 14 | B | 1208 | CLA | 6 | 0 |
| 14 | A | 1110 | CLA | 2 | 0 |
| 14 | B | 1228 | CLA | 2 | 0 |
| 17 | G | 4002 | BCR | 2 | 0 |
| 14 | Z | 505 | CLA | 5 | 0 |
| 14 | L | 1503 | CLA | 1 | 0 |
| 17 | 3 | 524 | BCR | 1 | 0 |
| 14 | 2 | 517 | CLA | 1 | 0 |
| 14 | G | 1109 | CLA | 2 | 0 |
| 14 | 6 | 512 | CLA | 4 | 0 |
| 14 | B | 1212 | CLA | 1 | 0 |
| 18 | A | 5006 | LHG | 4 | 0 |
| 17 | W | 4021 | BCR | 3 | 0 |
| 18 | V | 5218 | LHG | 2 | 0 |
| 14 | Z | 510 | CLA | 2 | 0 |
| 17 | L | 4022 | BCR | 6 | 0 |
| 14 | G | 1117 | CLA | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | H | 1207 | CLA | 3 | 0 |
| 14 | 1 | 502 | CLA | 2 | 0 |
| 14 | 4 | 503 | CLA | 1 | 0 |
| 14 | G | 1104 | CLA | 6 | 0 |
| 17 | U | 4104 | BCR | 3 | 0 |
| 14 | R | 1302 | CLA | 3 | 0 |
| 17 | B | 4006 | BCR | 4 | 0 |
| 14 | G | 1124 | CLA | 3 | 0 |
| 14 | 6 | 511 | CLA | 3 | 0 |
| 17 | 6 | 522 | BCR | 4 | 0 |
| 14 | 4 | 513 | CLA | 2 | 0 |
| 14 | H | 1012 | CLA | 4 | 0 |
| 14 | H | 1212 | CLA | 1 | 0 |
| 20 | H | 5002 | LMG | 6 | 0 |
| 14 | A | 1130 | CLA | 4 | 0 |
| 17 | 4 | 521 | BCR | 2 | 0 |
| 14 | A | 1104 | CLA | 6 | 0 |
| 14 | T | 1302 | CLA | 1 | 0 |
| 14 | H | 1238 | CLA | 1 | 0 |
| 14 | A | 1103 | CLA | 5 | 0 |
| 14 | H | 1021 | CLA | 4 | 0 |
| 14 | B | 1210 | CLA | 9 | 0 |
| 14 | G | 1110 | CLA | 1 | 0 |
| 14 | V | 1503 | CLA | 2 | 0 |
| 18 | G | 5003 | LHG | 2 | 0 |
| 14 | A | 1125 | CLA | 3 | 0 |
| 14 | F | 1301 | CLA | 1 | 0 |
| 14 | H | 1240 | CLA | 3 | 0 |
| 19 | B | 1843 | LMU | 1 | 0 |
| 17 | F | 4016 | BCR | 6 | 0 |
| 14 | G | 1135 | CLA | 2 | 0 |
| 14 | G | 1129 | CLA | 6 | 0 |
| 17 | A | 4003 | BCR | 1 | 0 |
| 14 | H | 1235 | CLA | 4 | 0 |
| 14 | Z | 502 | CLA | 3 | 0 |
| 14 | G | 1120 | CLA | 2 | 0 |
| 14 | Y | 505 | CLA | 7 | 0 |
| 14 | 3 | 518 | CLA | 1 | 0 |
| 14 | B | 1021 | CLA | 3 | 0 |
| 18 | L | 5221 | LHG | 1 | 0 |
| 14 | A | 1119 | CLA | 7 | 0 |
| 14 | L | 1502 | CLA | 4 | 0 |

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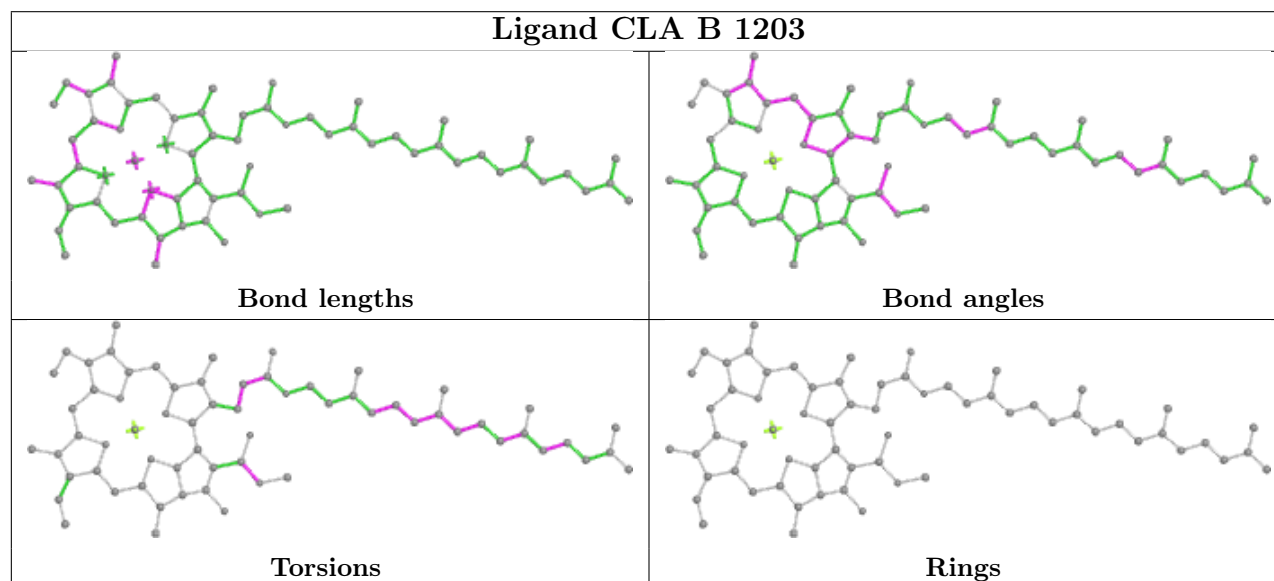
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18 | A | 5009 | LHG | 3 | 0 |
| 14 | J | 1303 | CLA | 3 | 0 |
| 14 | A | 1115 | CLA | 2 | 0 |
| 14 | L | 1501 | CLA | 5 | 0 |
| 17 | A | 4007 | BCR | 2 | 0 |
| 17 | G | 4007 | BCR | 3 | 0 |
| 14 | H | 1223 | CLA | 4 | 0 |
| 14 | B | 1207 | CLA | 10 | 0 |
| 14 | Z | 511 | CLA | 2 | 0 |
| 17 | 6 | 523 | BCR | 4 | 0 |
| 18 | G | 5007 | LHG | 2 | 0 |
| 14 | H | 1220 | CLA | 3 | 0 |
| 17 | 4 | 524 | BCR | 2 | 0 |
| 14 | B | 1227 | CLA | 4 | 0 |
| 14 | 1 | 505 | CLA | 5 | 0 |
| 14 | 6 | 519 | CLA | 1 | 0 |
| 14 | B | 1211 | CLA | 1 | 0 |
| 14 | A | 1121 | CLA | 4 | 0 |
| 14 | G | 1103 | CLA | 5 | 0 |
| 14 | A | 1102 | CLA | 2 | 0 |
| 17 | I | 4018 | BCR | 4 | 0 |
| 14 | T | 1303 | CLA | 3 | 0 |
| 14 | G | 1121 | CLA | 4 | 0 |
| 14 | A | 1106 | CLA | 6 | 0 |
| 21 | Y | 822 | SQD | 1 | 0 |
| 20 | B | 5002 | LMG | 5 | 0 |
| 14 | 5 | 505 | CLA | 1 | 0 |
| 17 | G | 4001 | BCR | 3 | 0 |
| 14 | 6 | 506 | CLA | 2 | 0 |
| 14 | G | 1115 | CLA | 3 | 0 |
| 17 | H | 4005 | BCR | 3 | 0 |
| 14 | 4 | 510 | CLA | 3 | 0 |
| 14 | A | 1129 | CLA | 6 | 0 |
| 14 | A | 1132 | CLA | 1 | 0 |
| 14 | G | 1125 | CLA | 3 | 0 |
| 14 | B | 1235 | CLA | 4 | 0 |
| 14 | A | 1123 | CLA | 1 | 0 |
| 14 | G | 1105 | CLA | 2 | 0 |
| 14 | G | 1116 | CLA | 7 | 0 |
| 17 | A | 4011 | BCR | 4 | 0 |
| 14 | 4 | 507 | CLA | 1 | 0 |
| 14 | 2 | 509 | CLA | 3 | 0 |

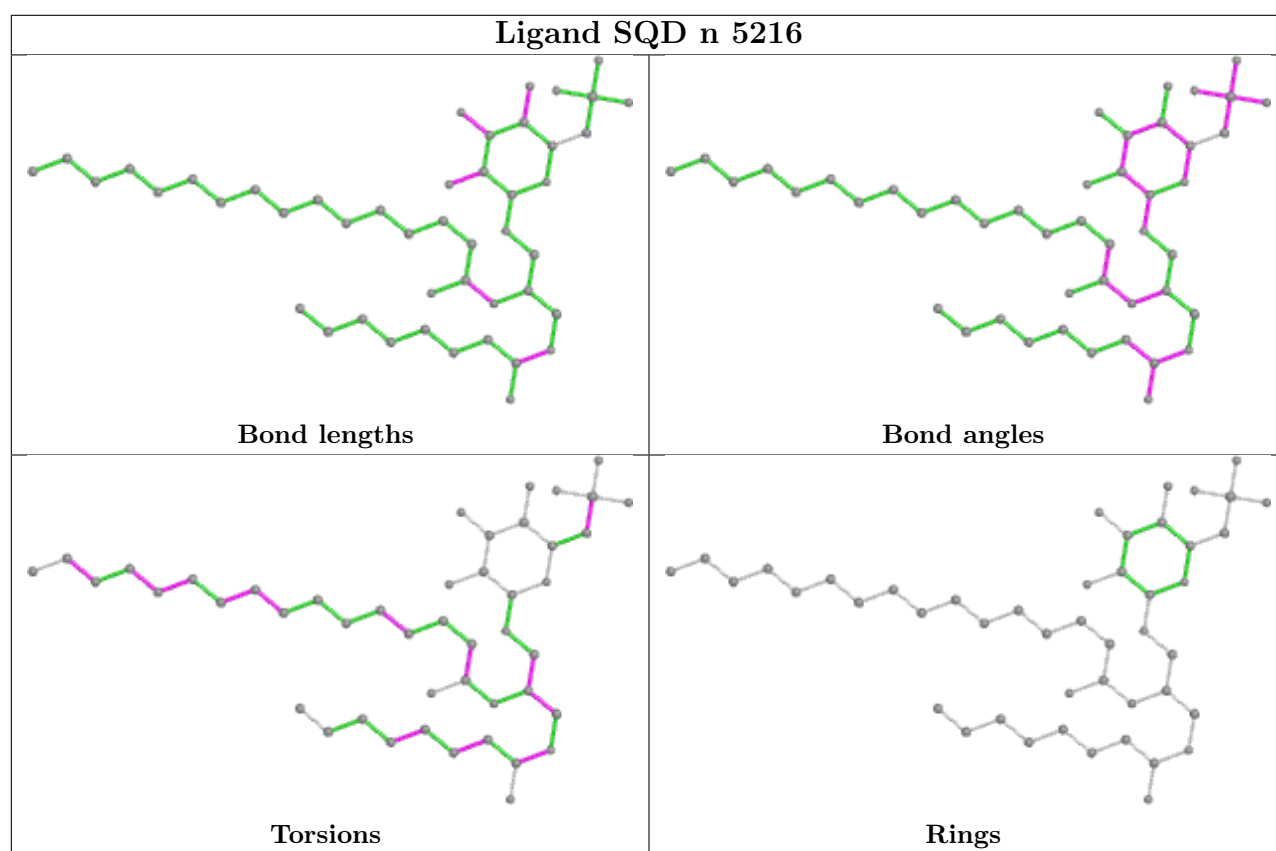
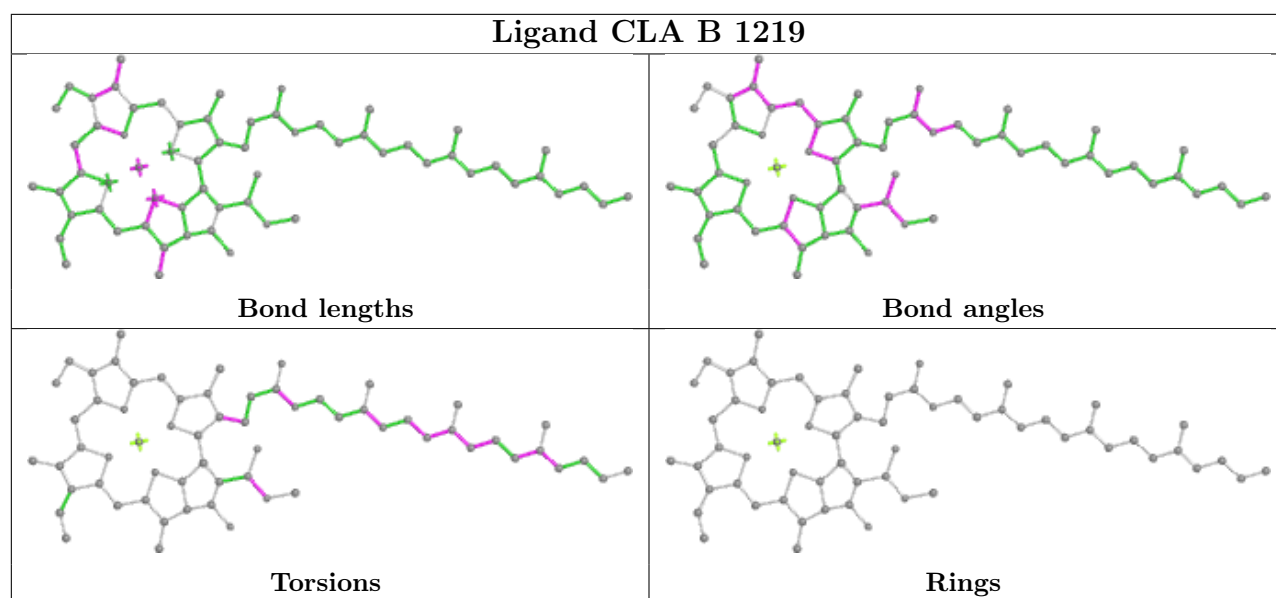
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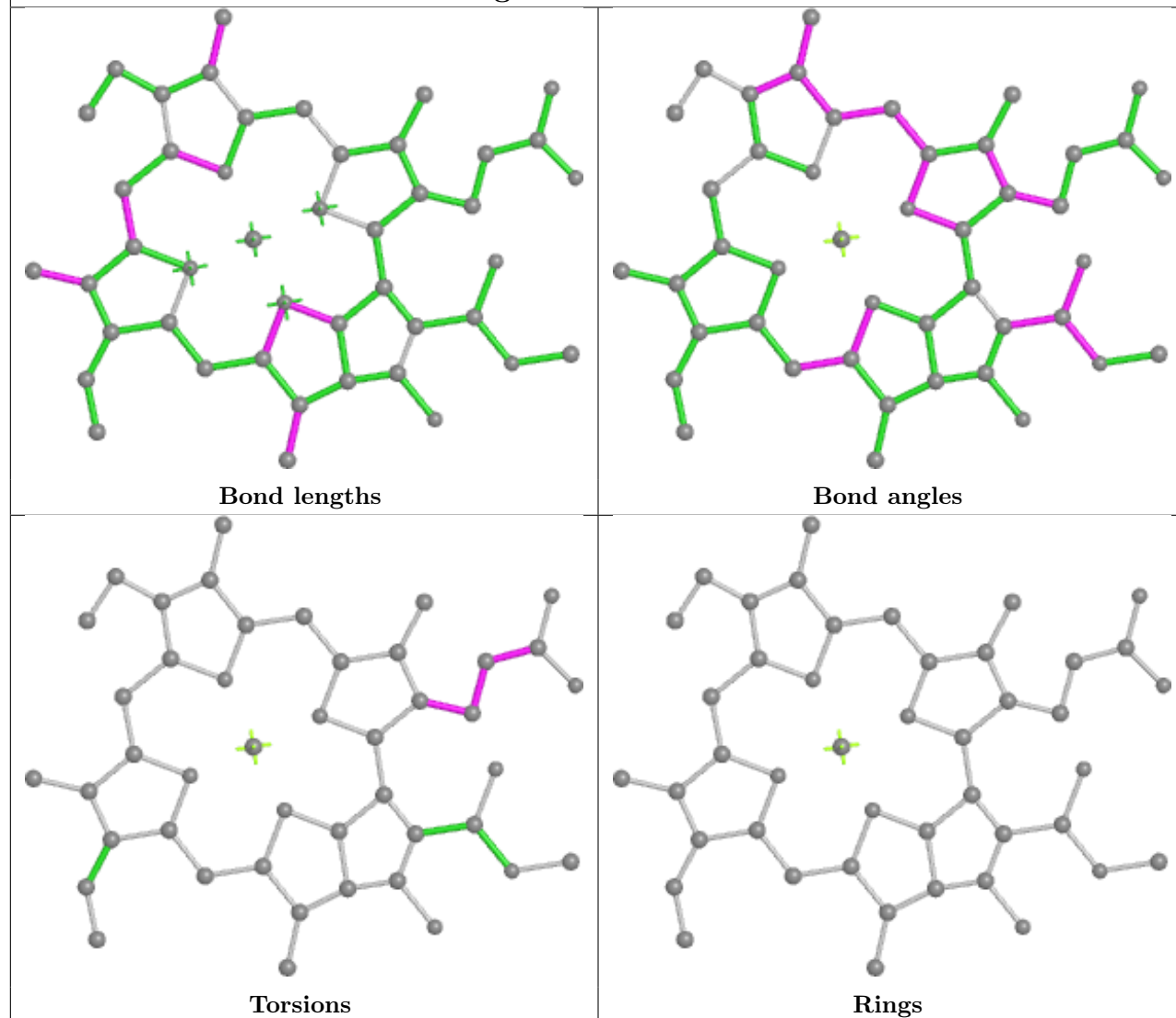
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18 | A | 5001 | LHG | 5 | 0 |

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

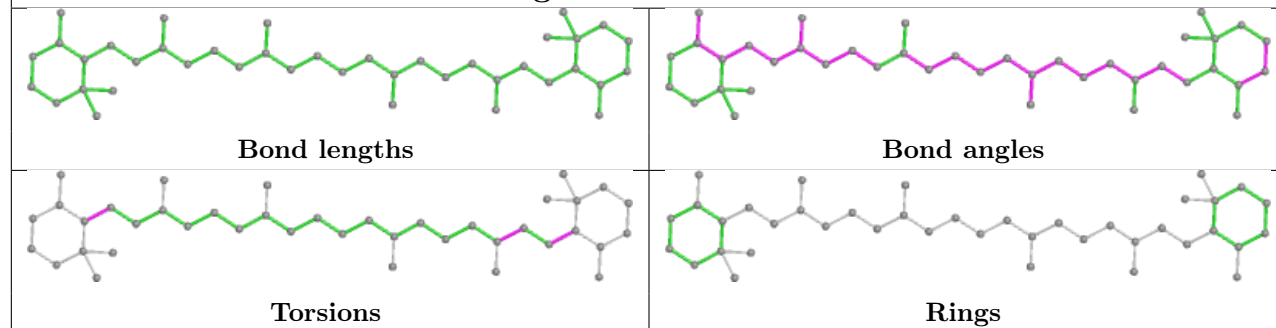


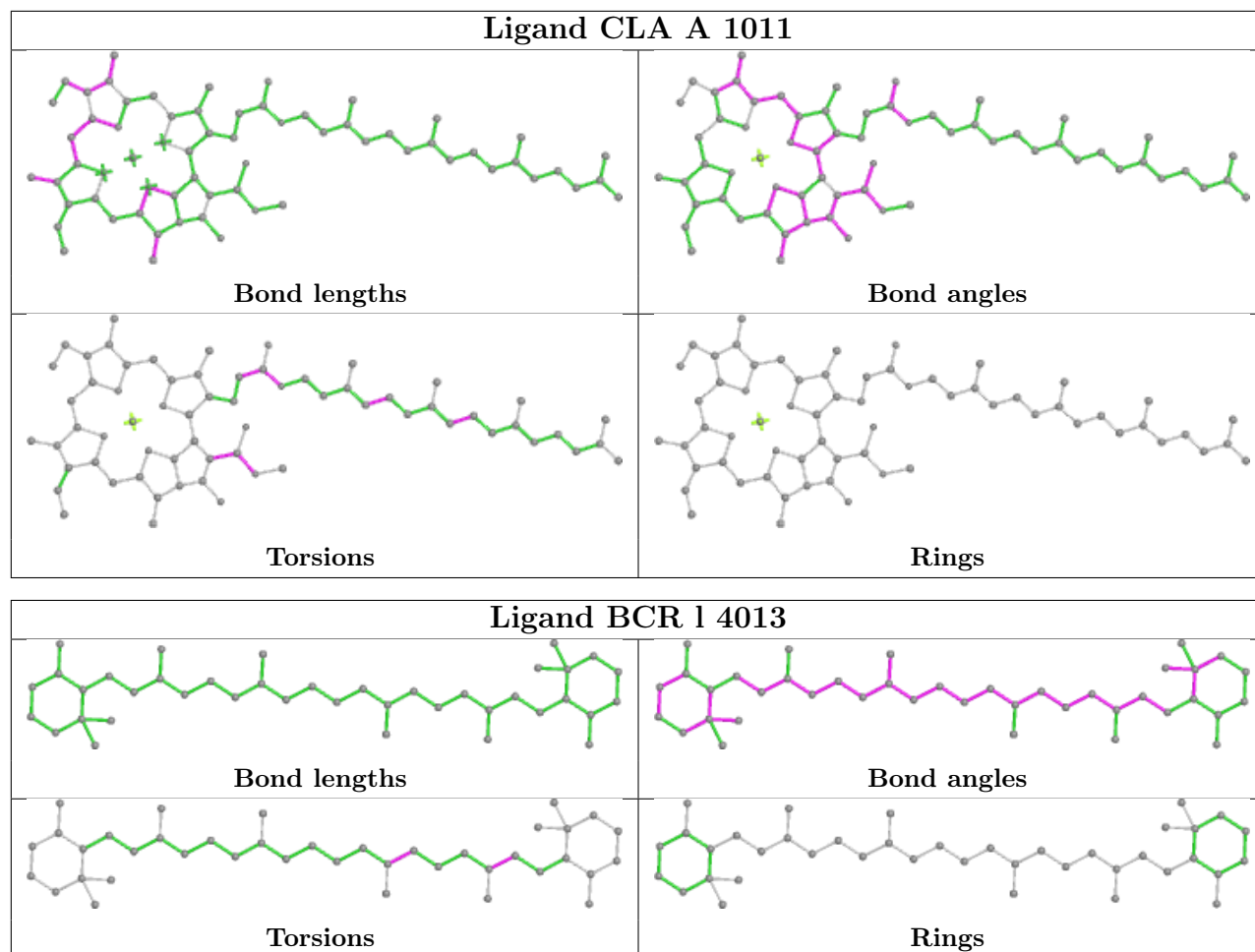


Ligand CLA 3 501

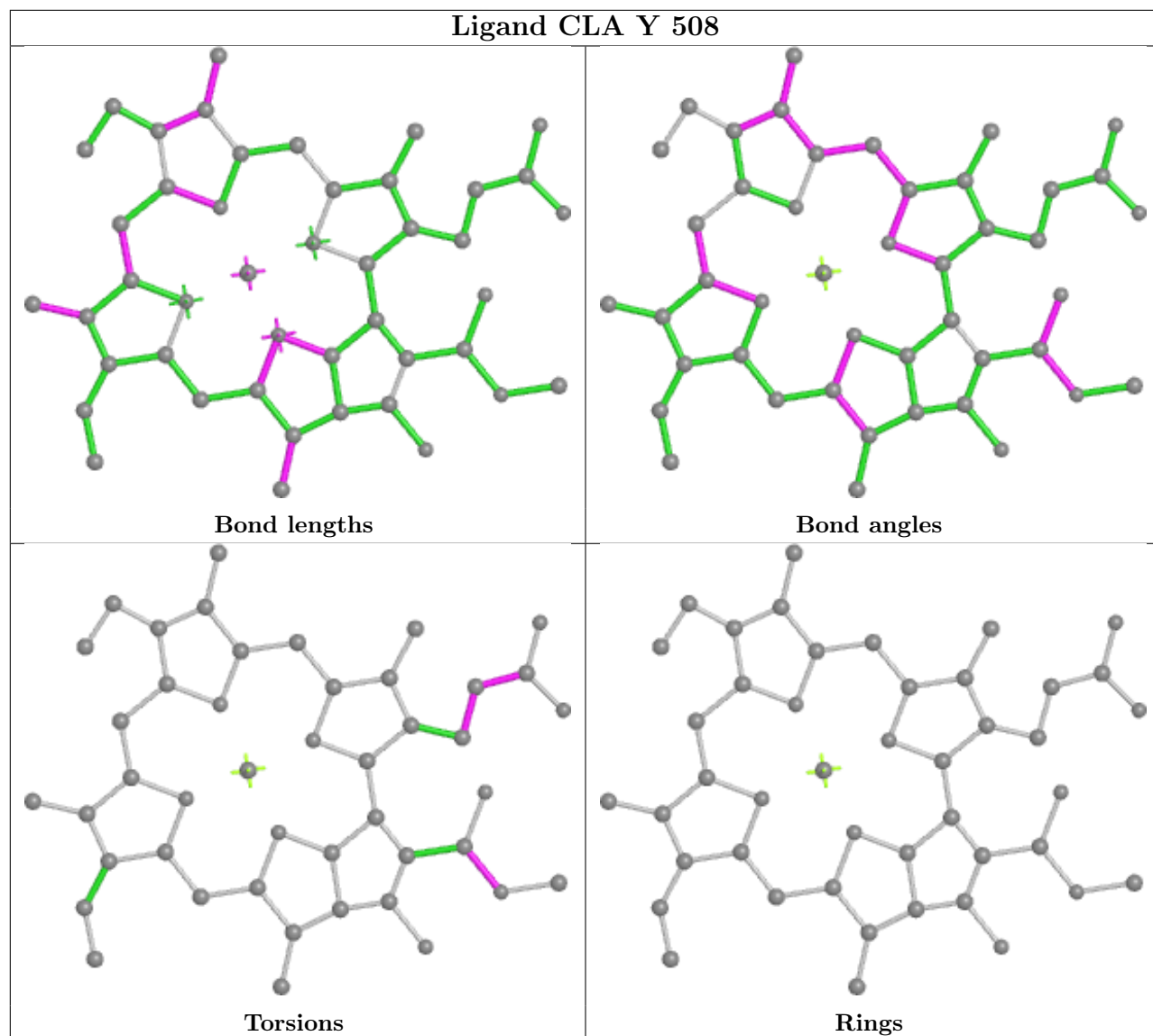


Ligand BCR b 523

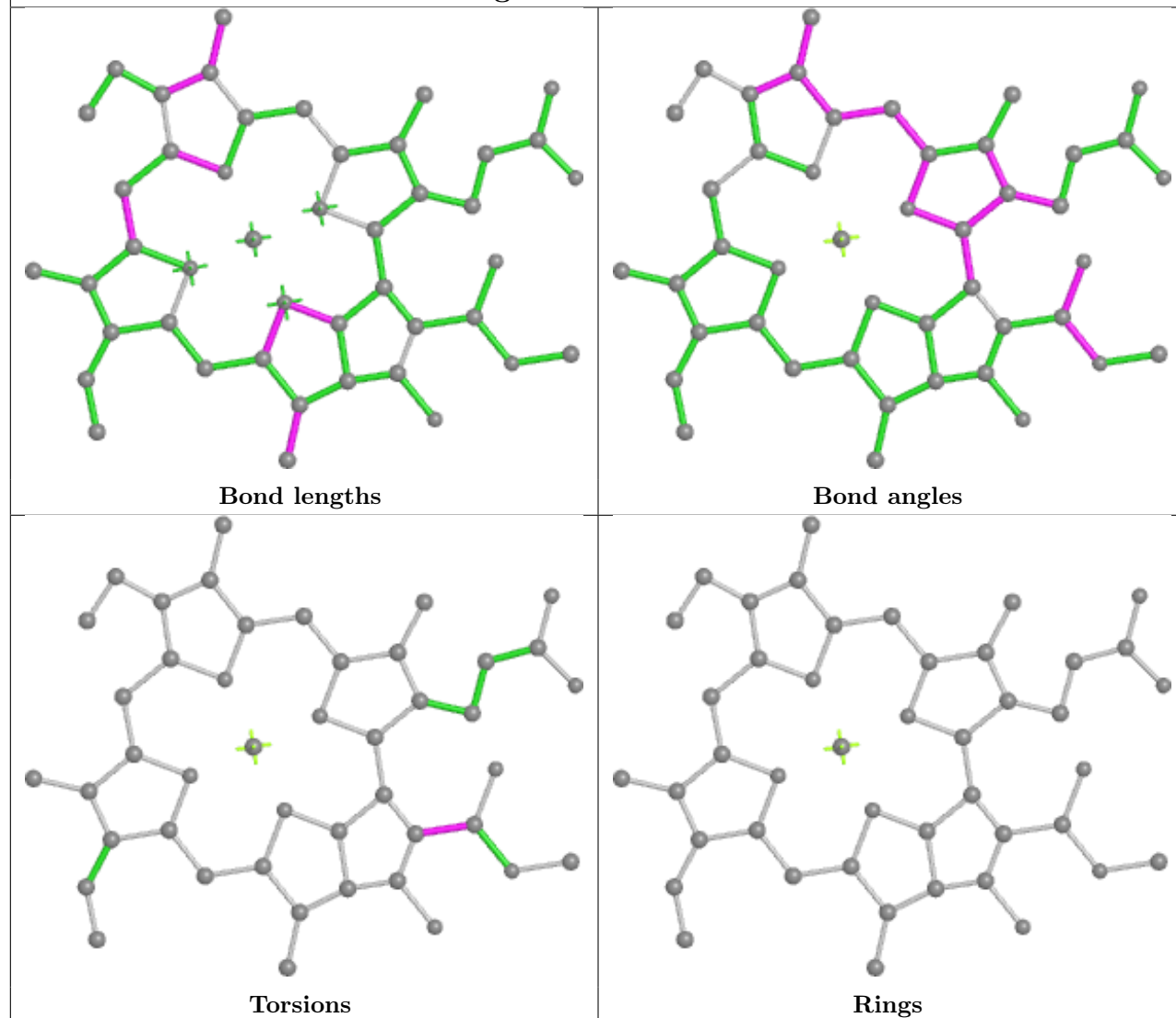




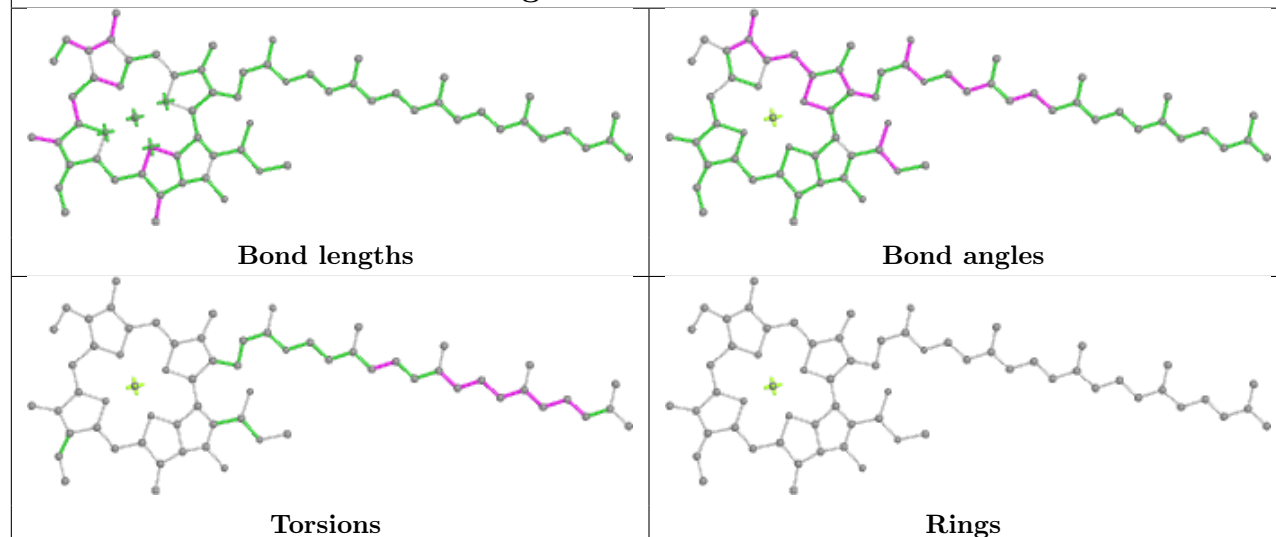
Ligand CLA Y 508

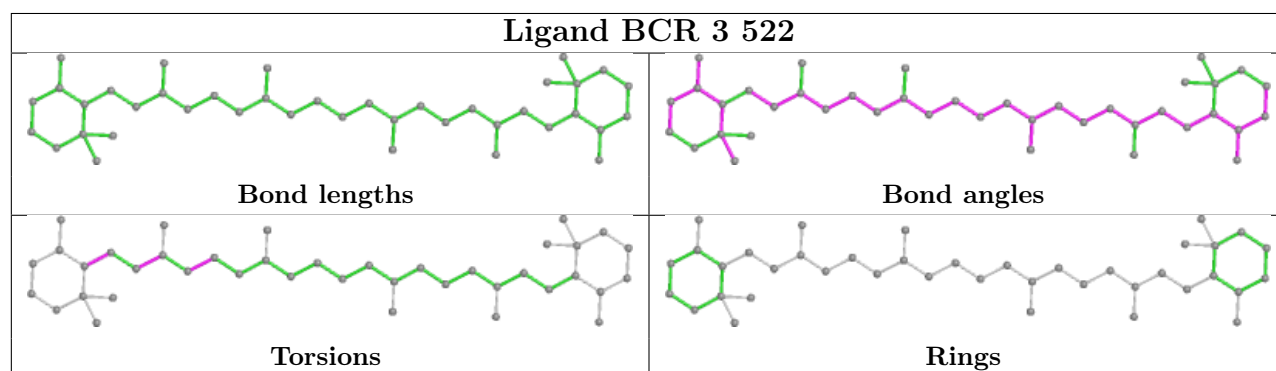
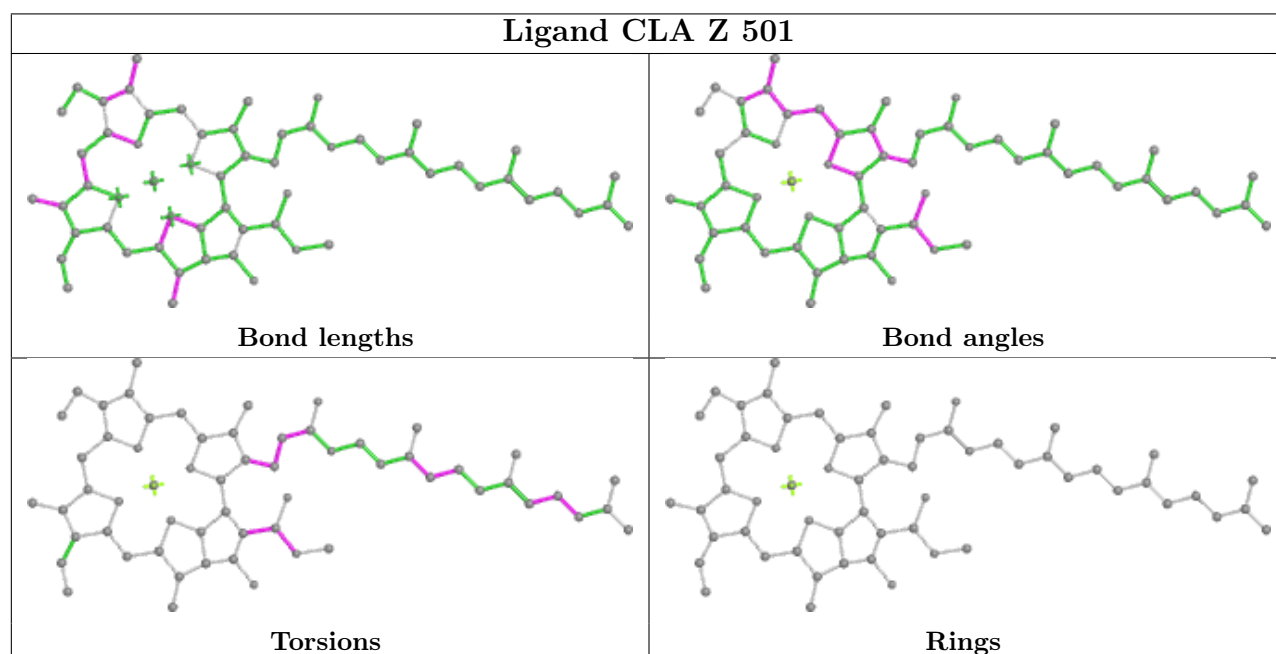
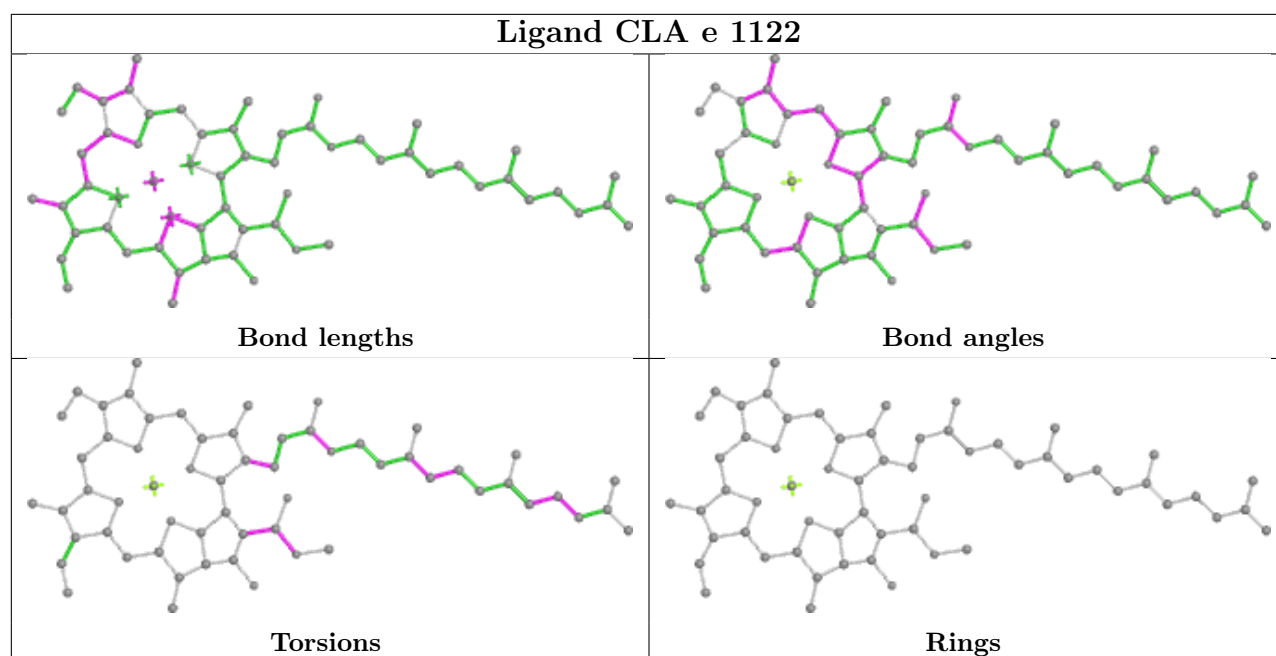


Ligand CLA 6 502

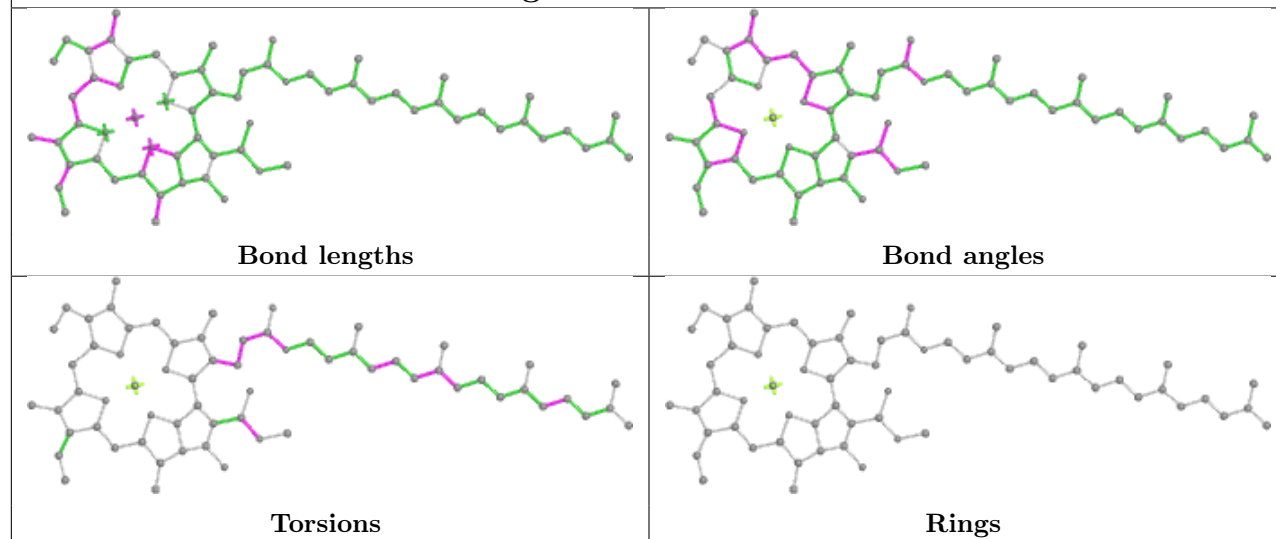


Ligand CLA G 1136

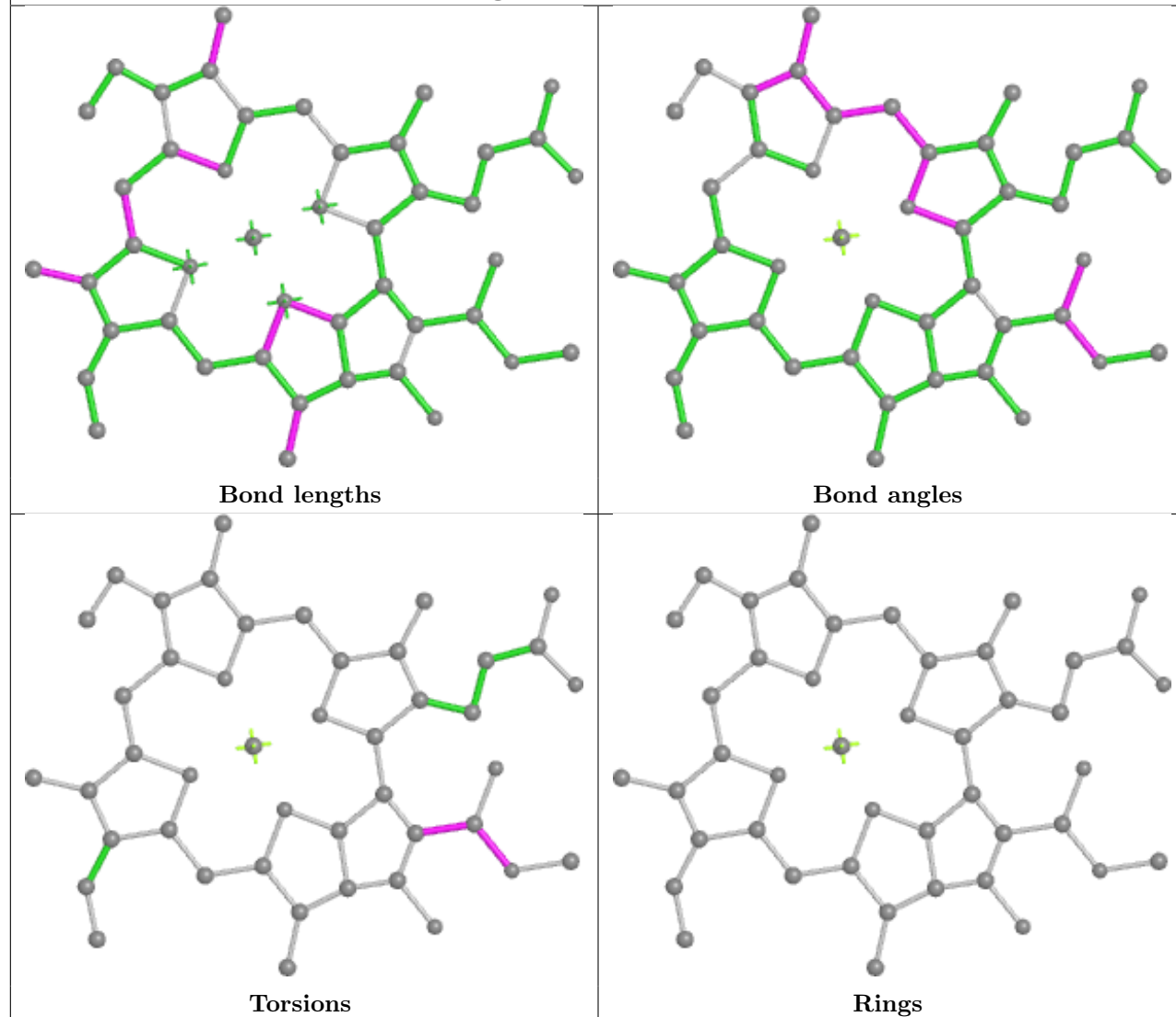


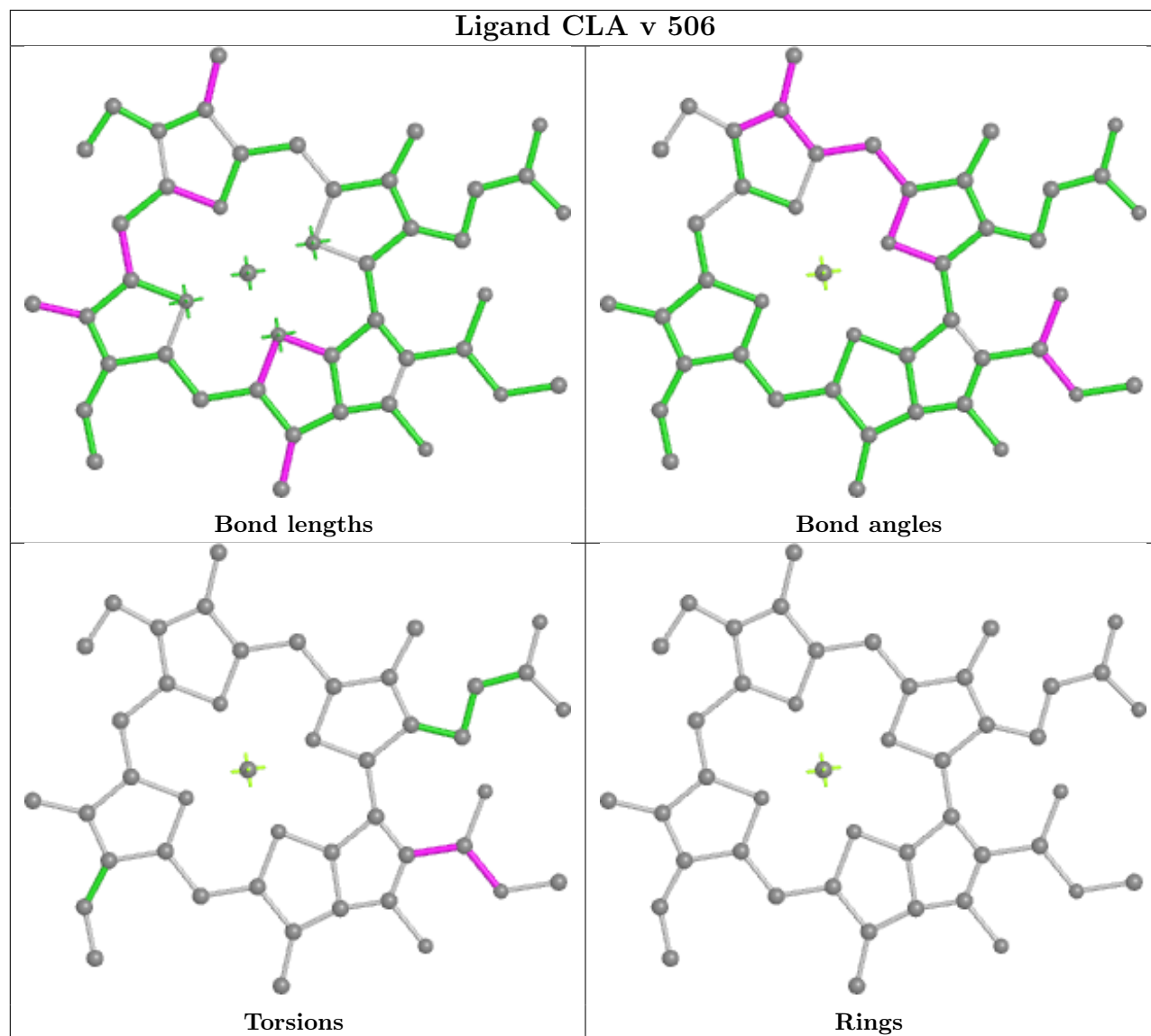
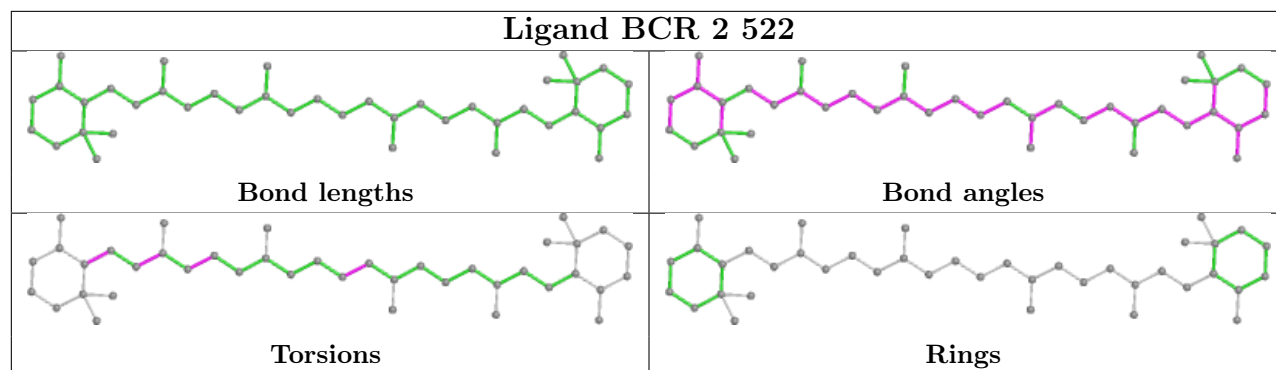


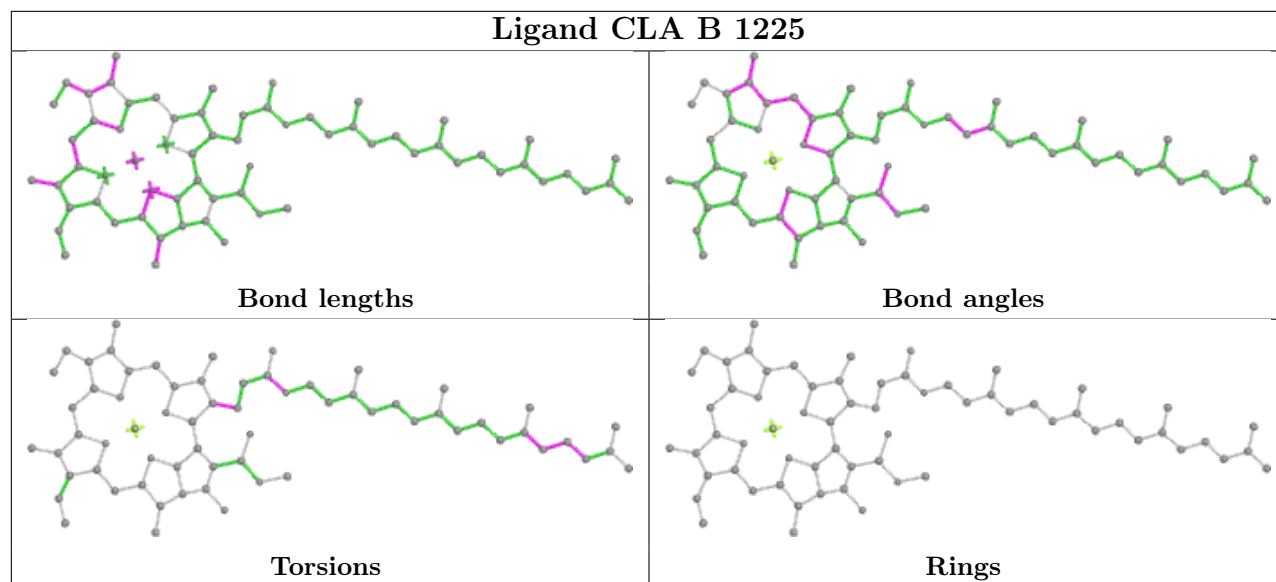
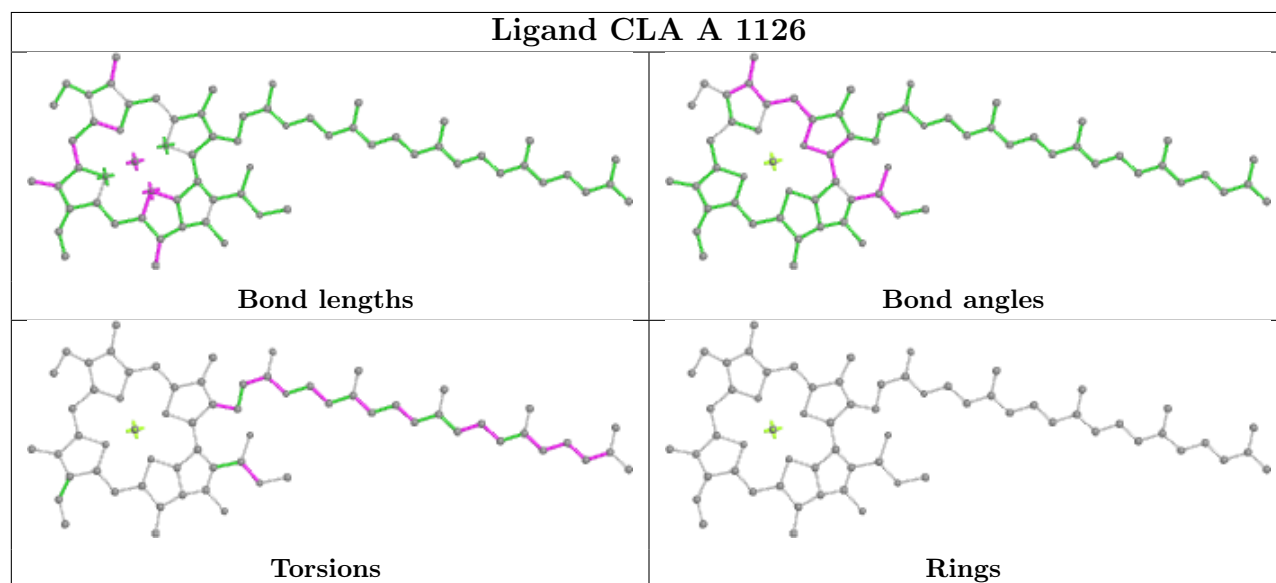
Ligand CLA H 1206



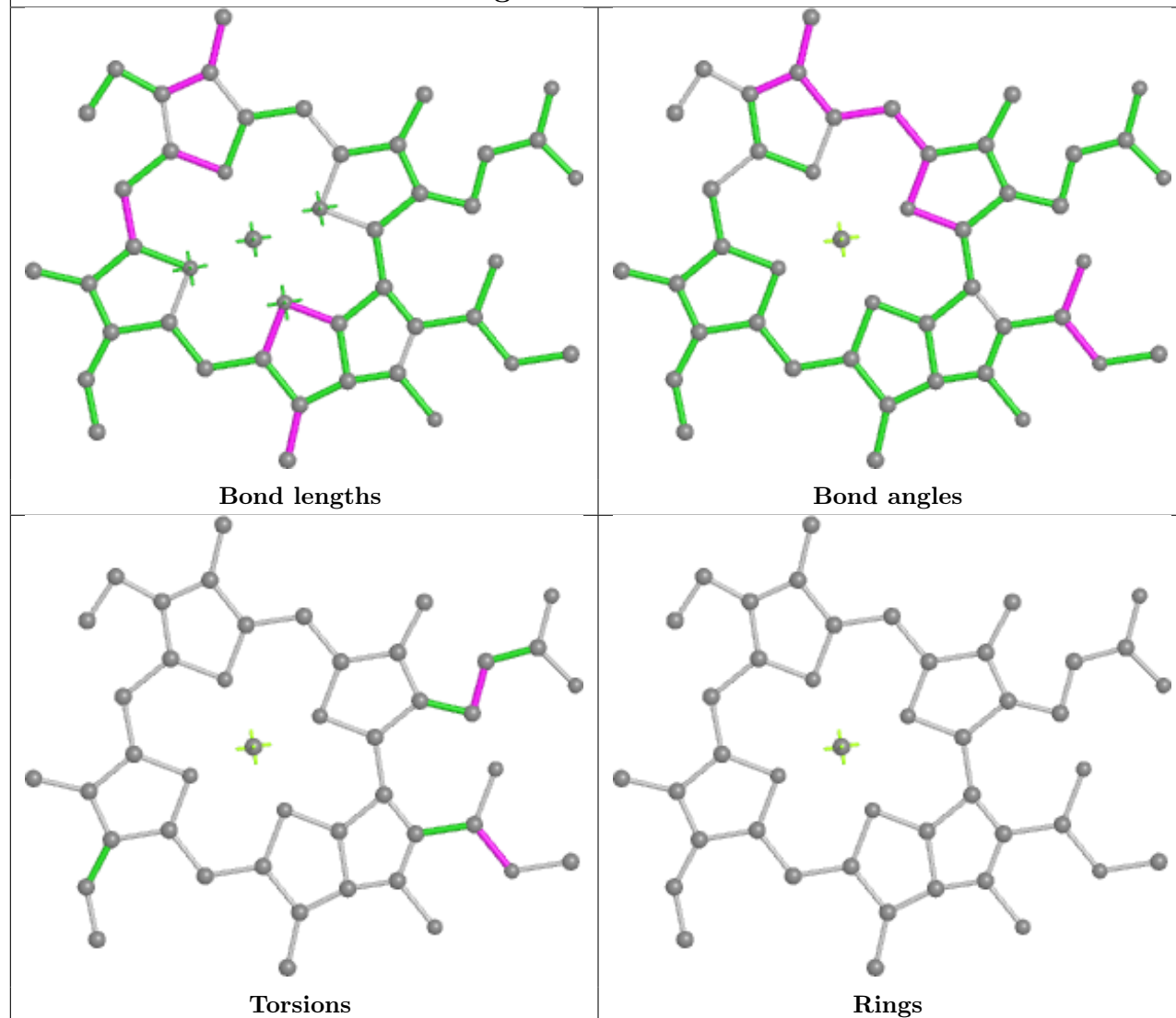
Ligand CLA Y 506



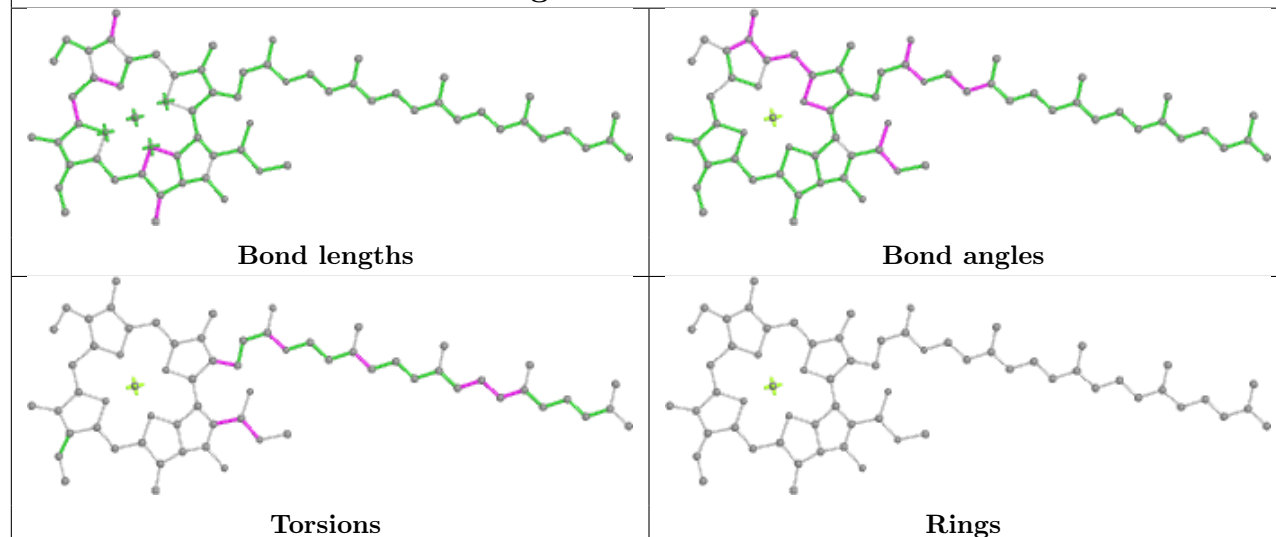


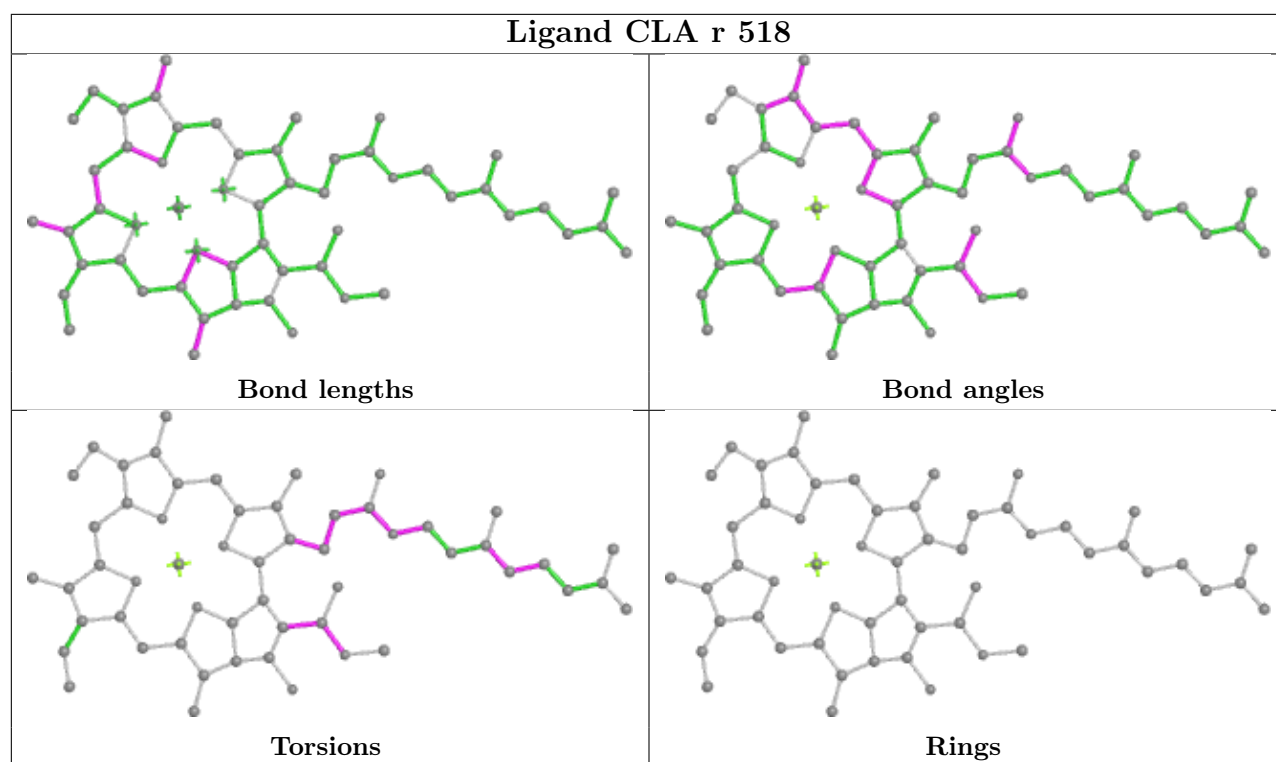
Ligand CLA B 1225**Ligand CLA A 1126**

Ligand CLA 6 513

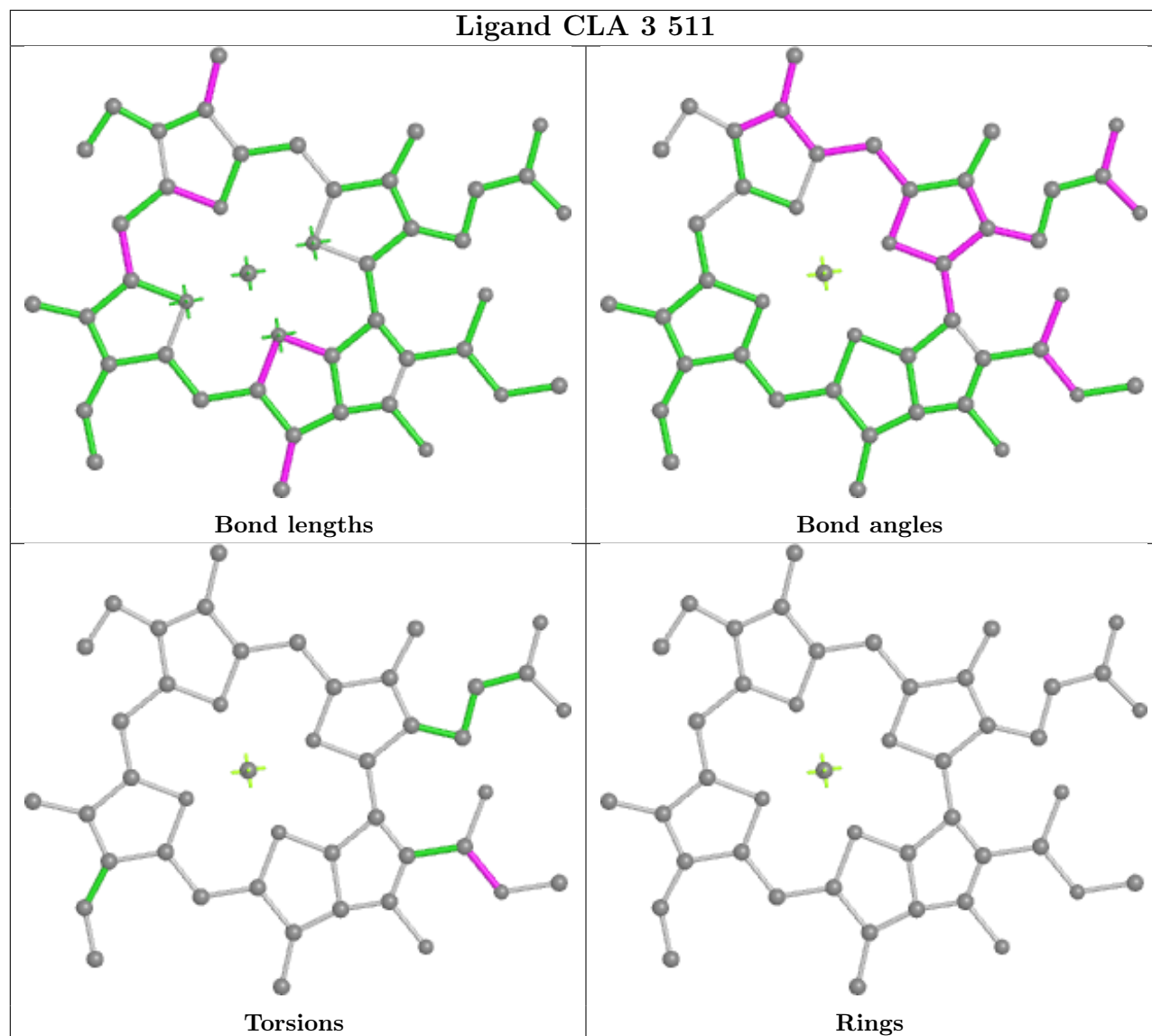


Ligand CLA f 1240

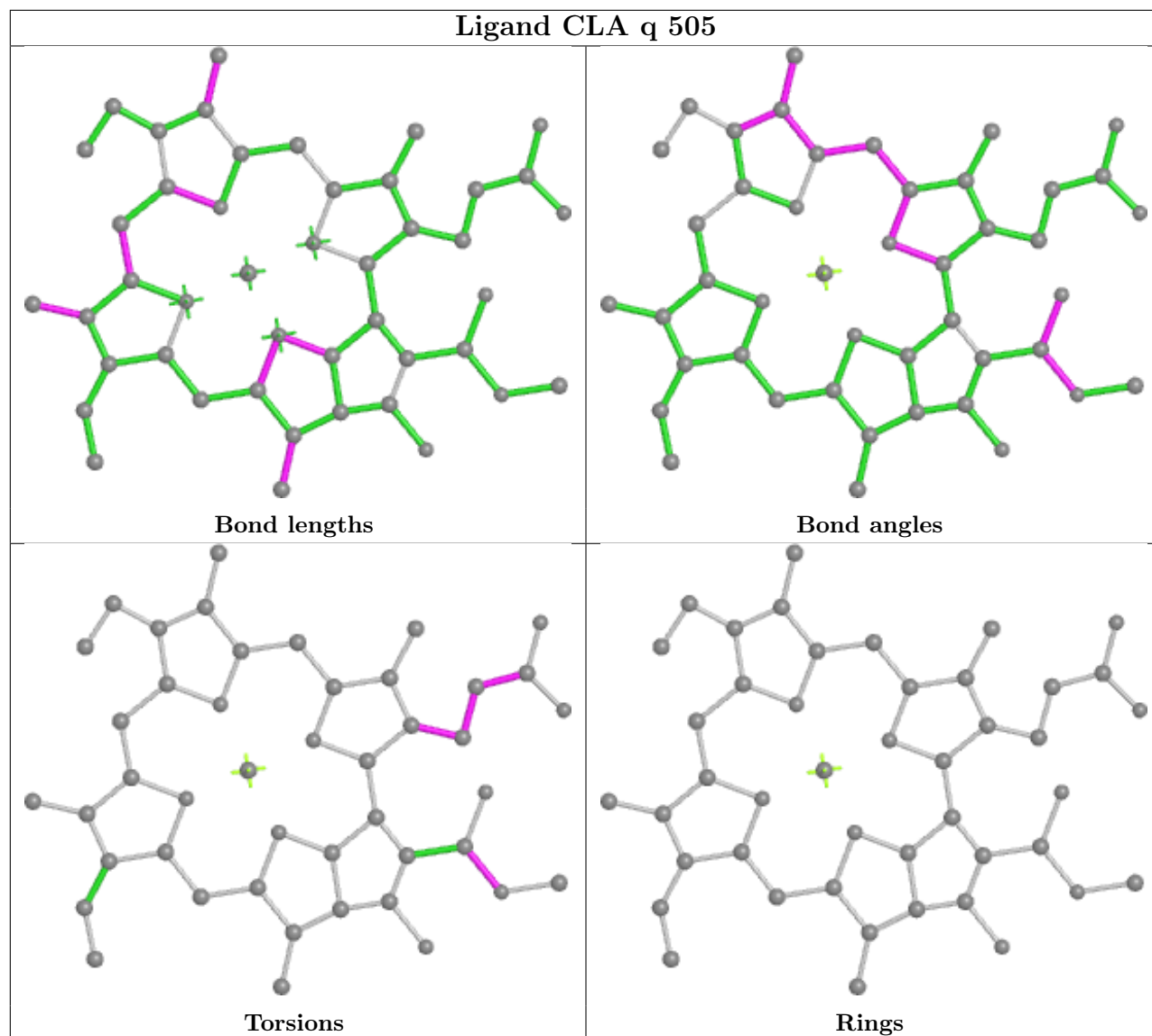




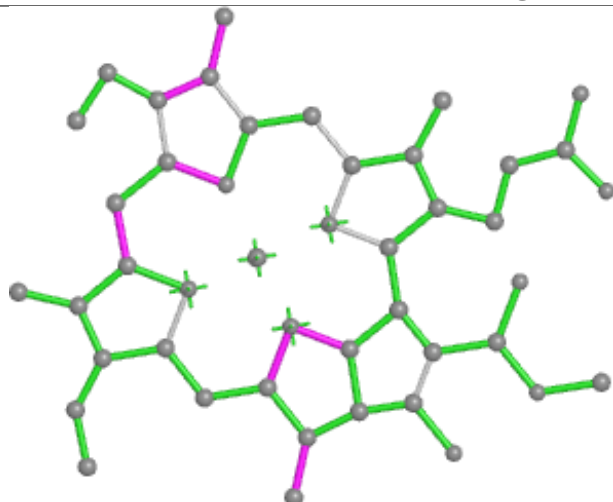
Ligand CLA 3 511



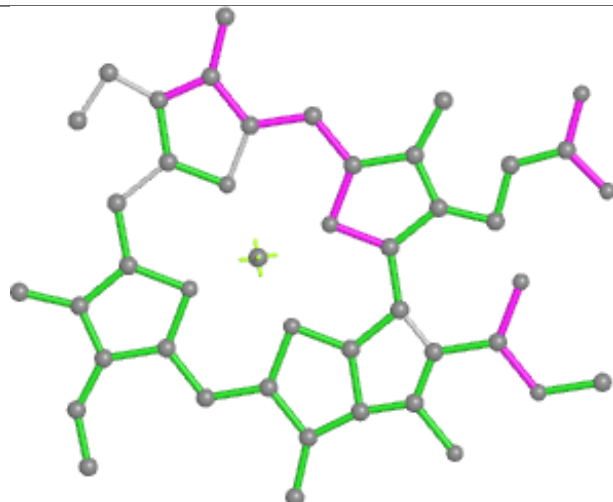
Ligand CLA q 505



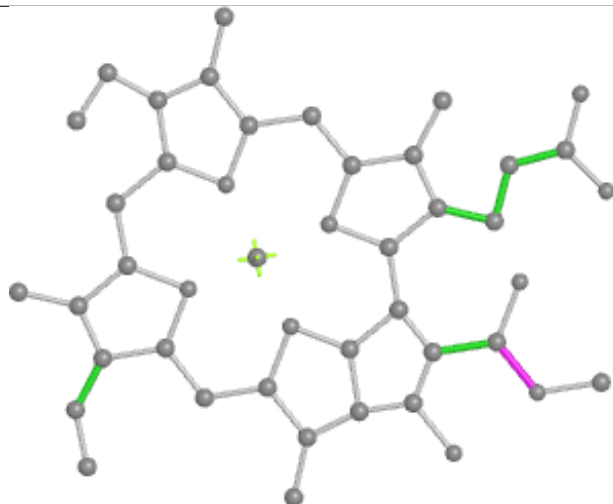
Ligand CLA Y 511



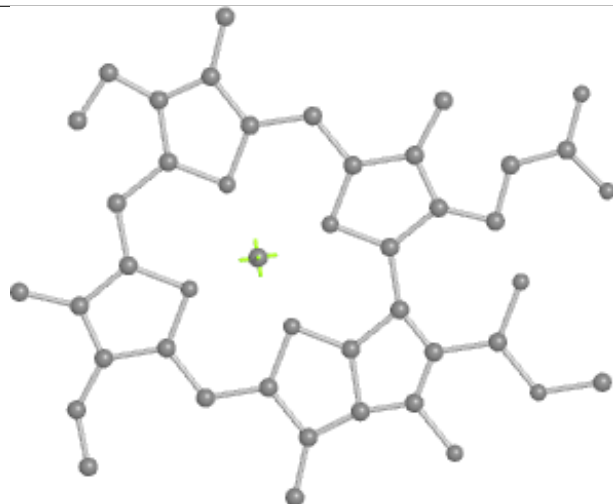
Bond lengths



Bond angles

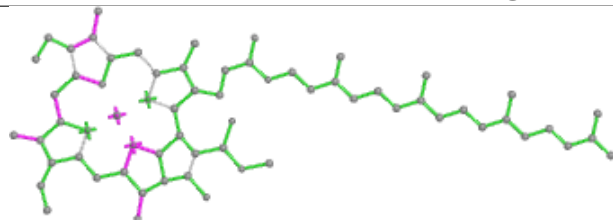


Torsions

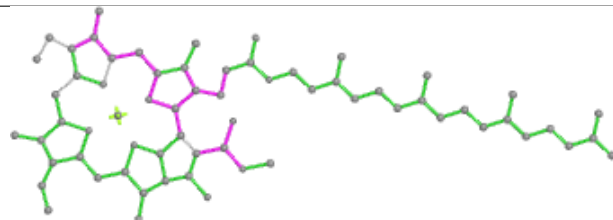


Rings

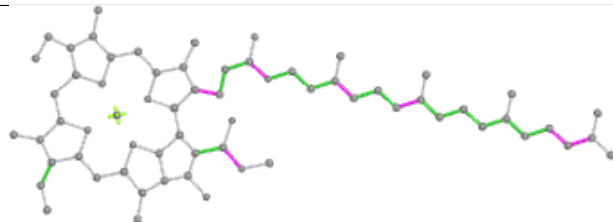
Ligand CLA G 1140



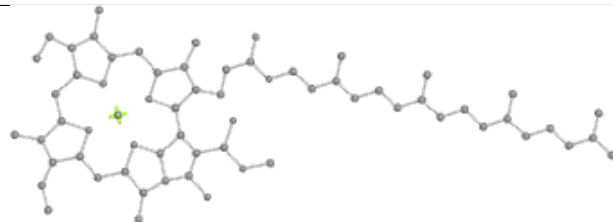
Bond lengths



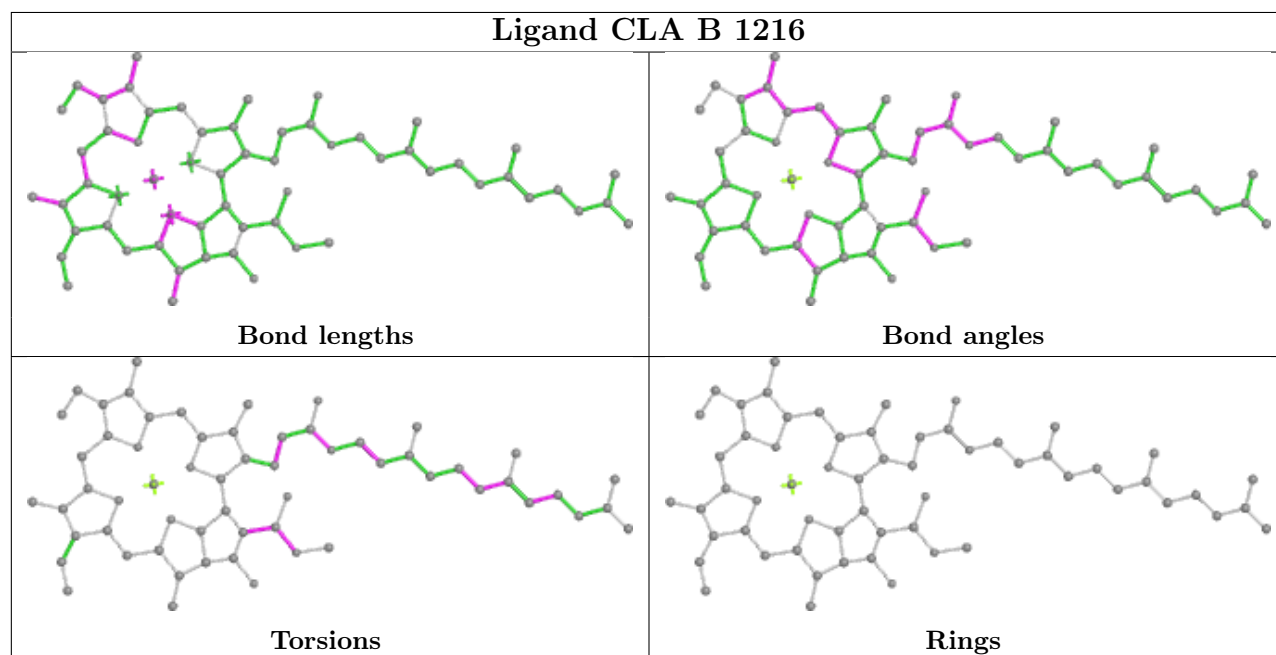
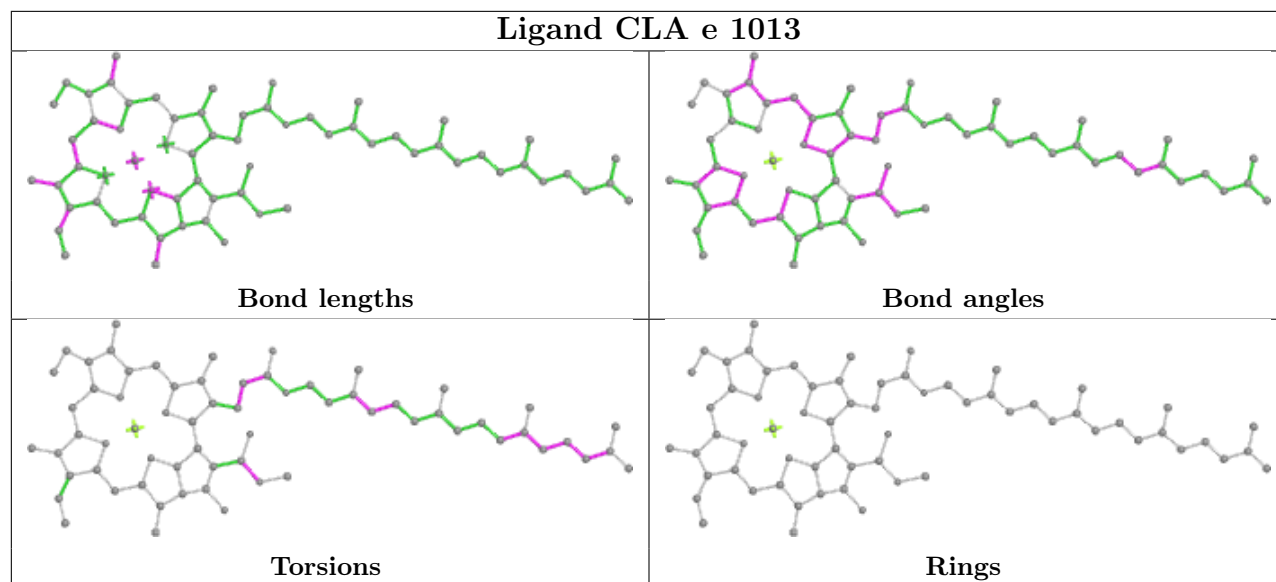
Bond angles



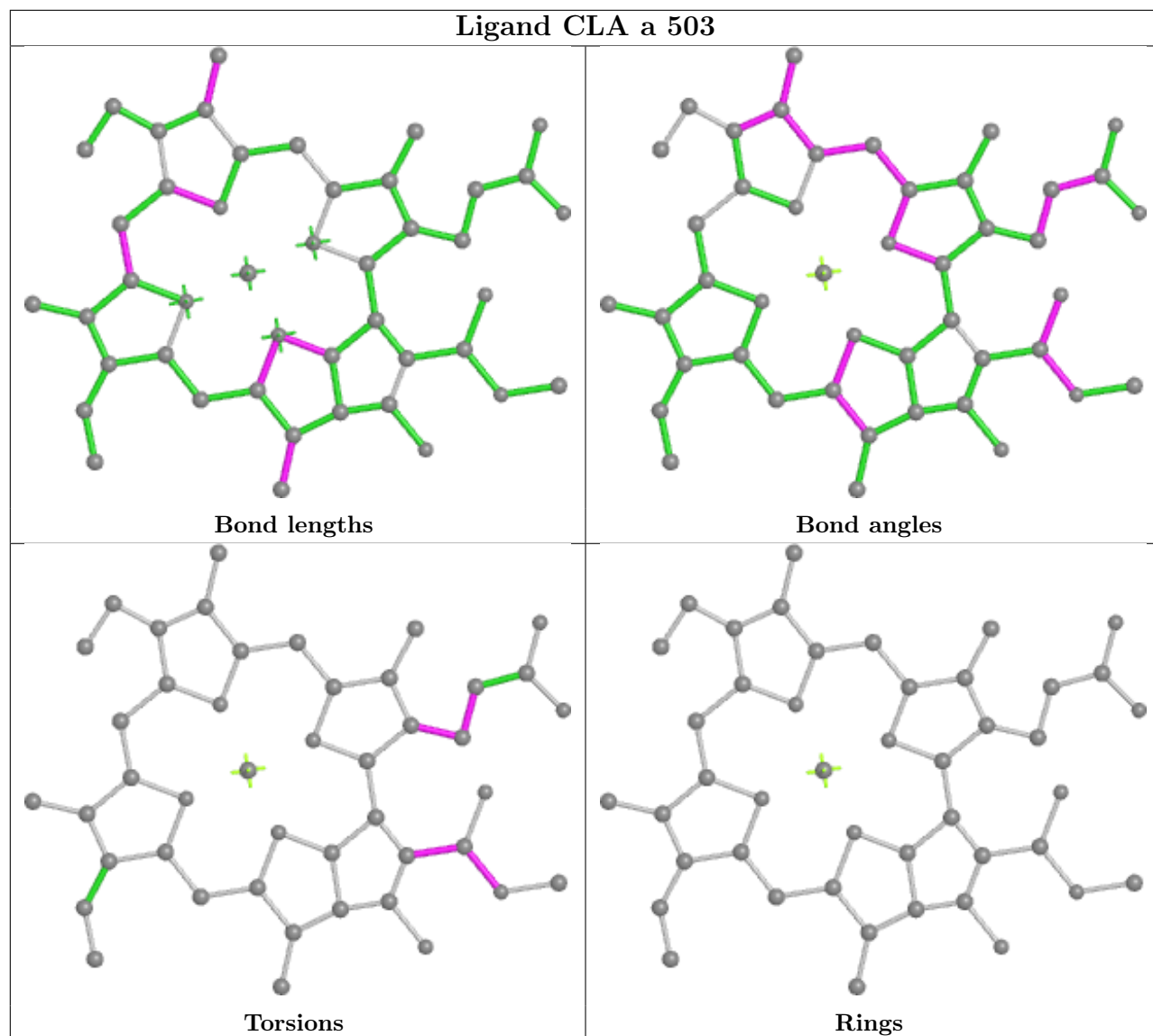
Torsions



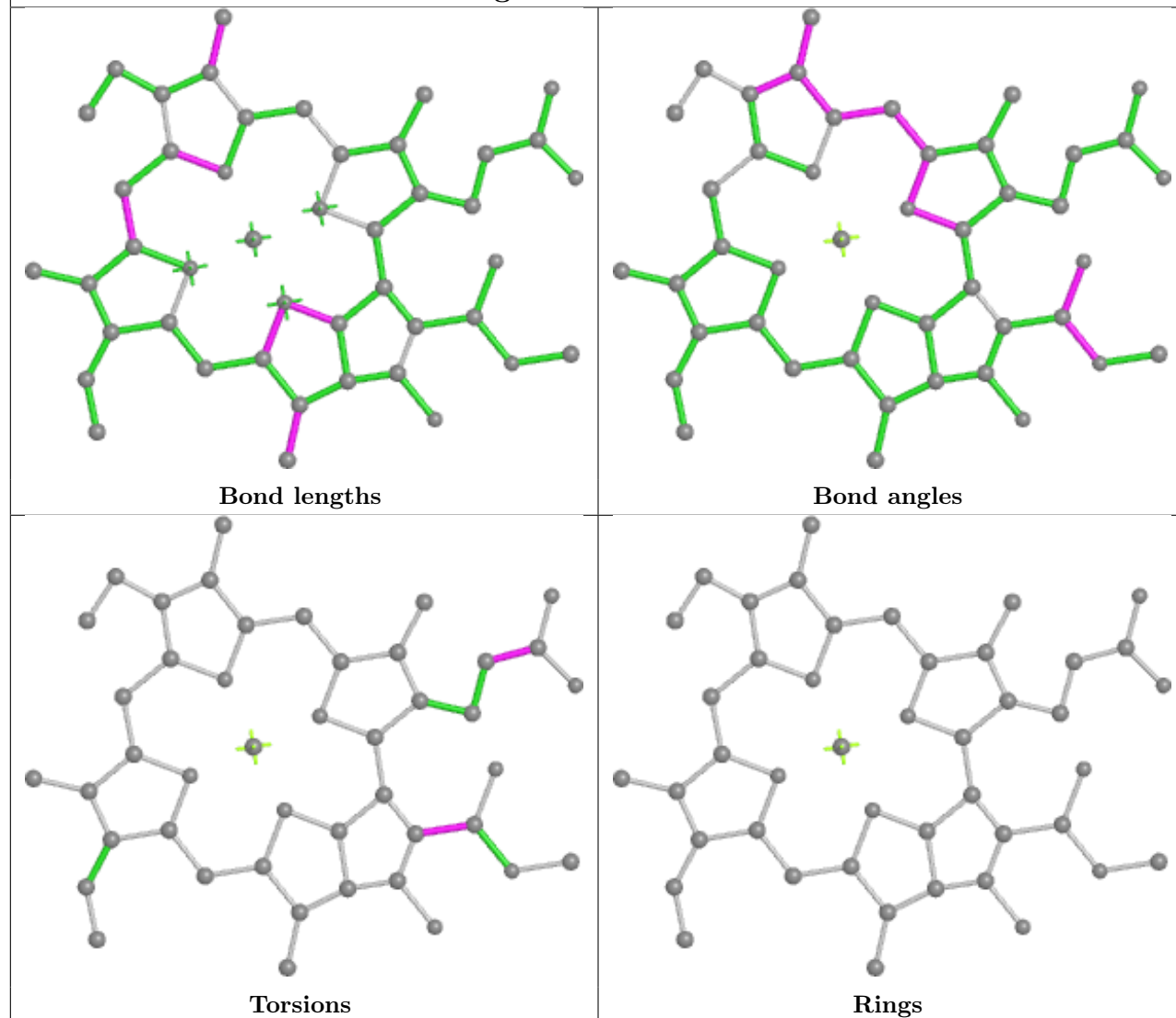
Rings



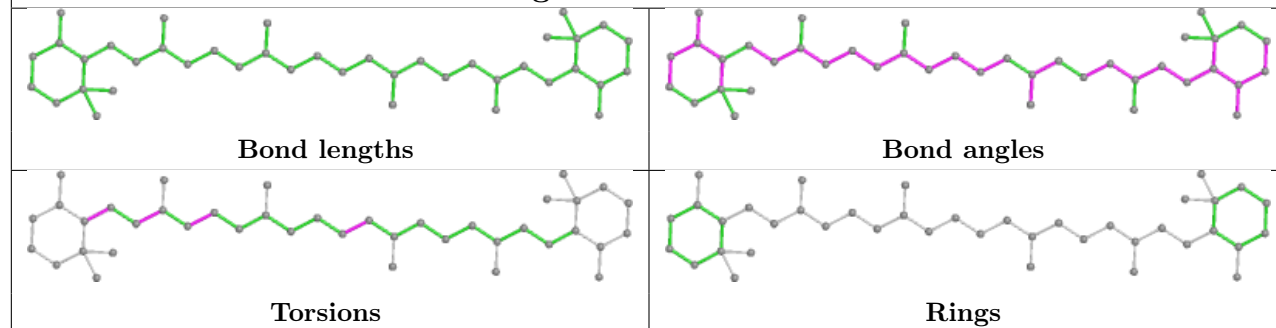
Ligand CLA a 503

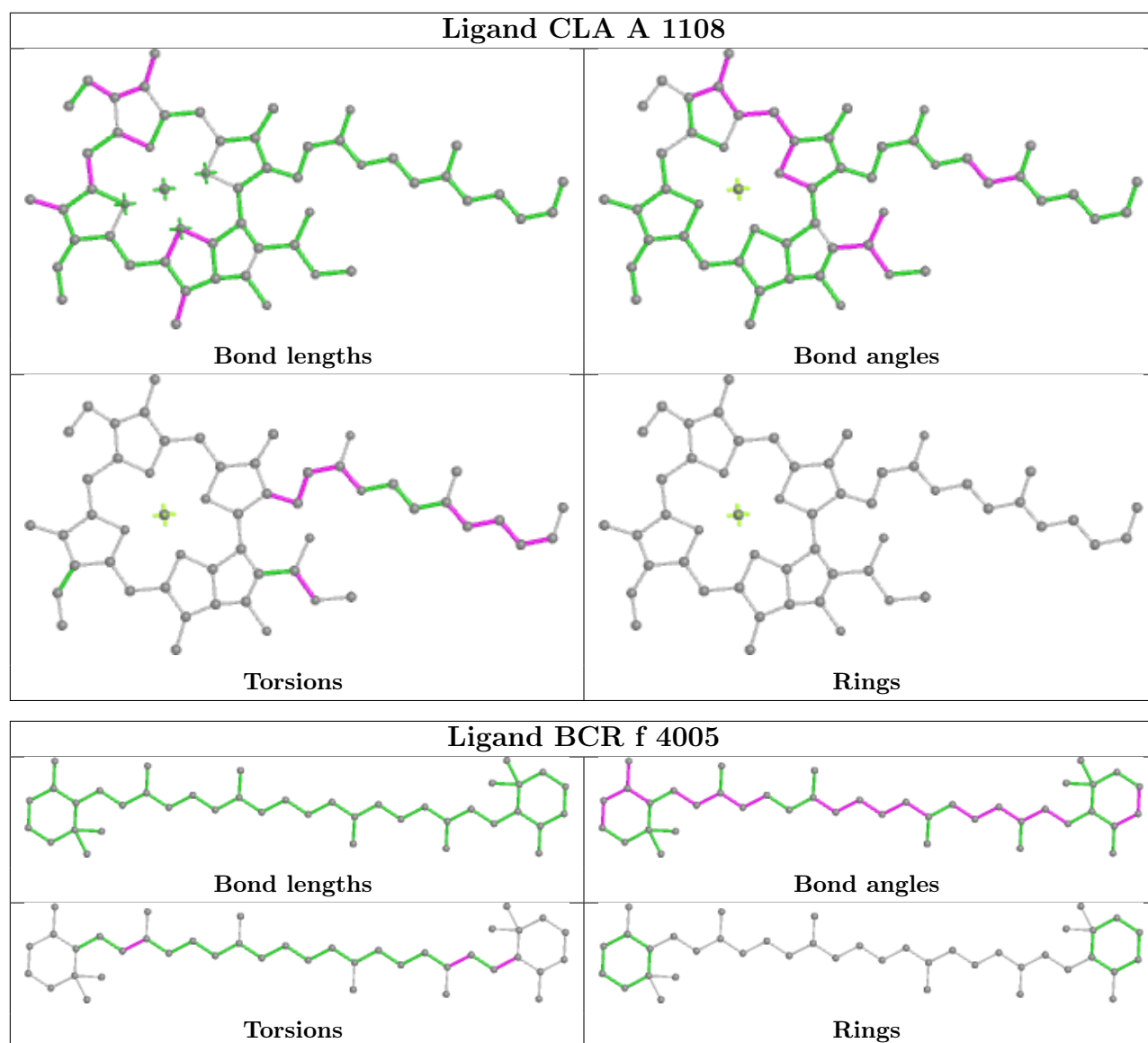


Ligand CLA 4 512

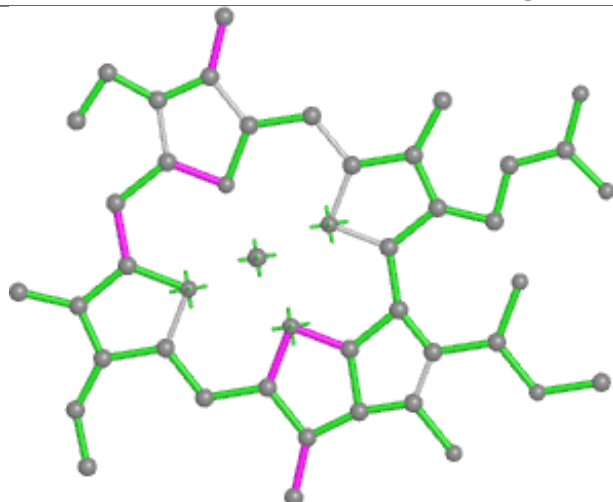


Ligand BCR Z 522

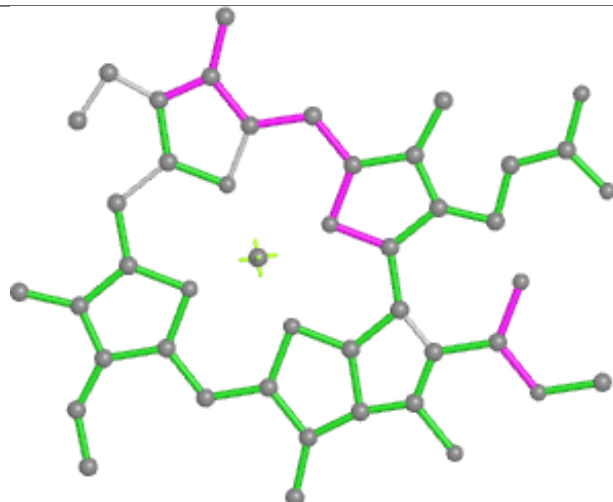




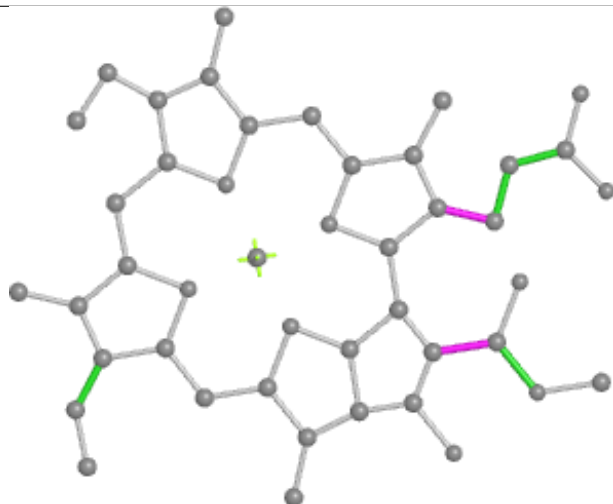
Ligand CLA c 516



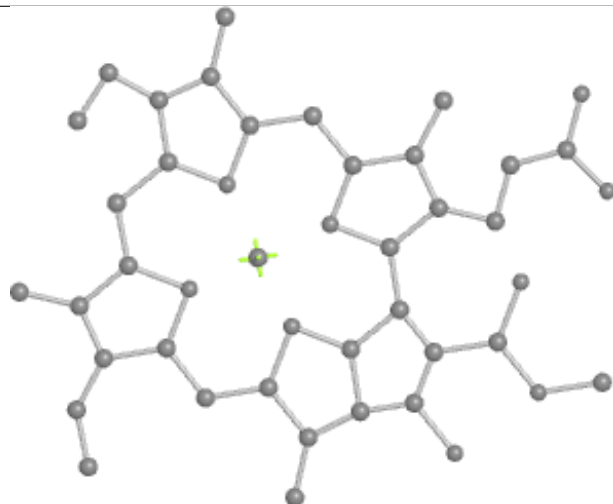
Bond lengths



Bond angles

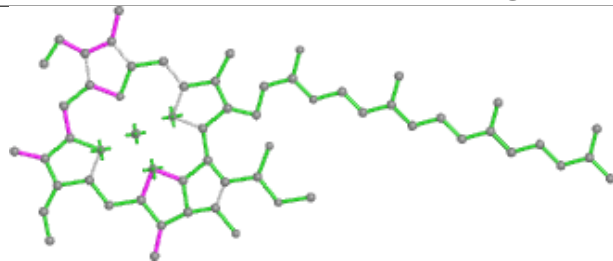


Torsions

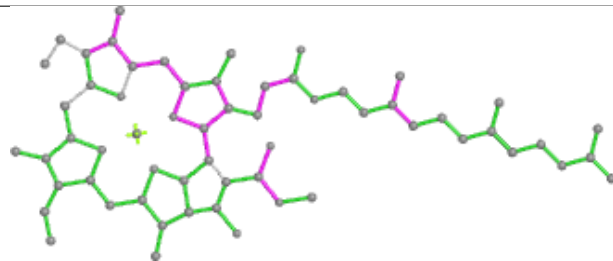


Rings

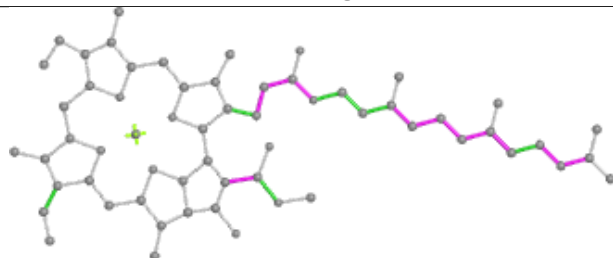
Ligand CLA G 1137



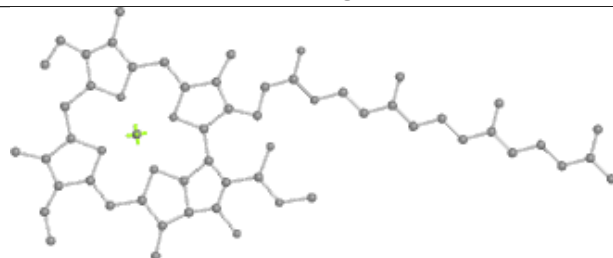
Bond lengths



Bond angles

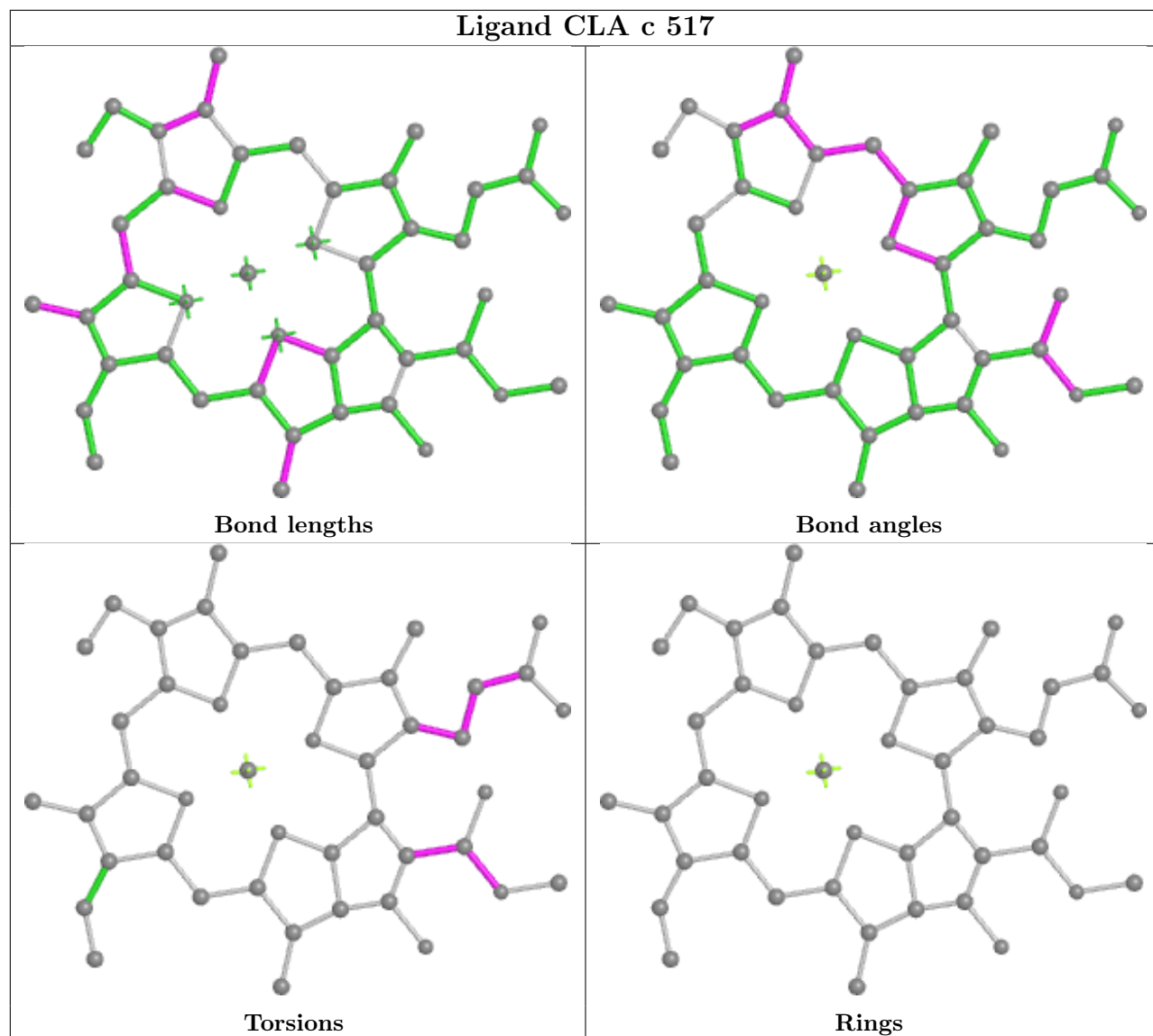


Torsions

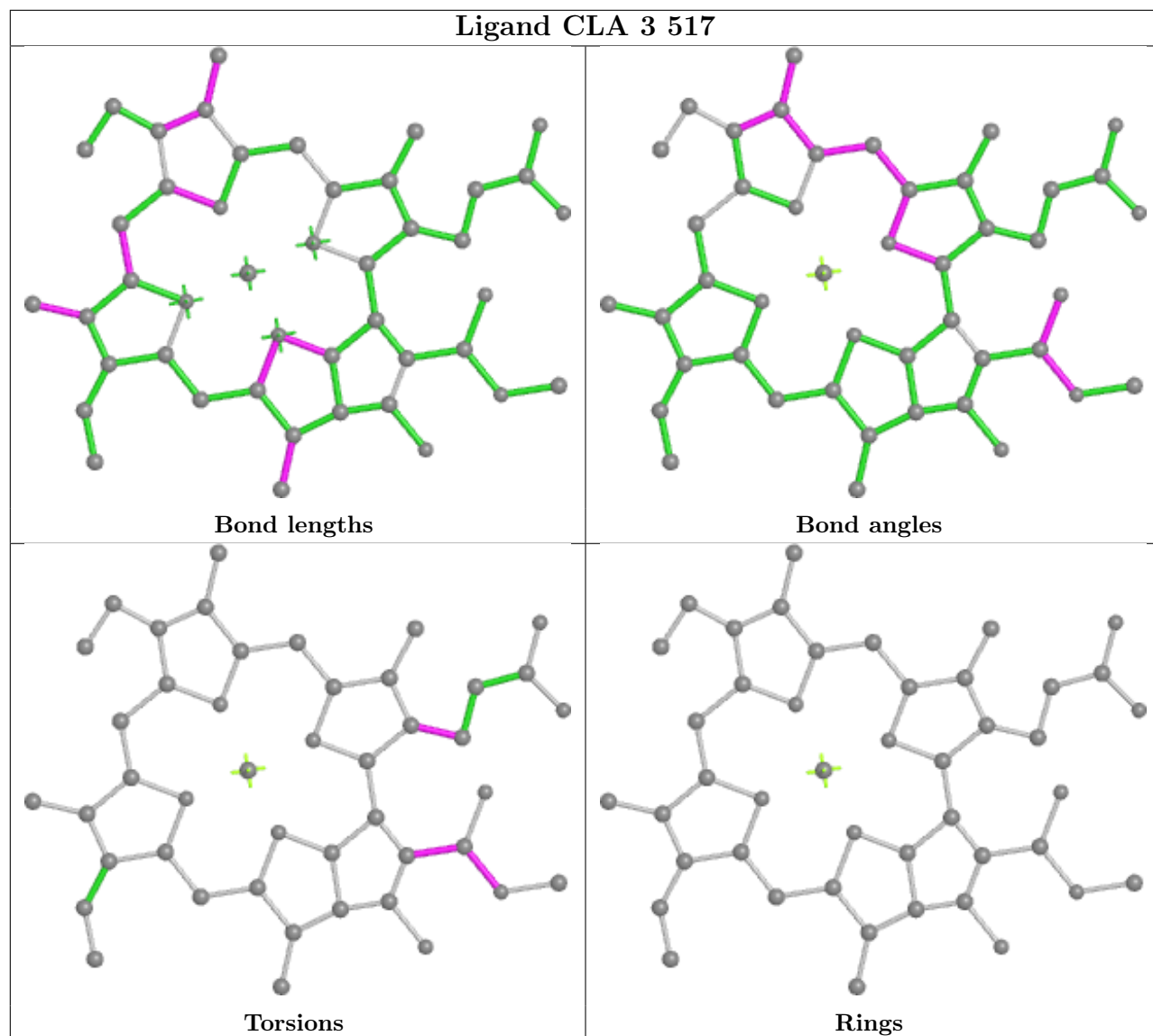


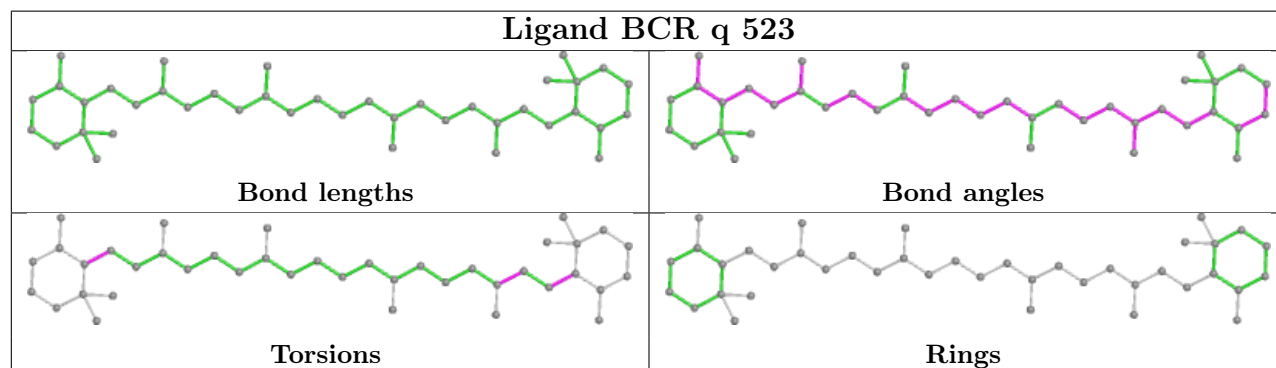
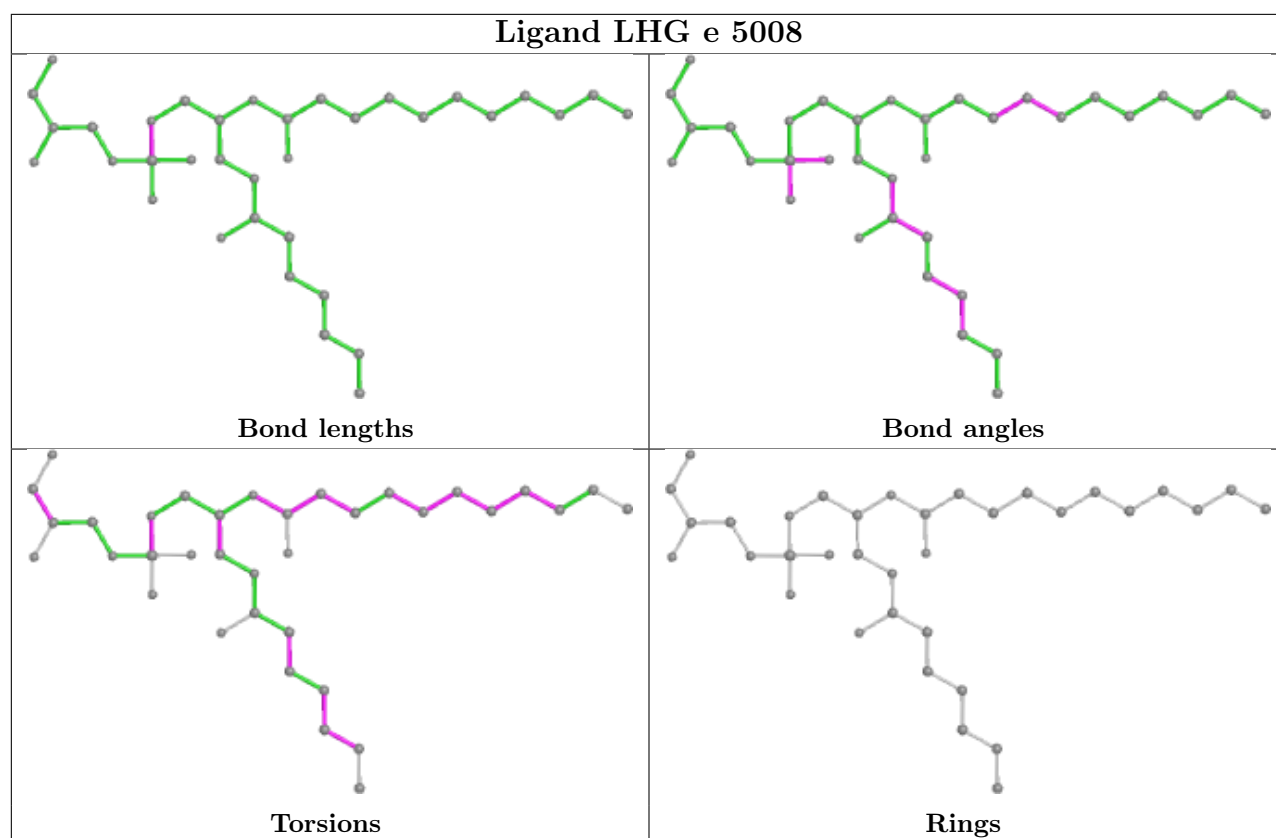
Rings

Ligand CLA c 517

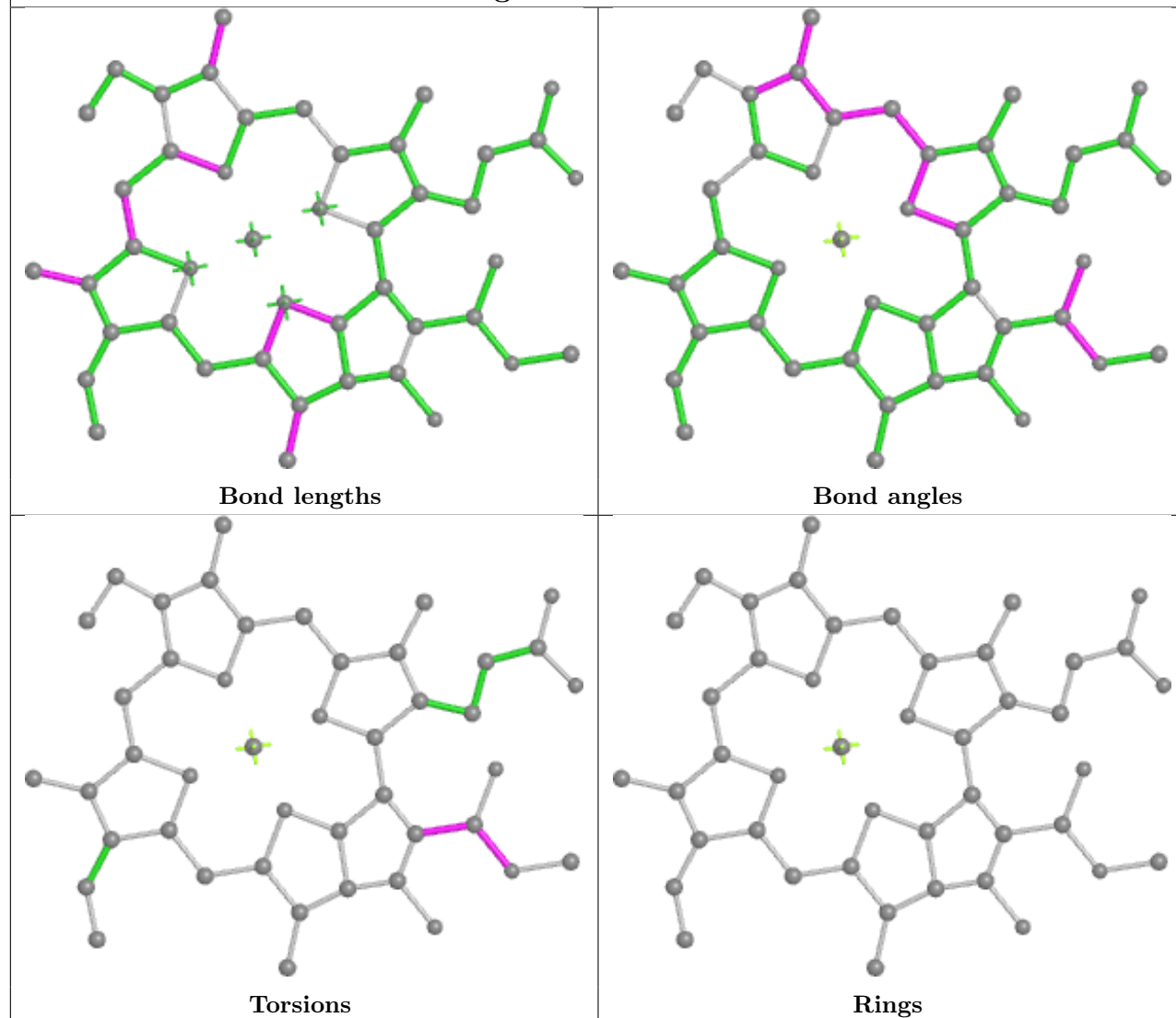


Ligand CLA 3 517

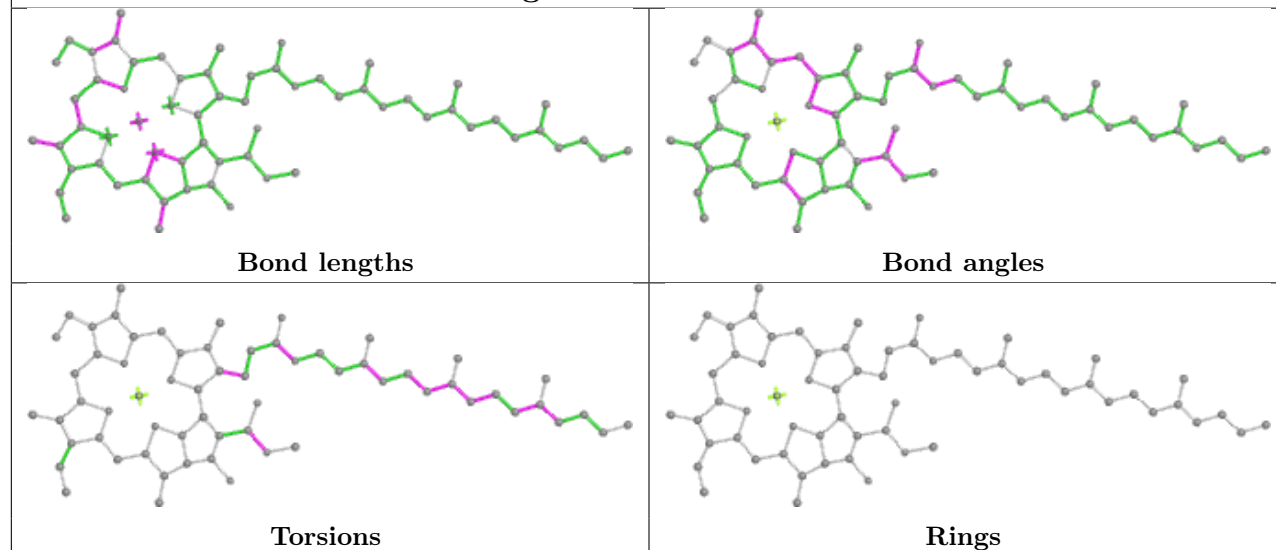




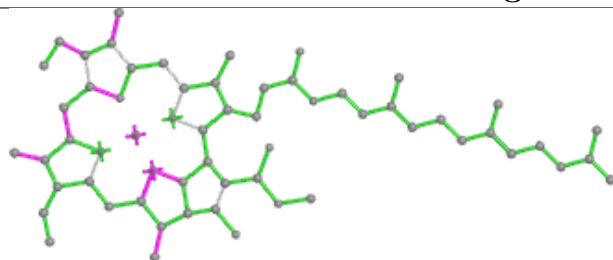
Ligand CLA 1 506



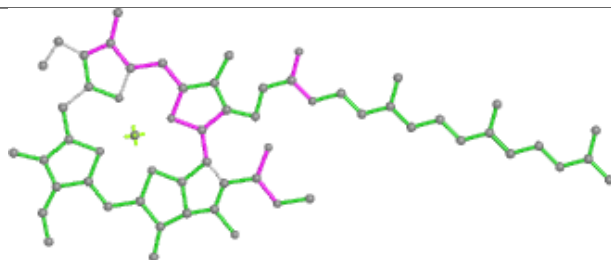
Ligand CLA H 1219



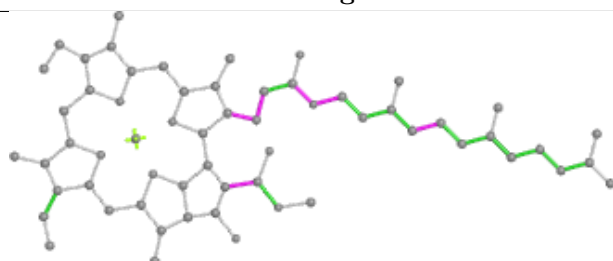
Ligand CLA G 1118



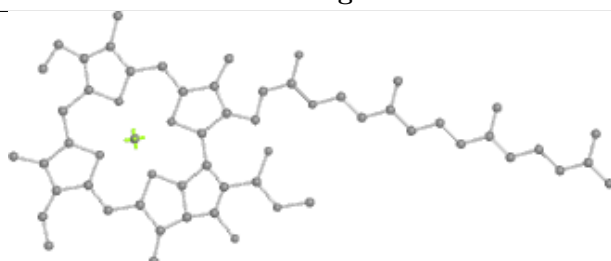
Bond lengths



Bond angles

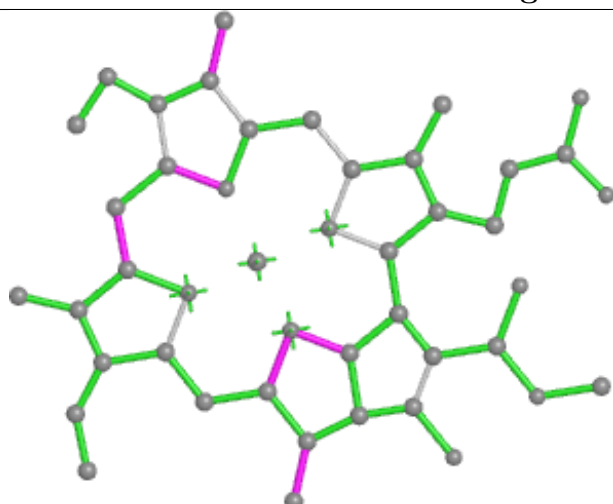


Torsions

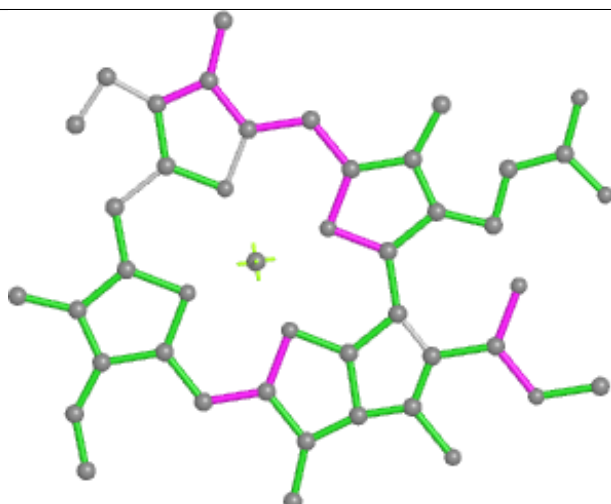


Rings

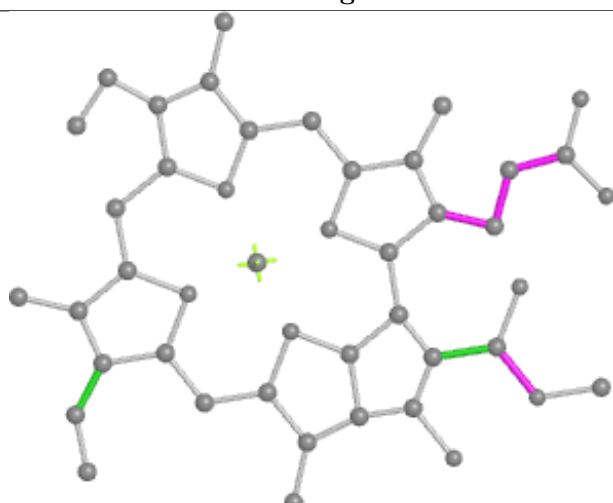
Ligand CLA t 501



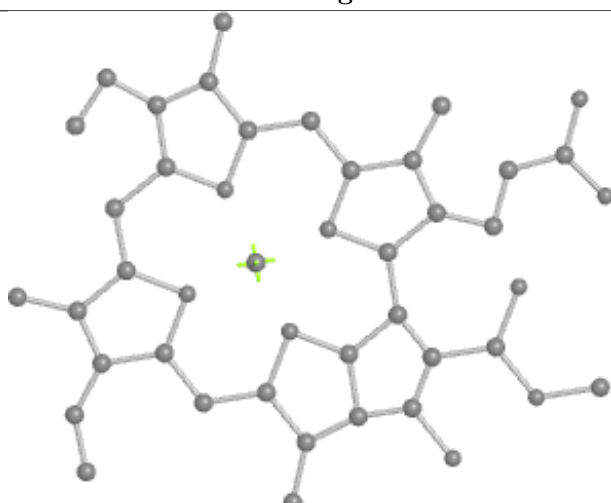
Bond lengths



Bond angles

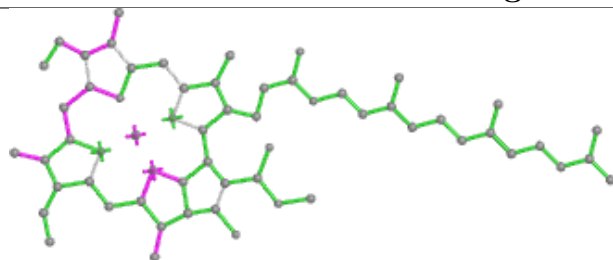


Torsions

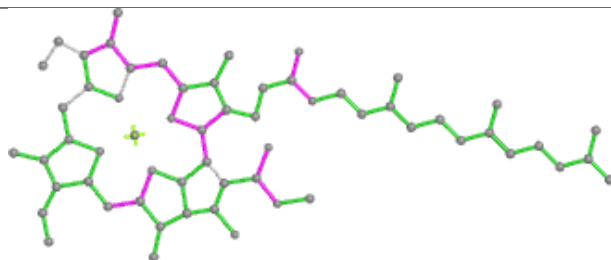


Rings

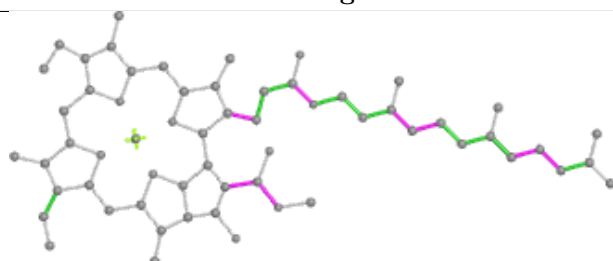
Ligand CLA G 1122



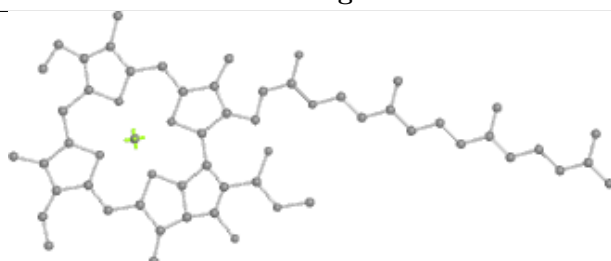
Bond lengths



Bond angles

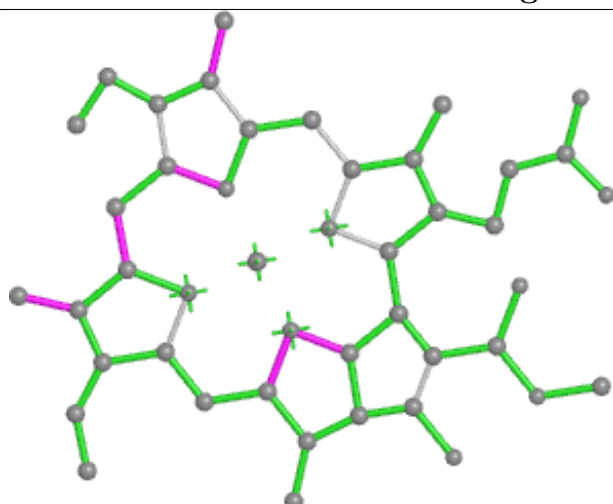


Torsions

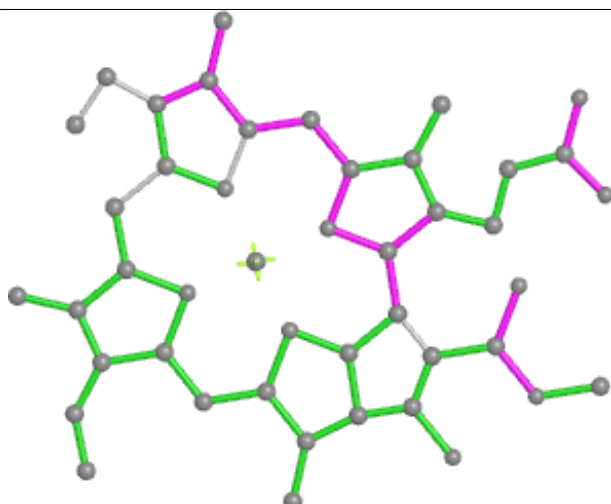


Rings

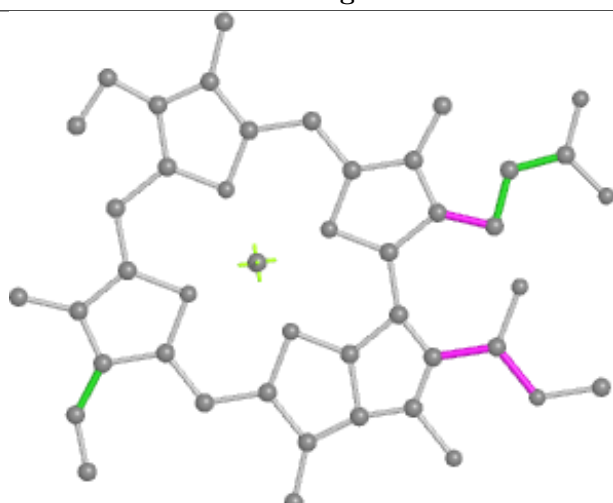
Ligand CLA t 517



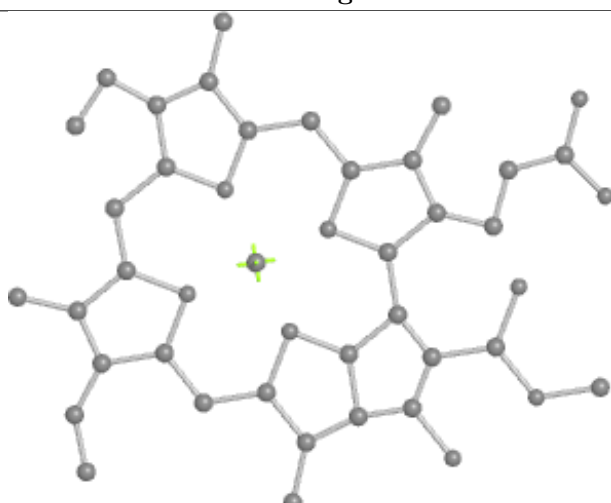
Bond lengths



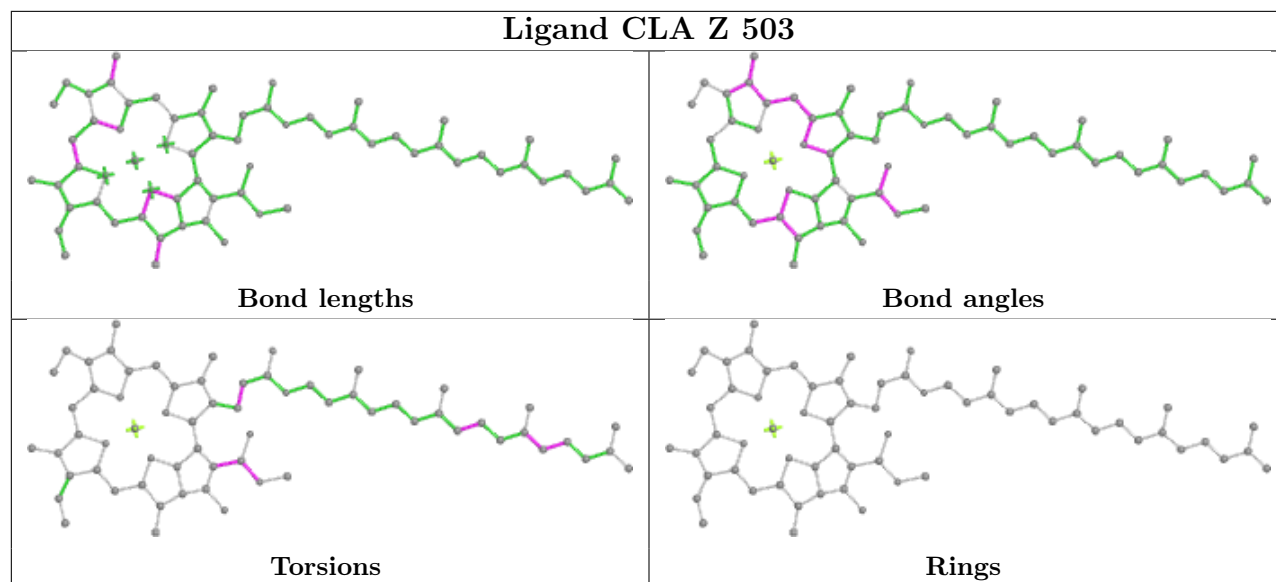
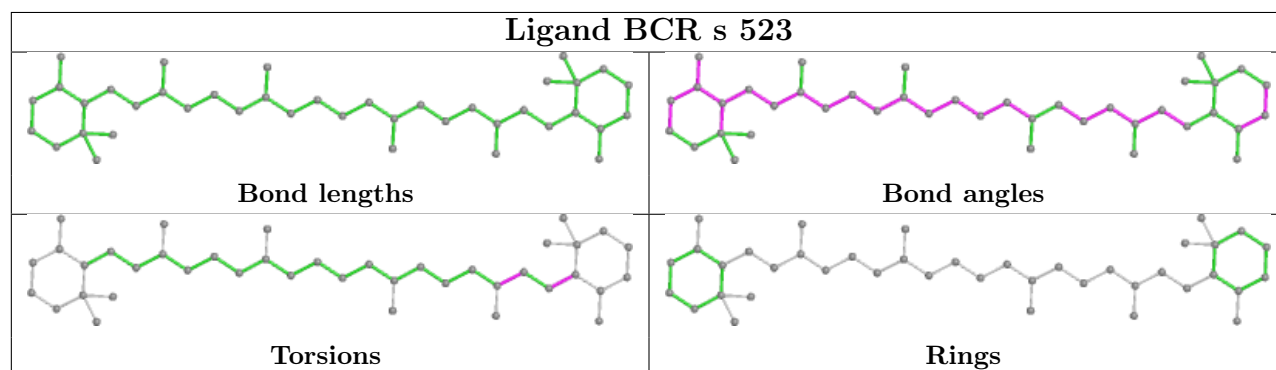
Bond angles



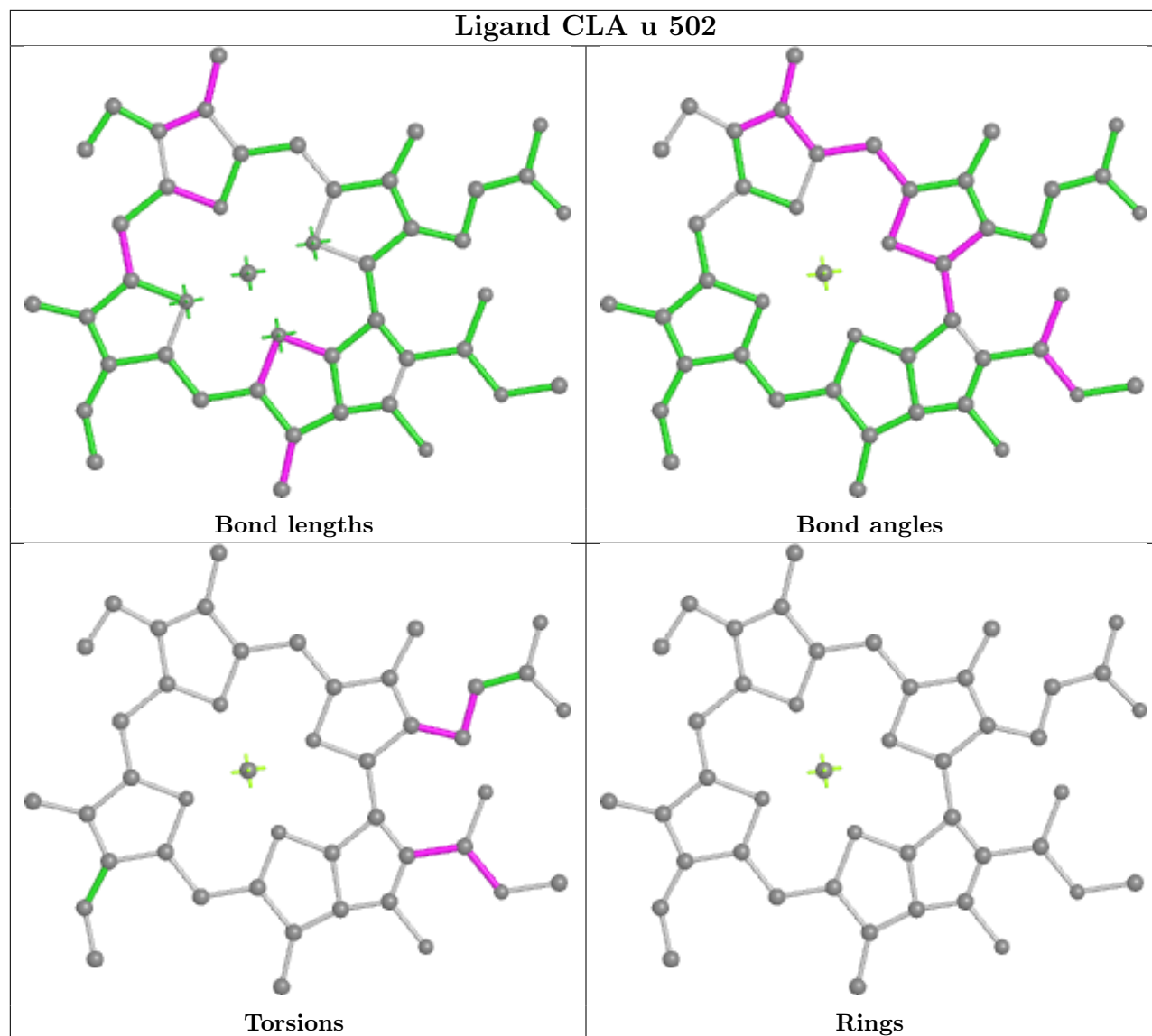
Torsions

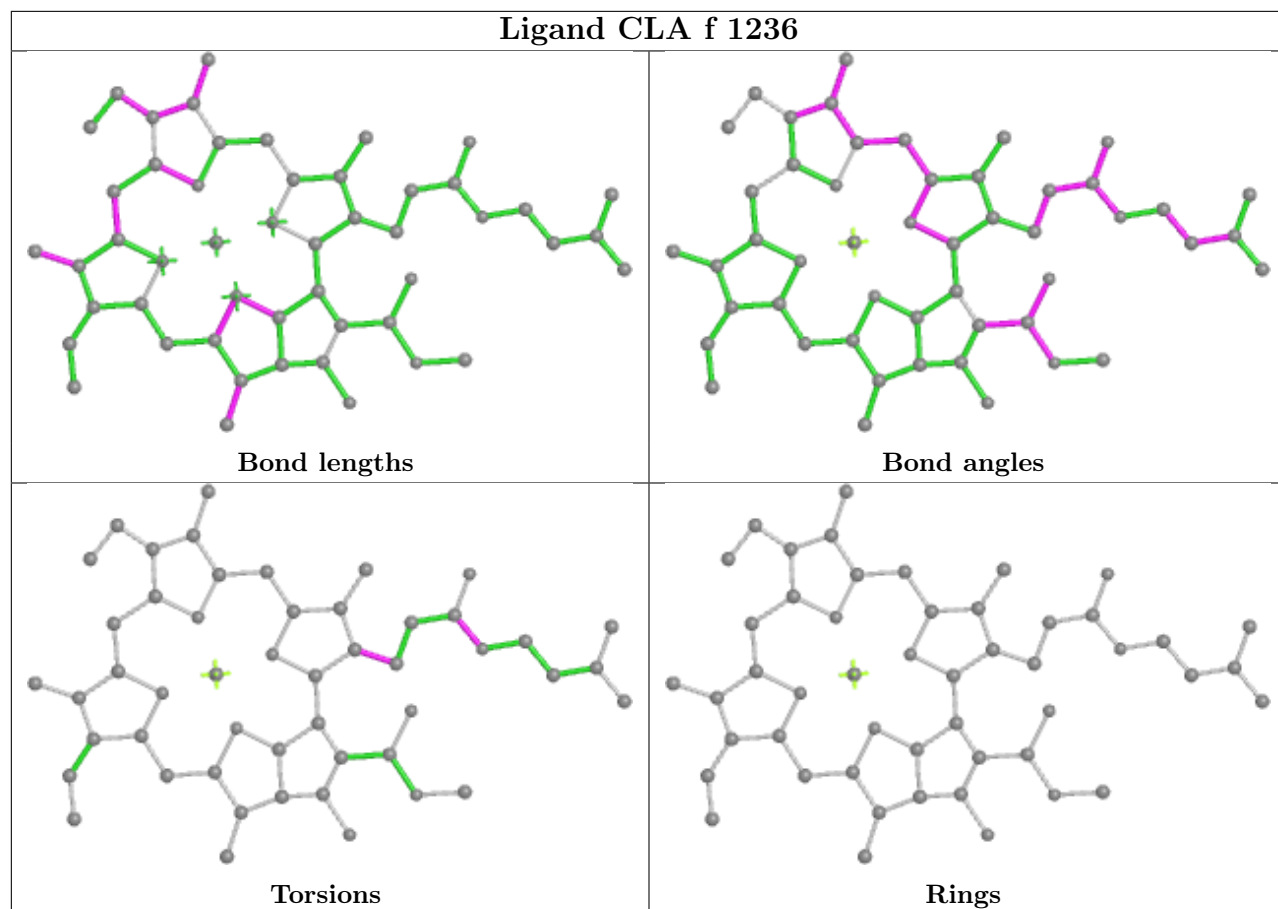


Rings

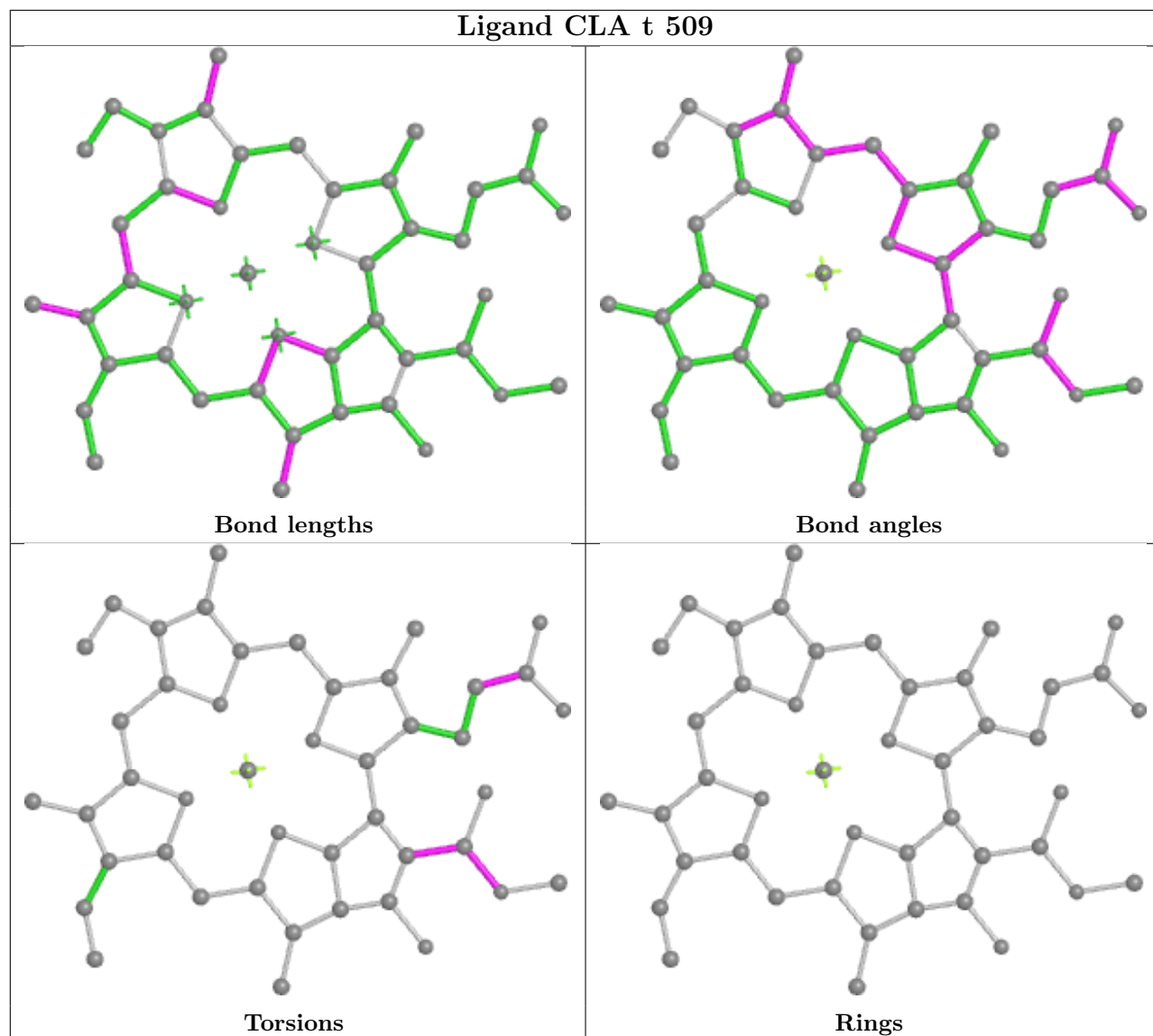
Ligand CLA Z 503**Ligand BCR s 523**

Ligand CLA u 502

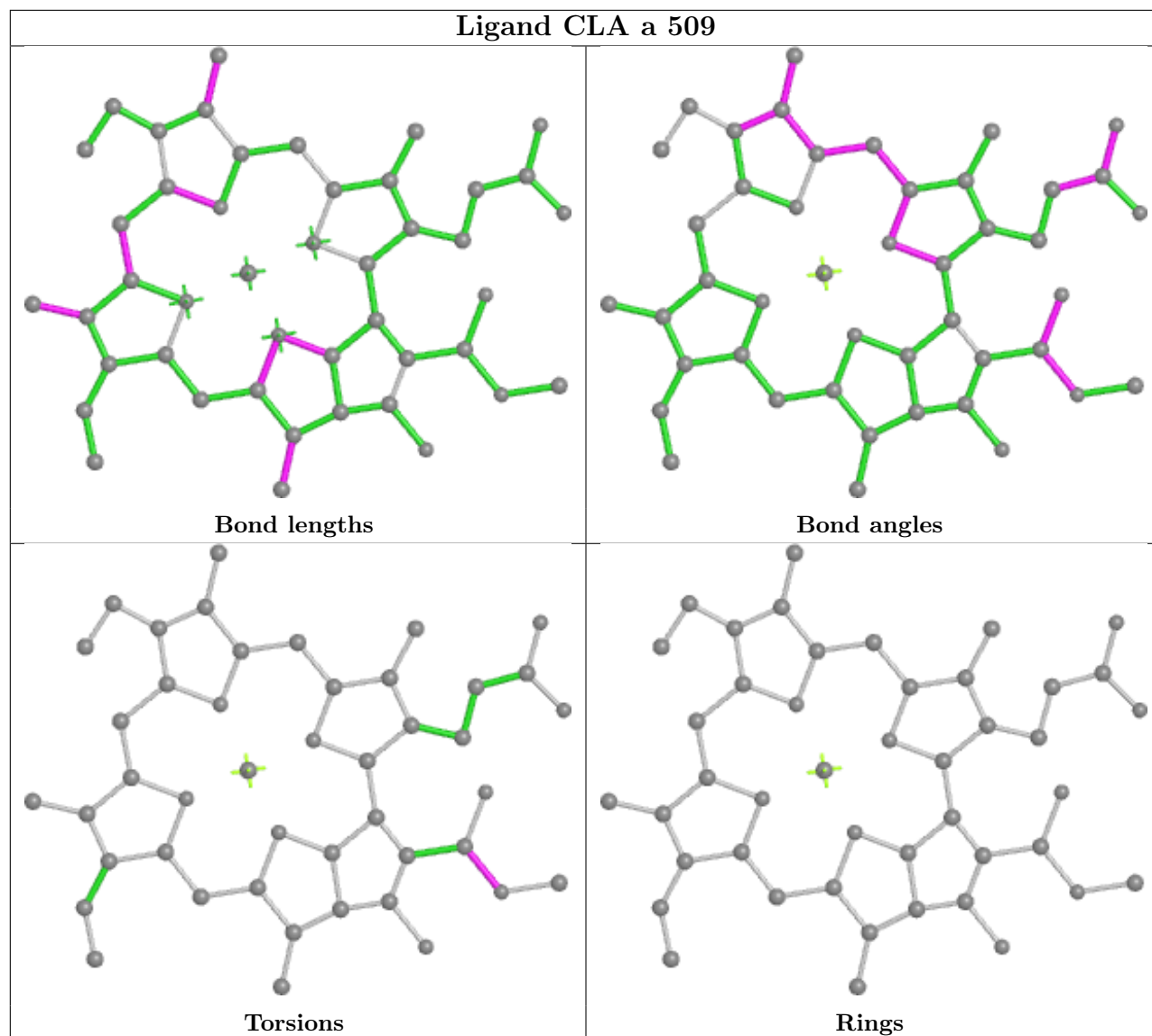




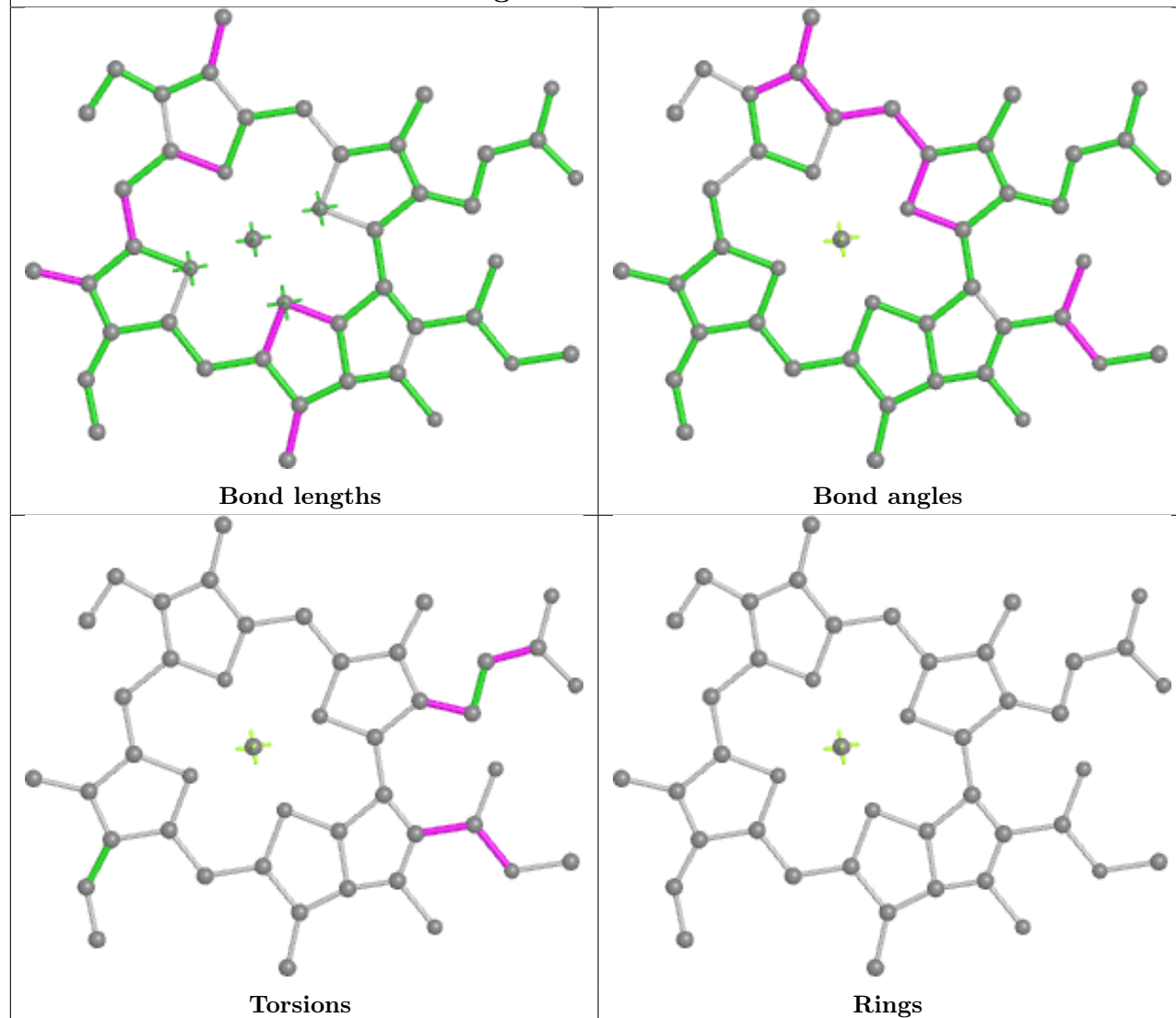
Ligand CLA t 509



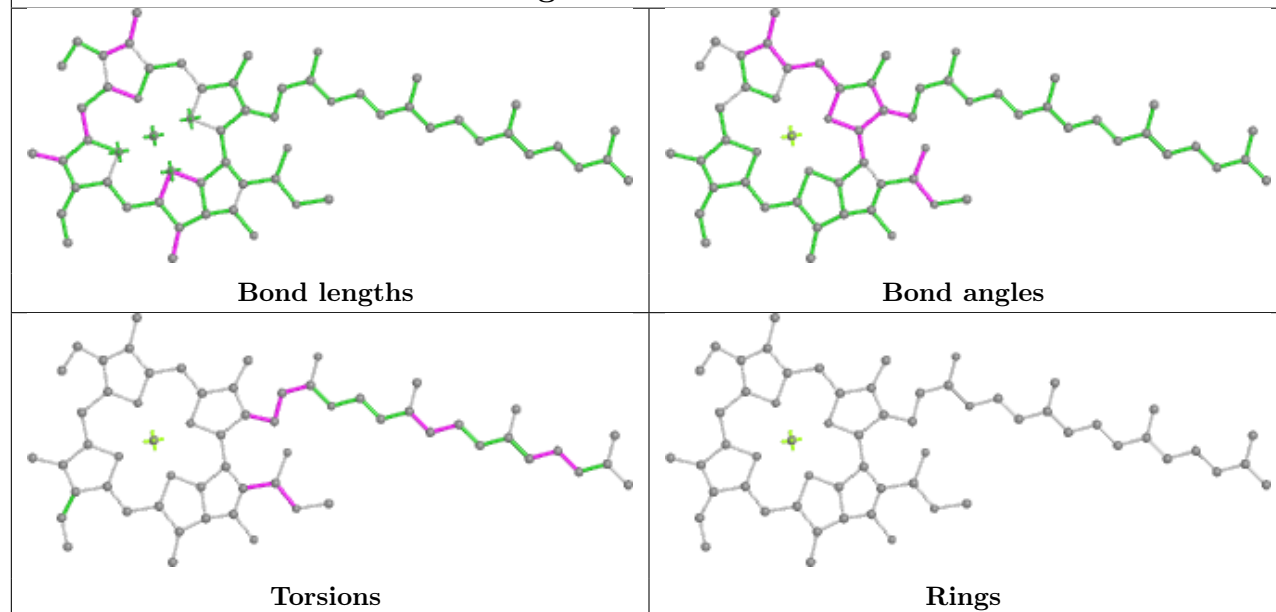
Ligand CLA a 509



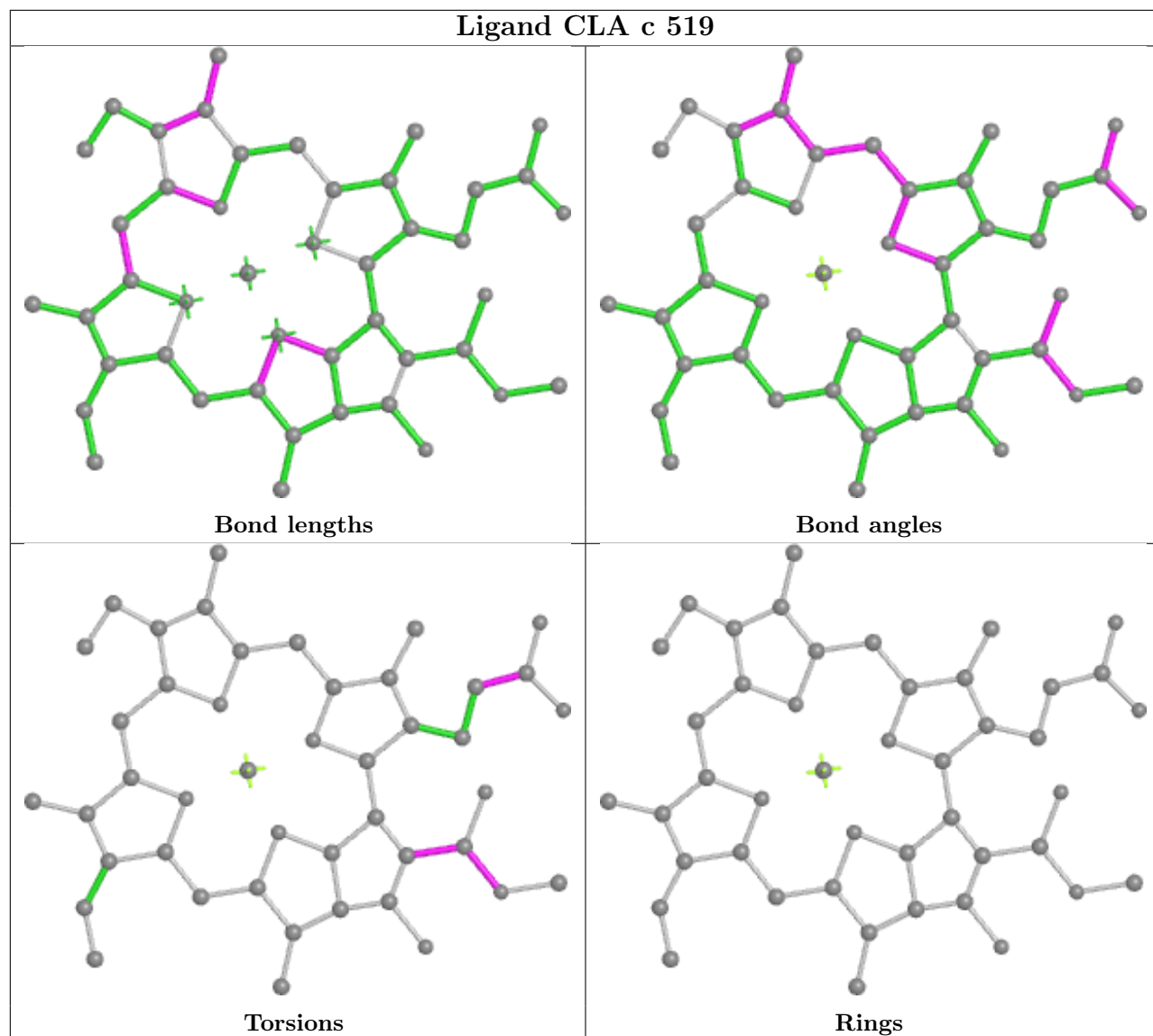
Ligand CLA v 512

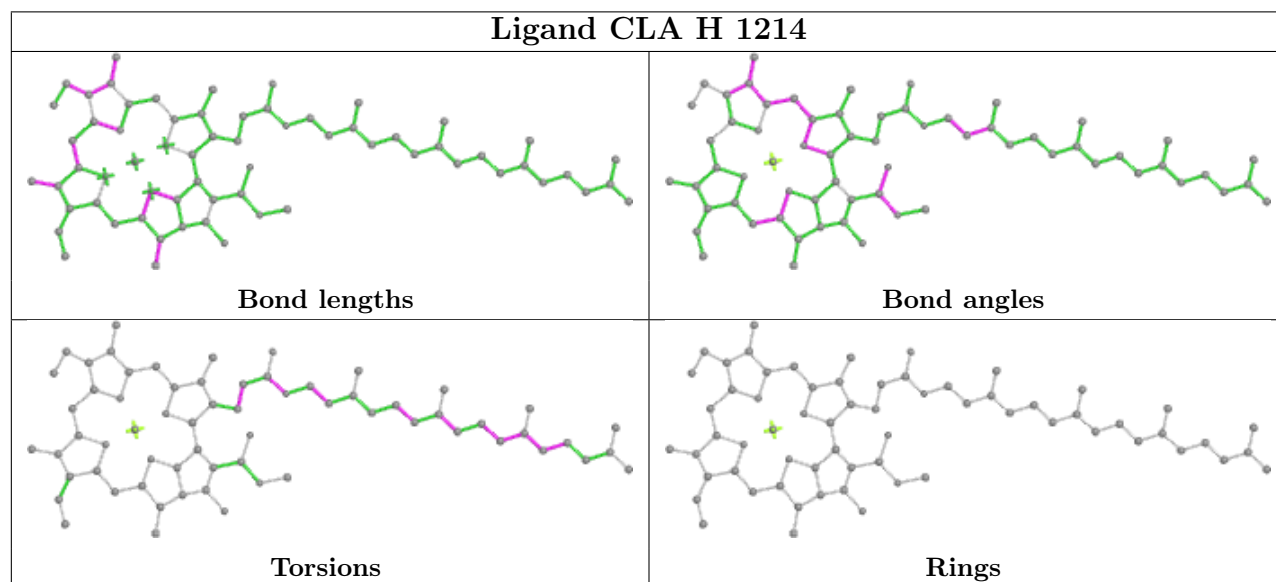
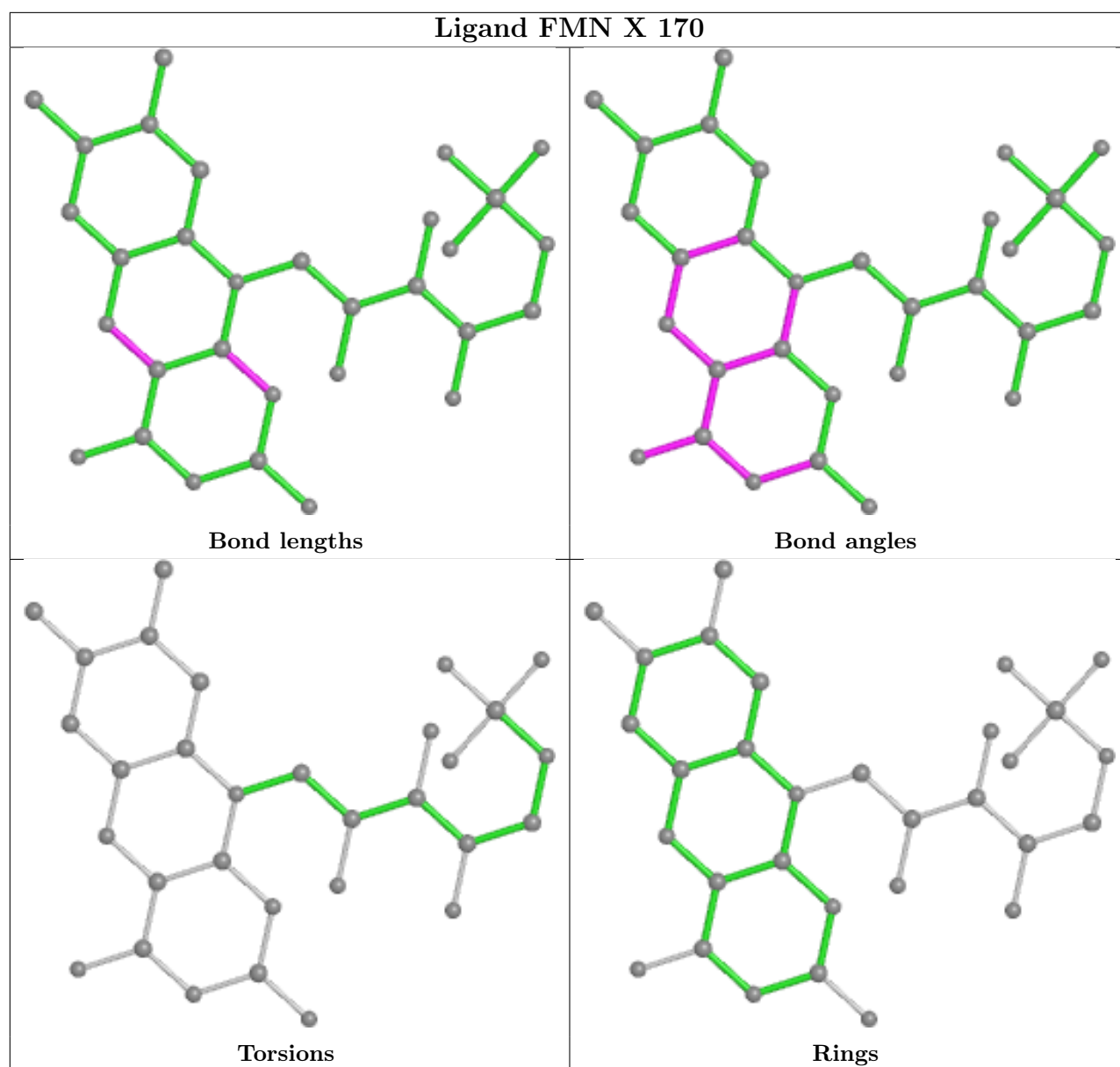


Ligand CLA r 501

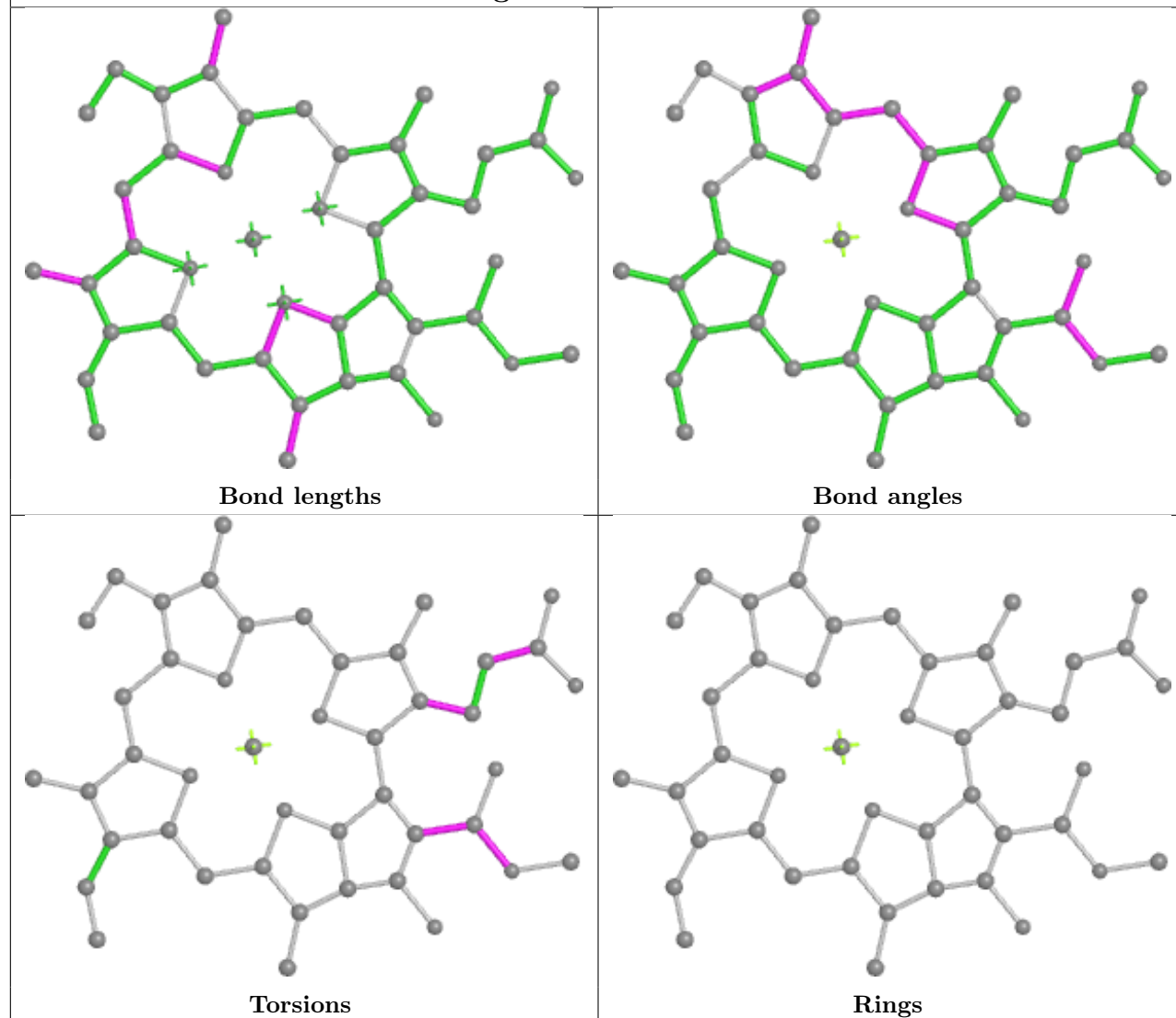


Ligand CLA c 519

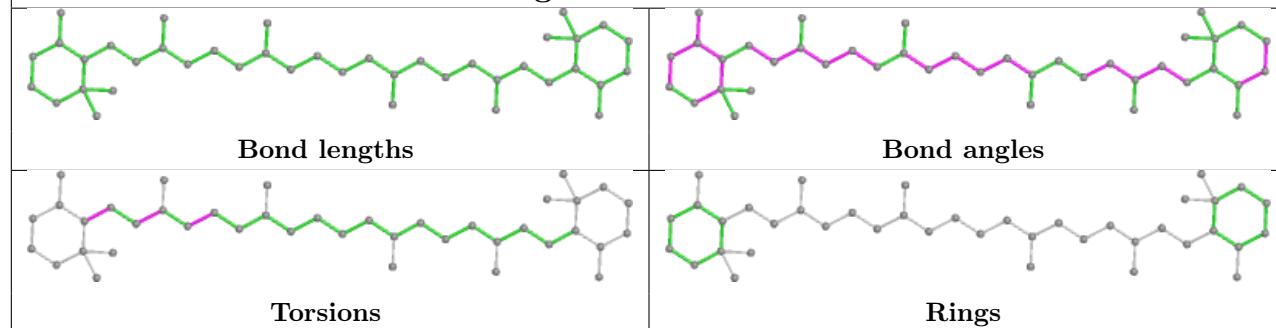




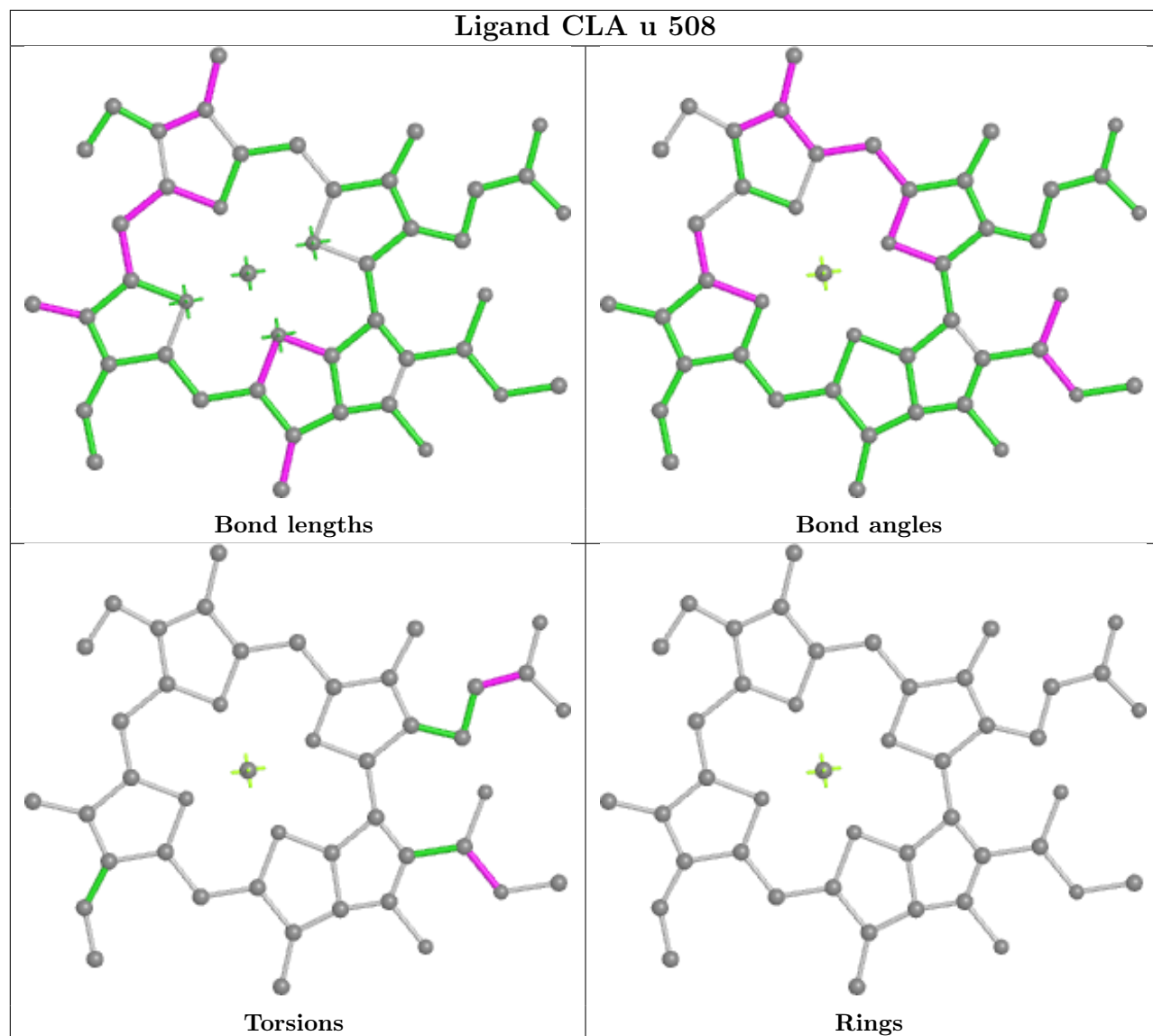
Ligand CLA d 512

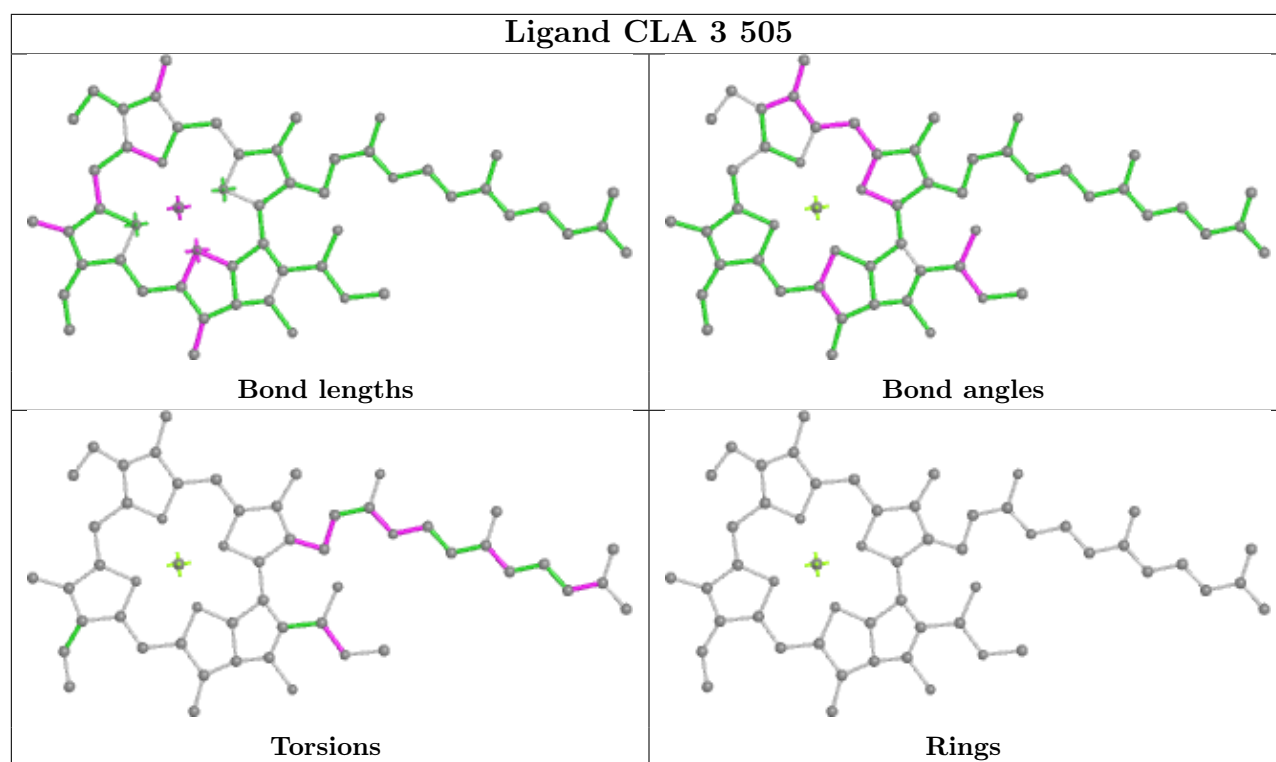


Ligand BCR 6 521

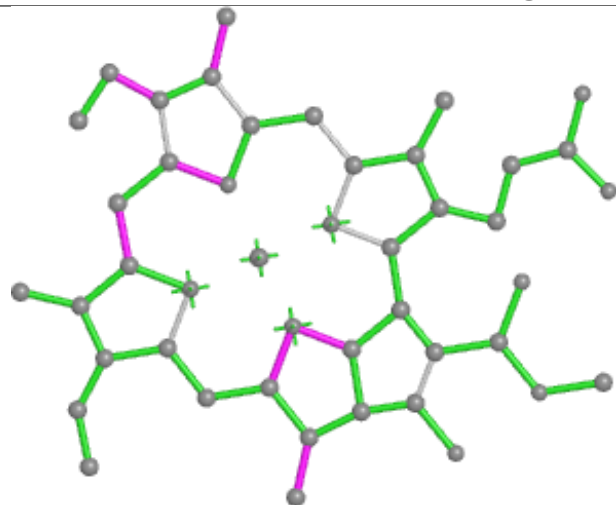


Ligand CLA u 508

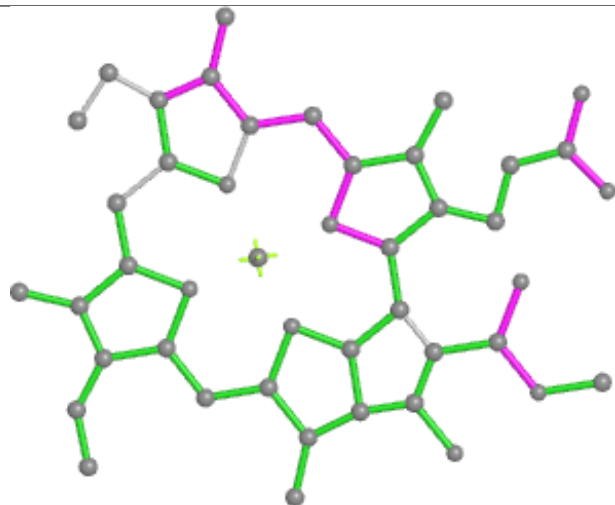




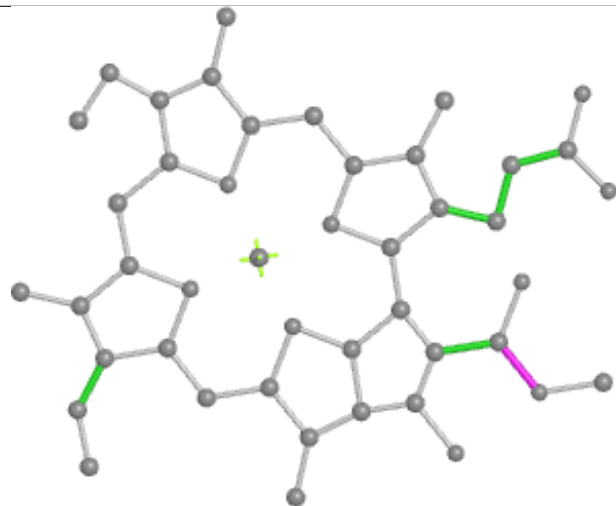
Ligand CLA 1 511



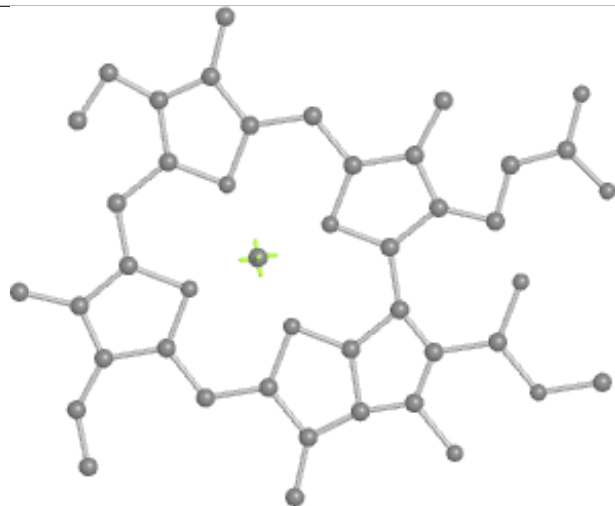
Bond lengths



Bond angles

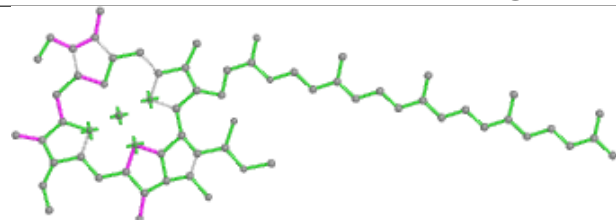


Torsions

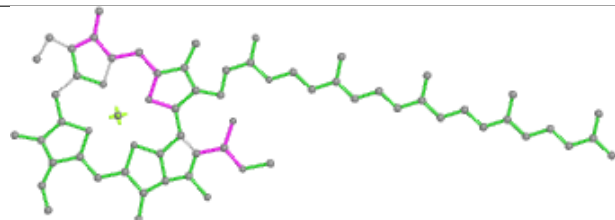


Rings

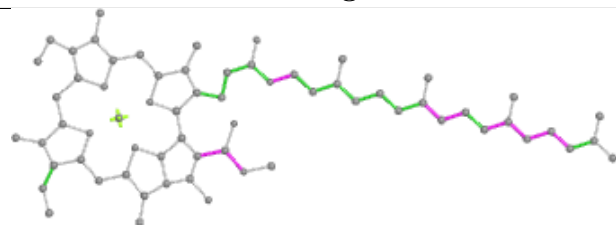
Ligand CLA A 1138



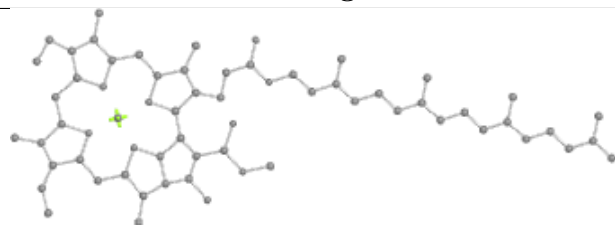
Bond lengths



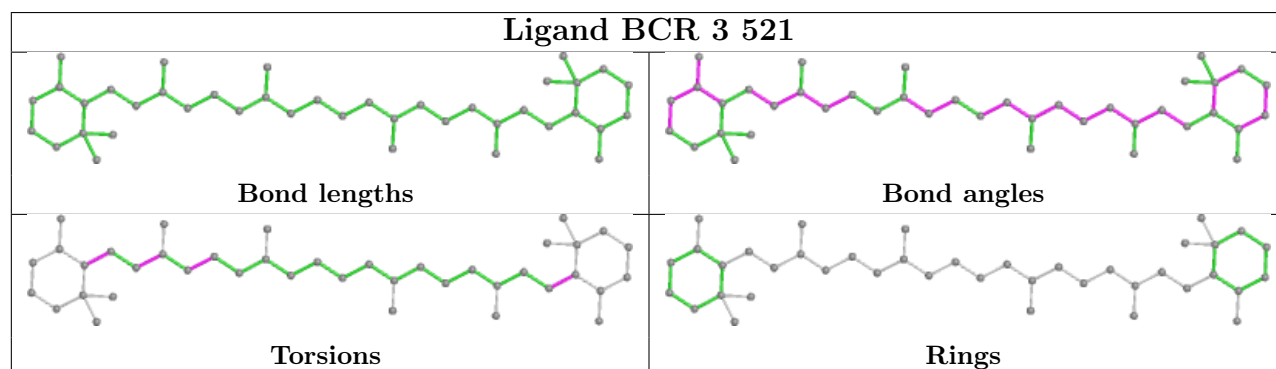
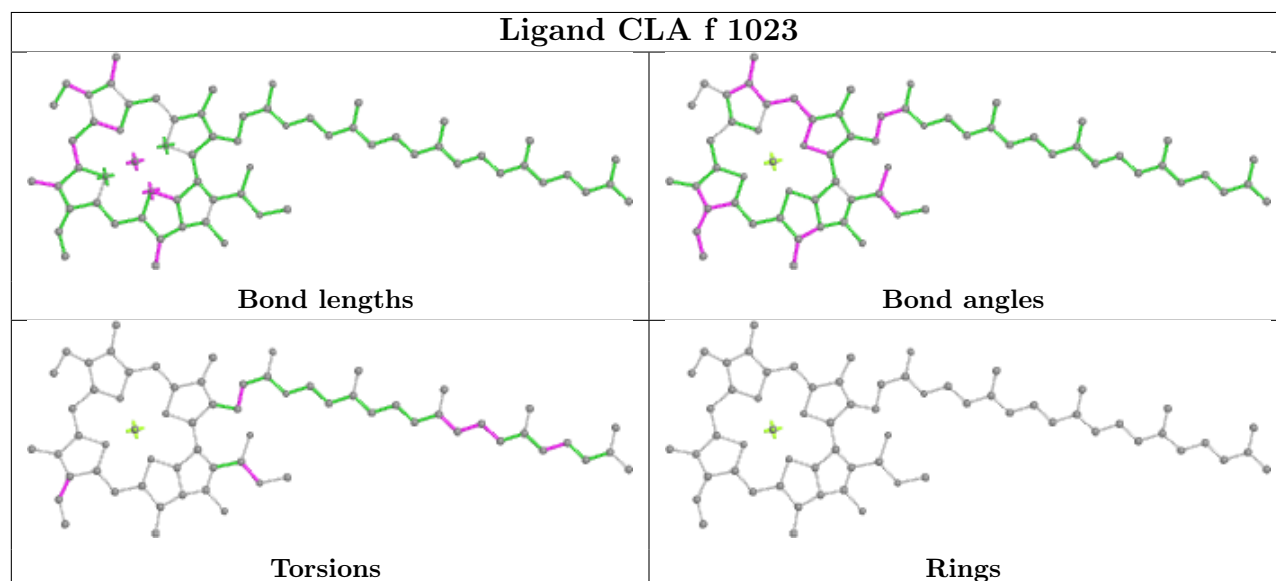
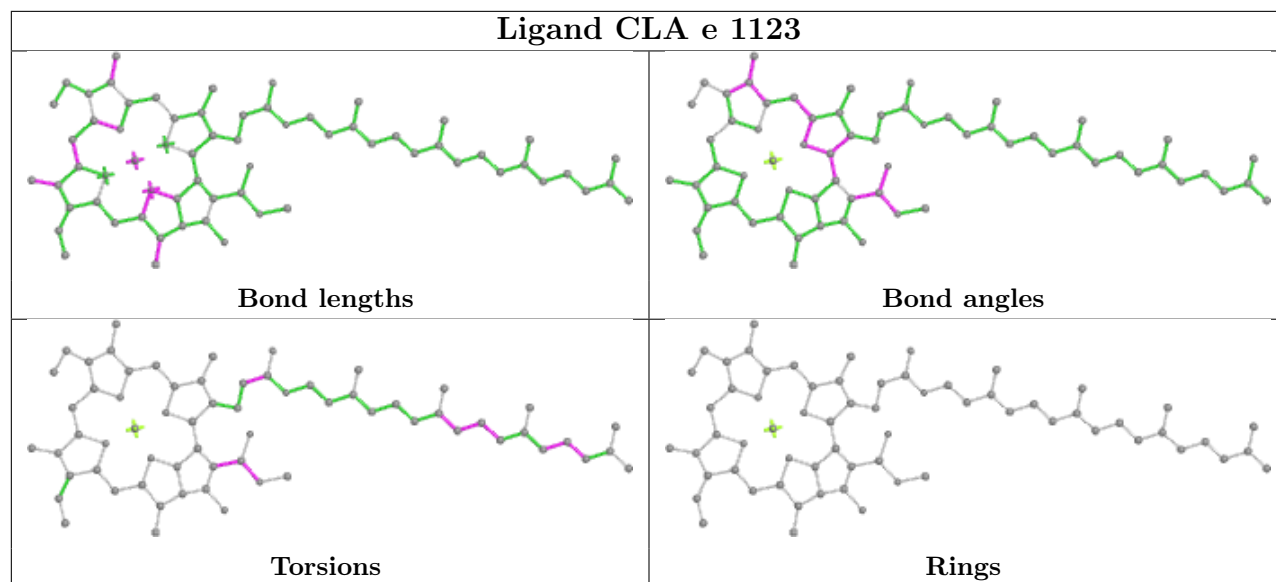
Bond angles



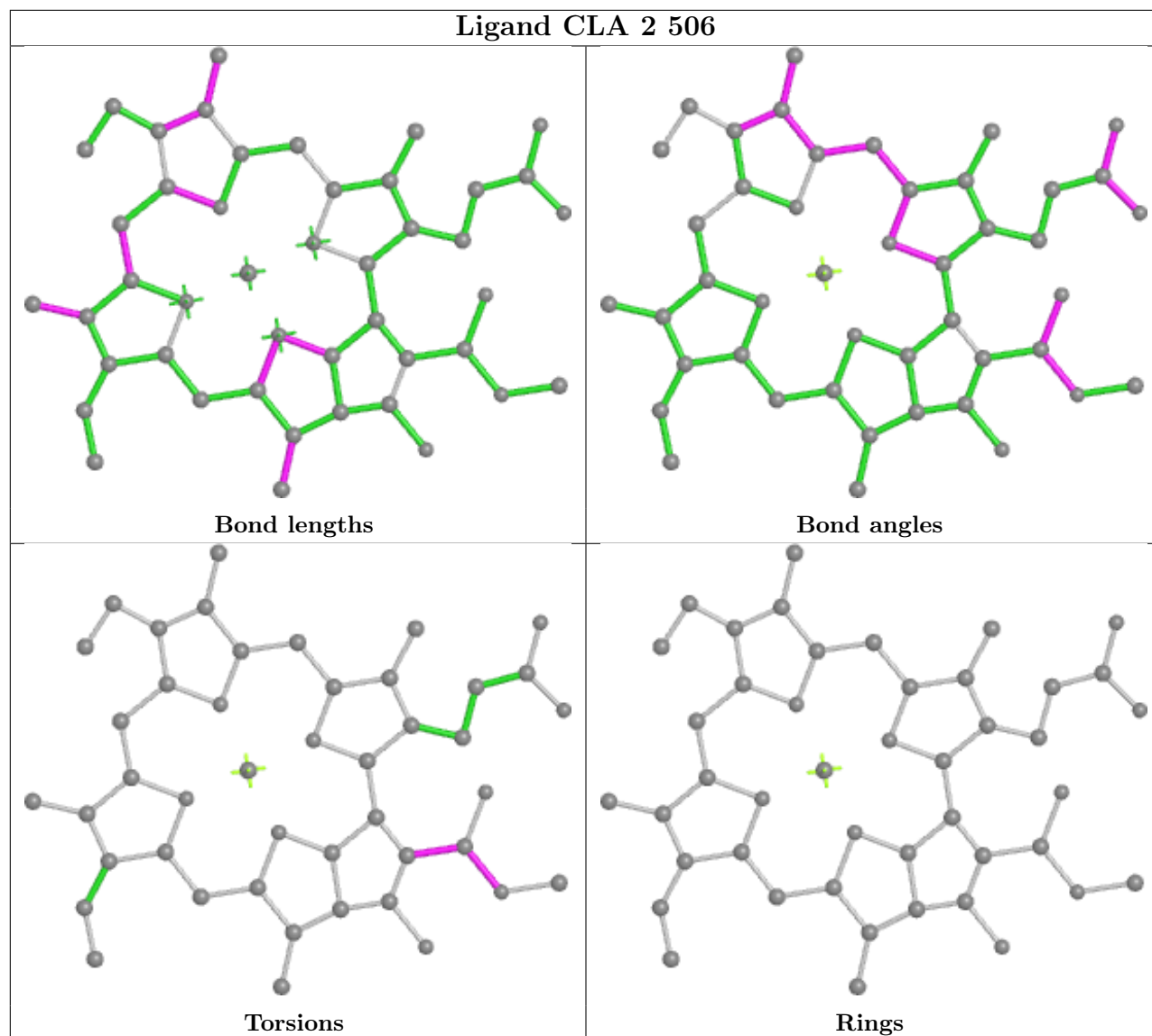
Torsions



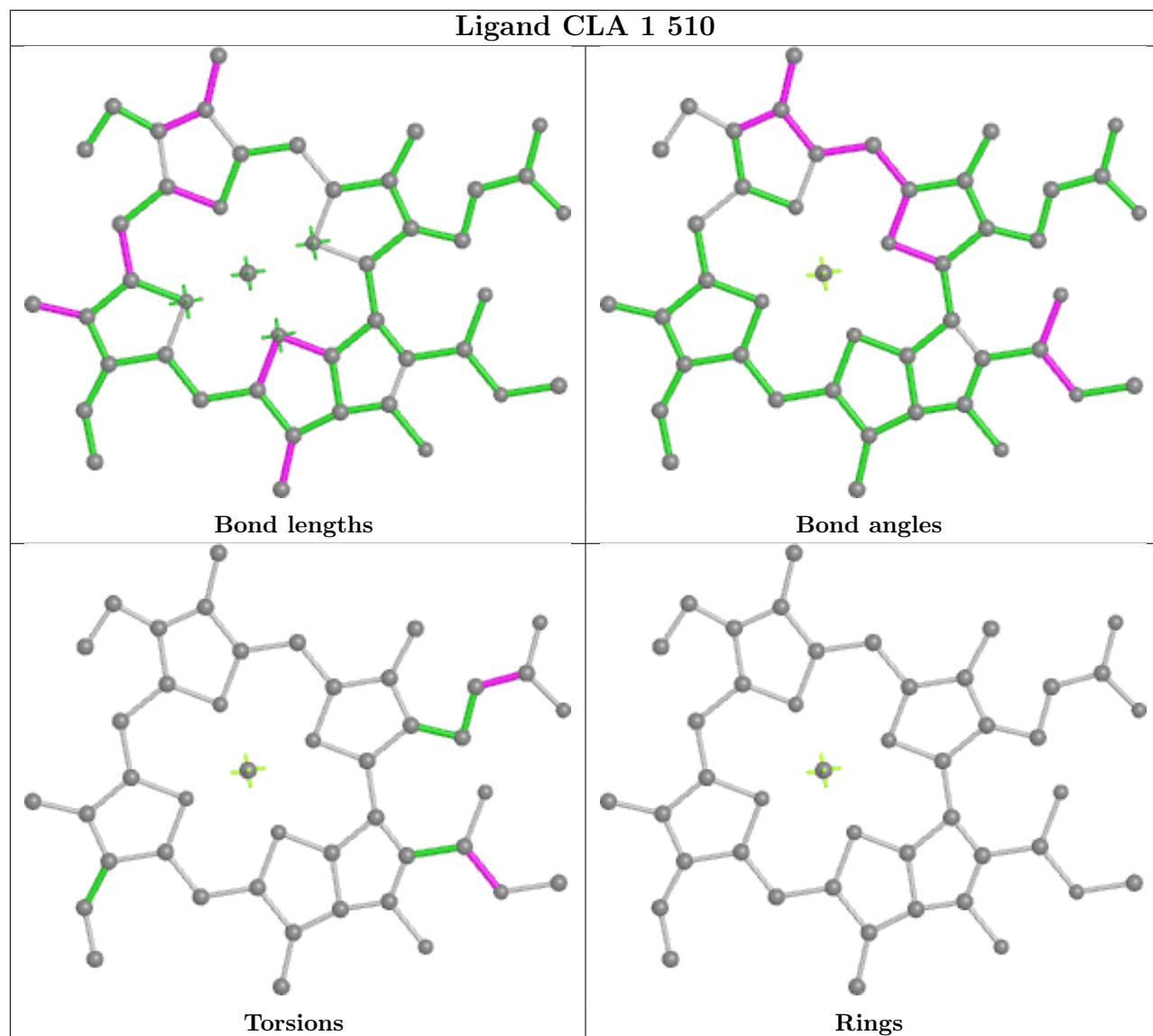
Rings



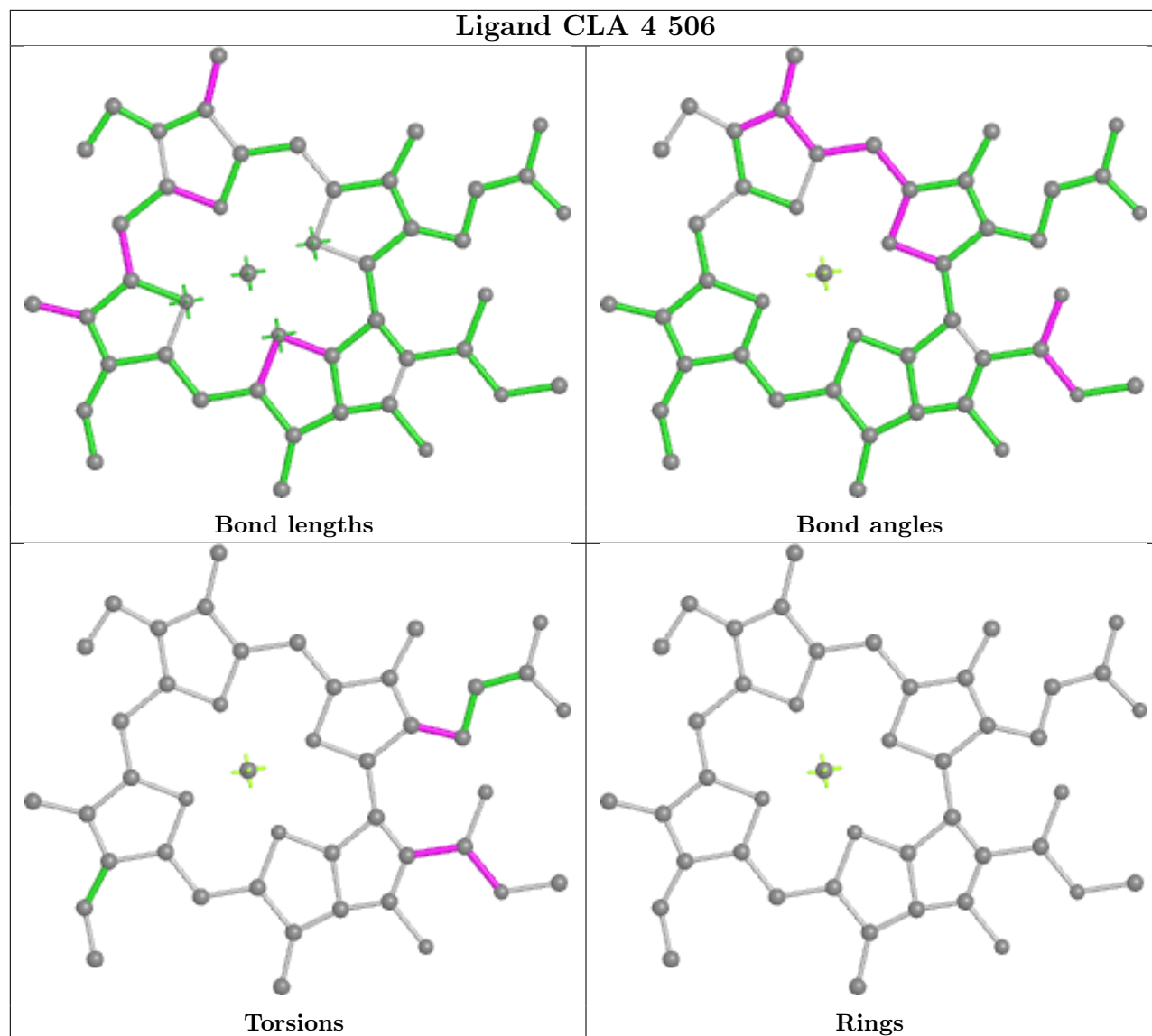
Ligand CLA 2 506



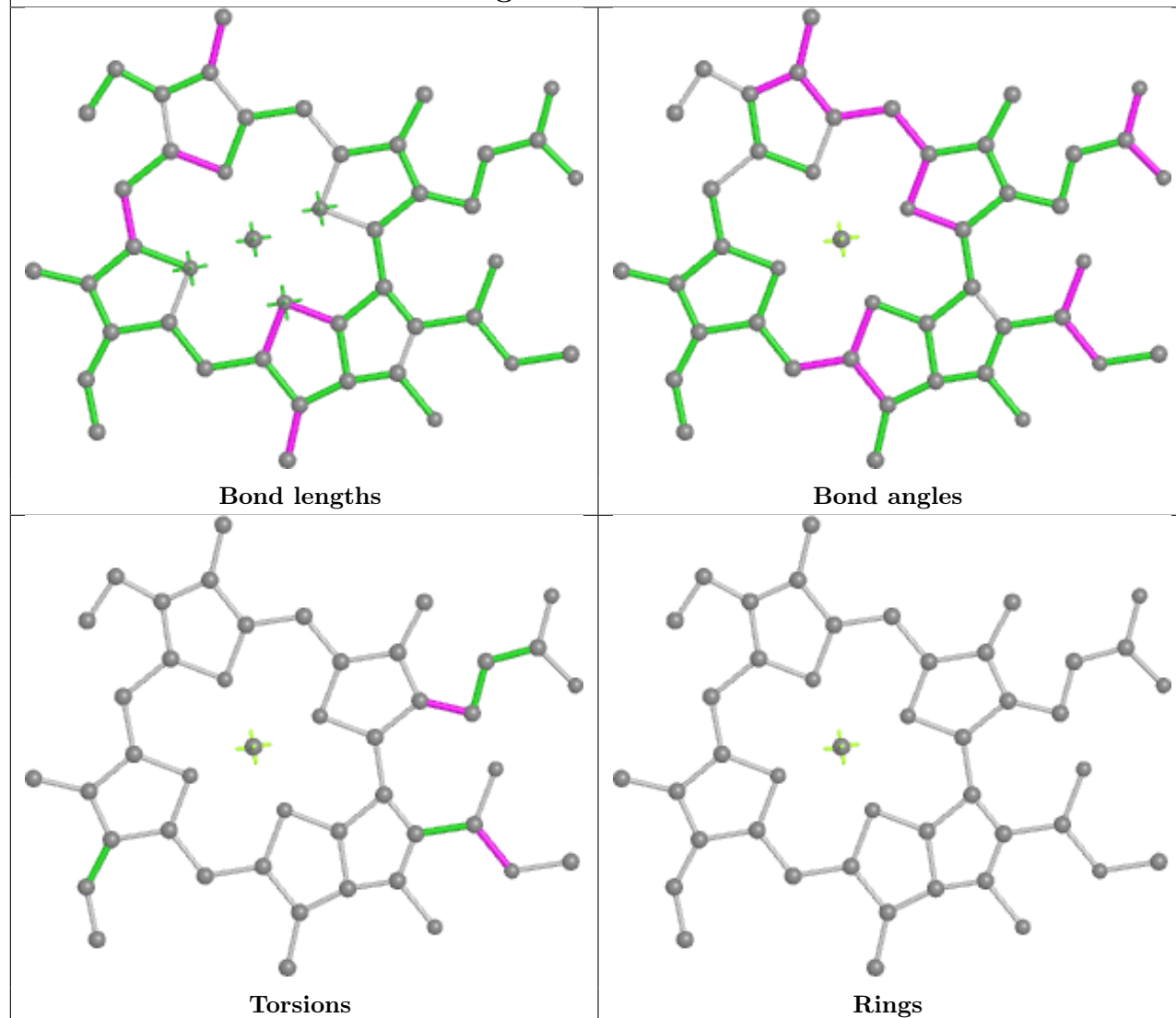
Ligand CLA 1 510



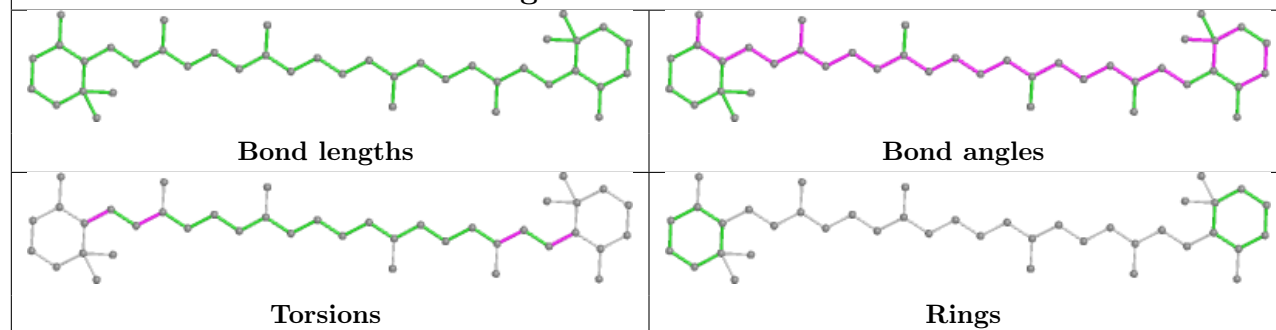
Ligand CLA 4 506



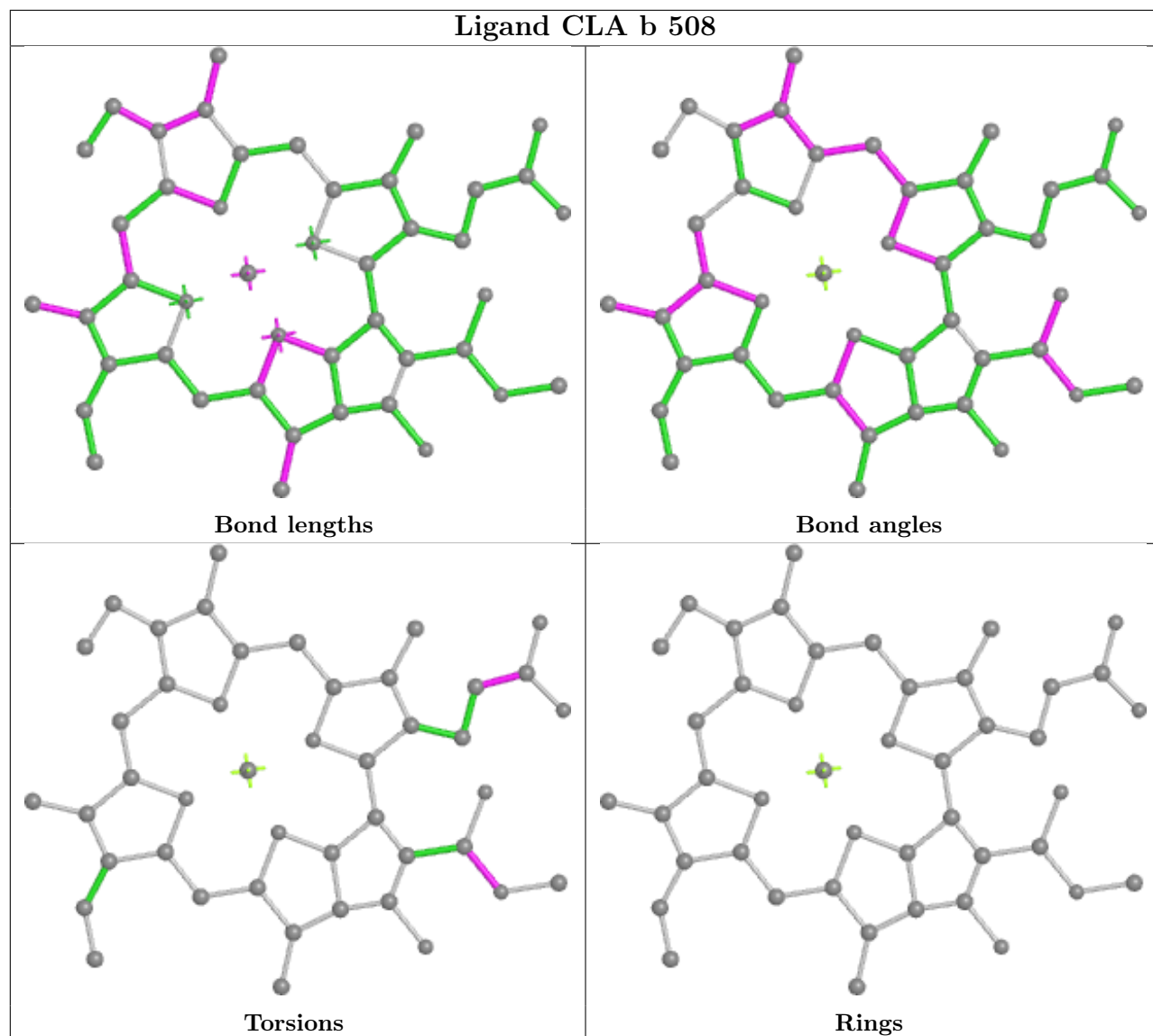
Ligand CLA t 511

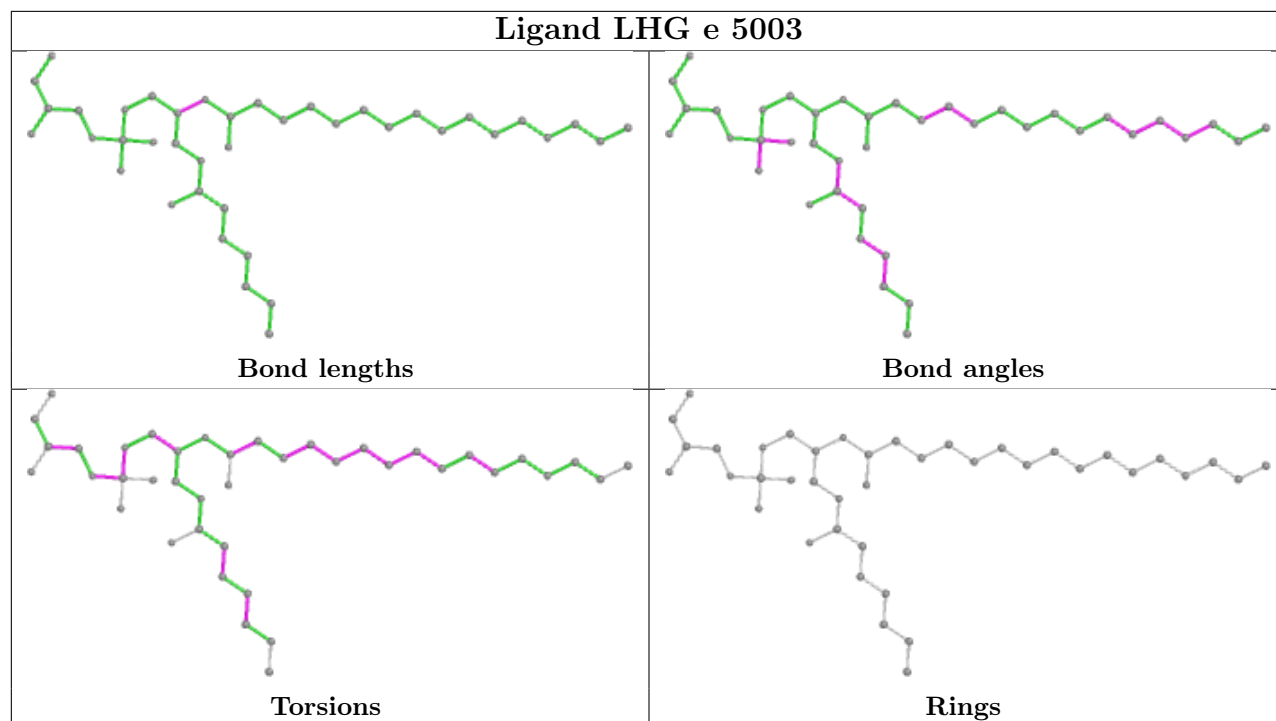


Ligand BCR H 4004

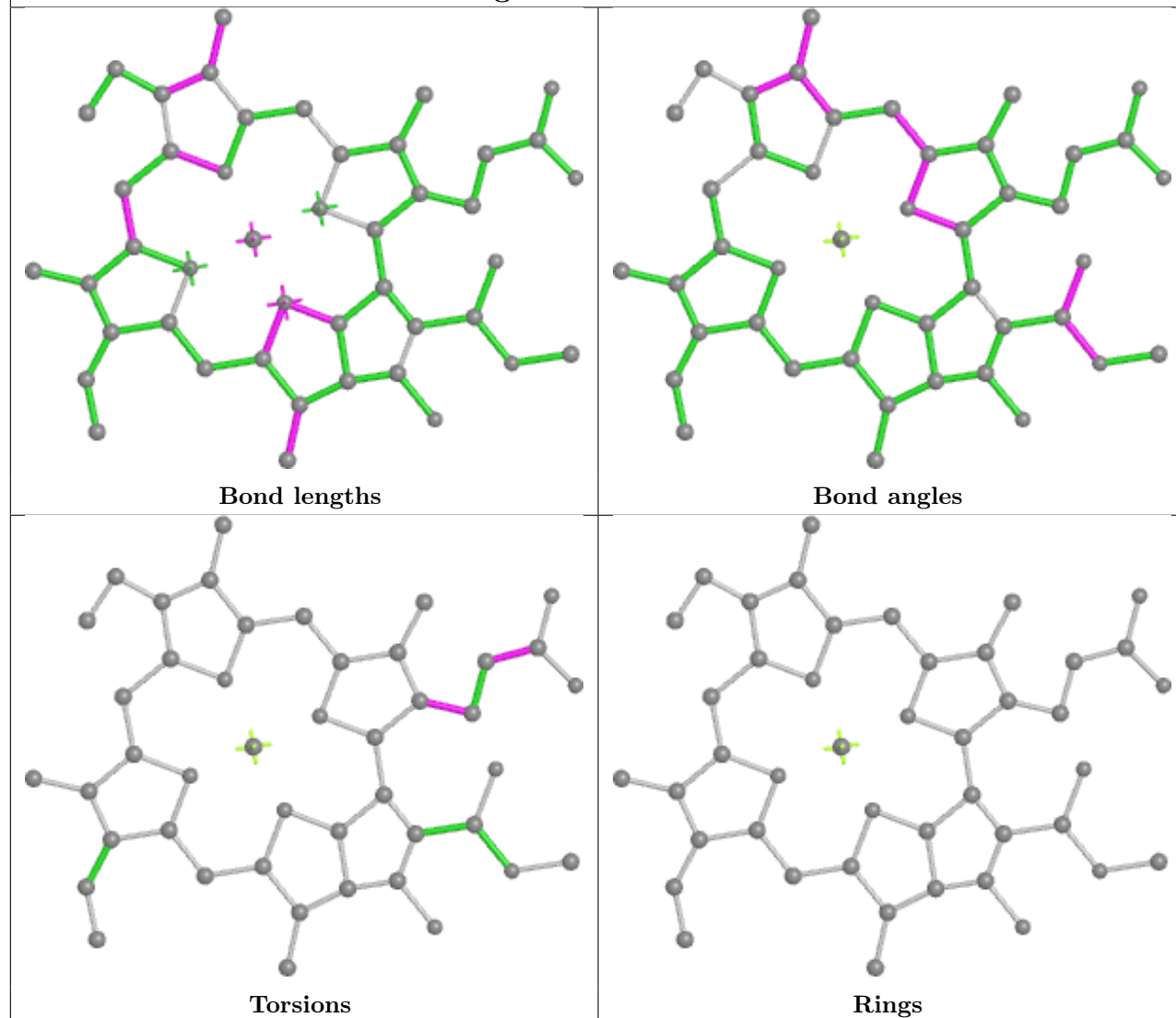


Ligand CLA b 508

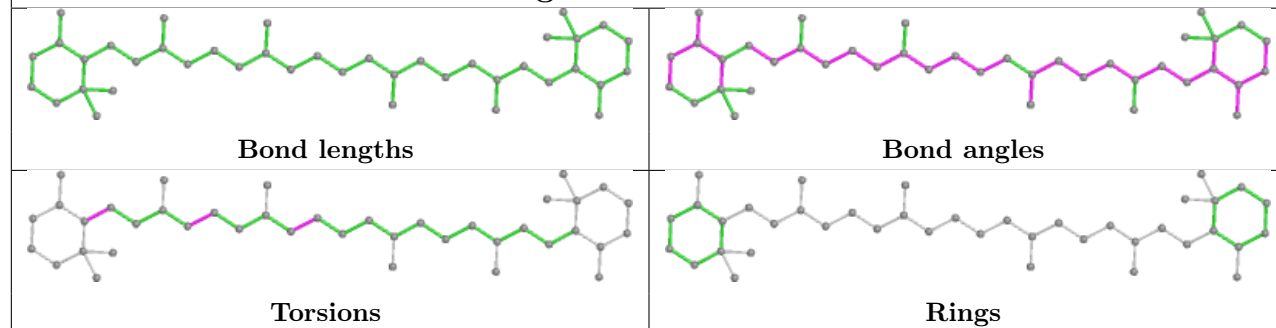




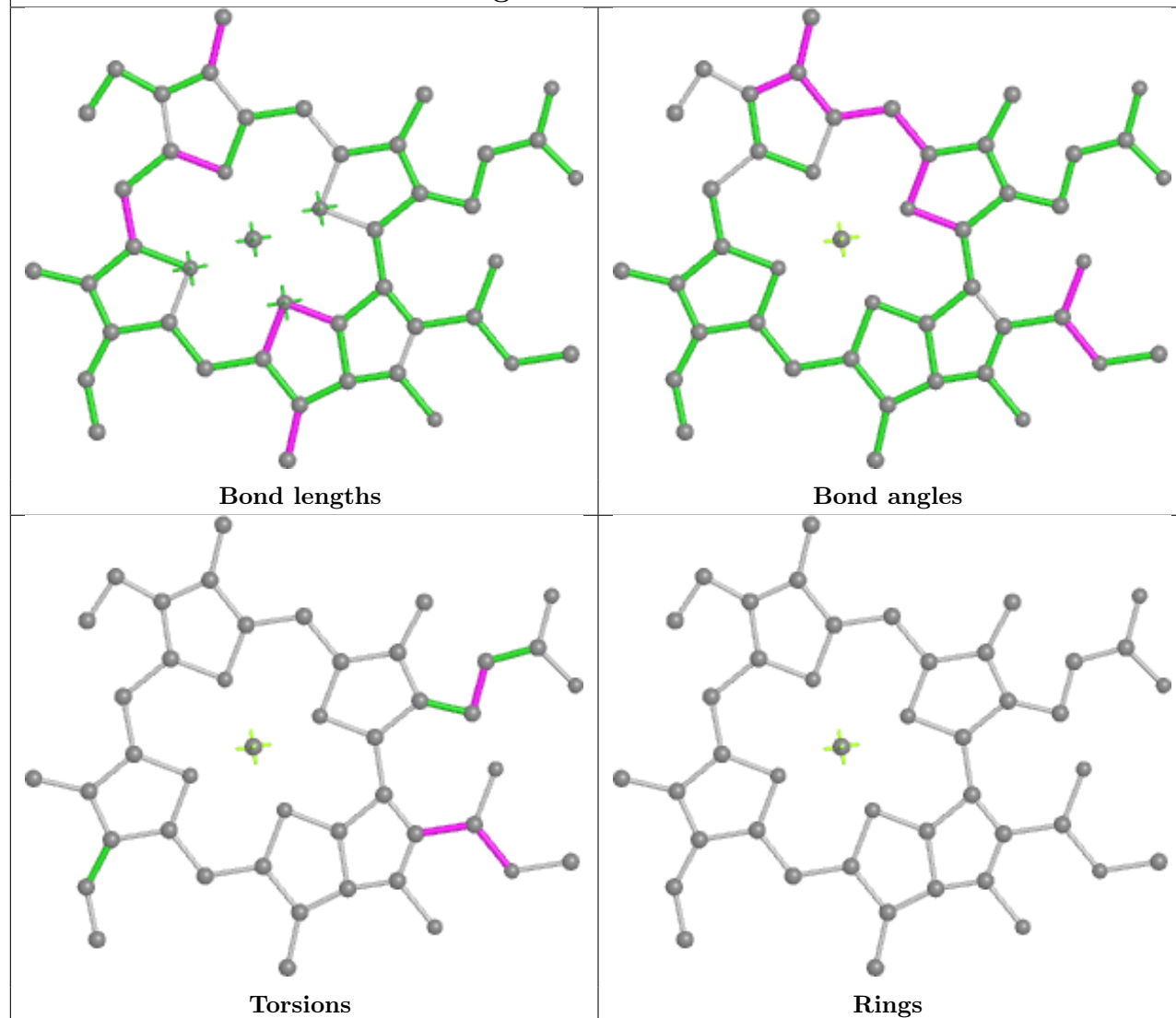
Ligand CLA 2 512



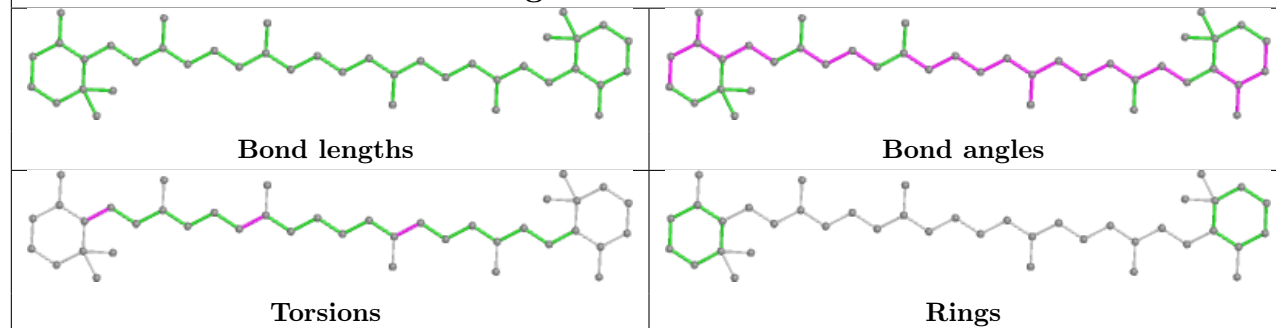
Ligand BCR t 522

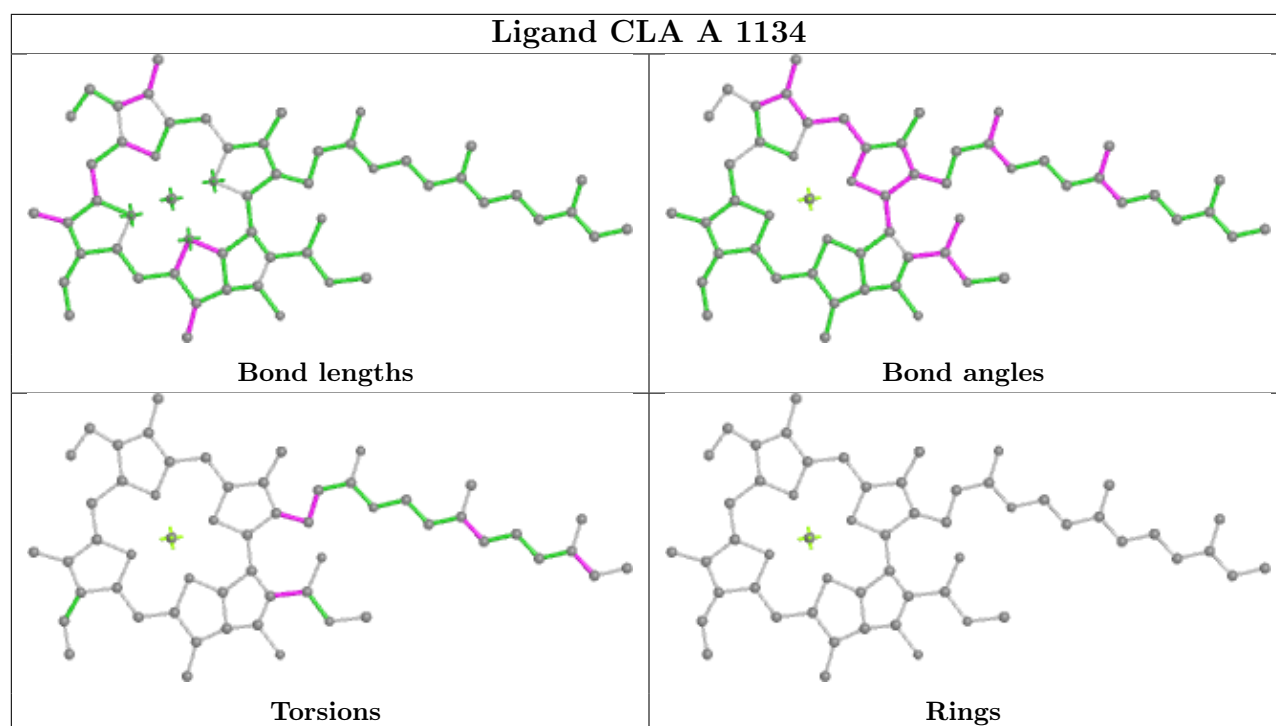


Ligand CLA b 518

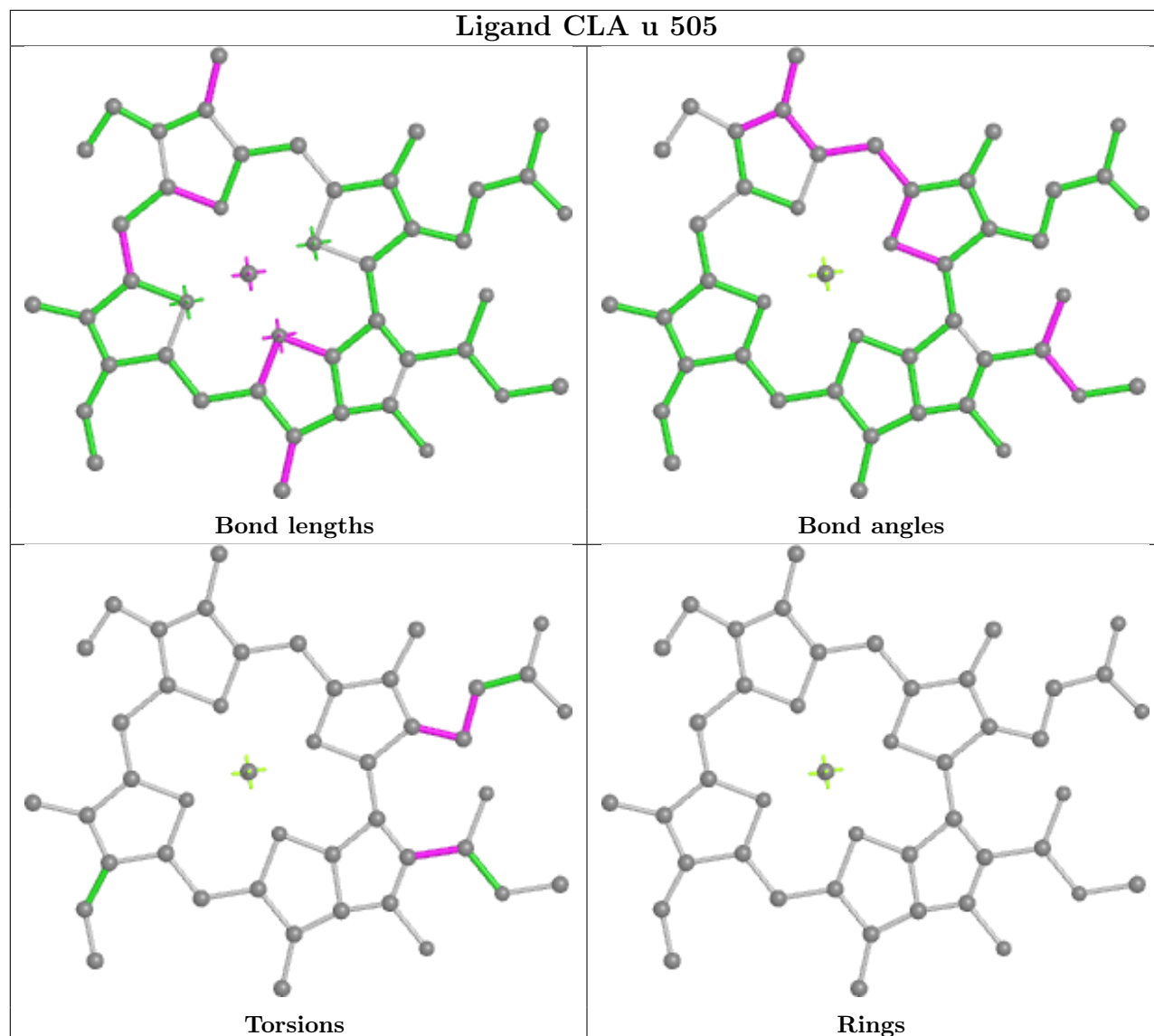


Ligand BCR o 4021

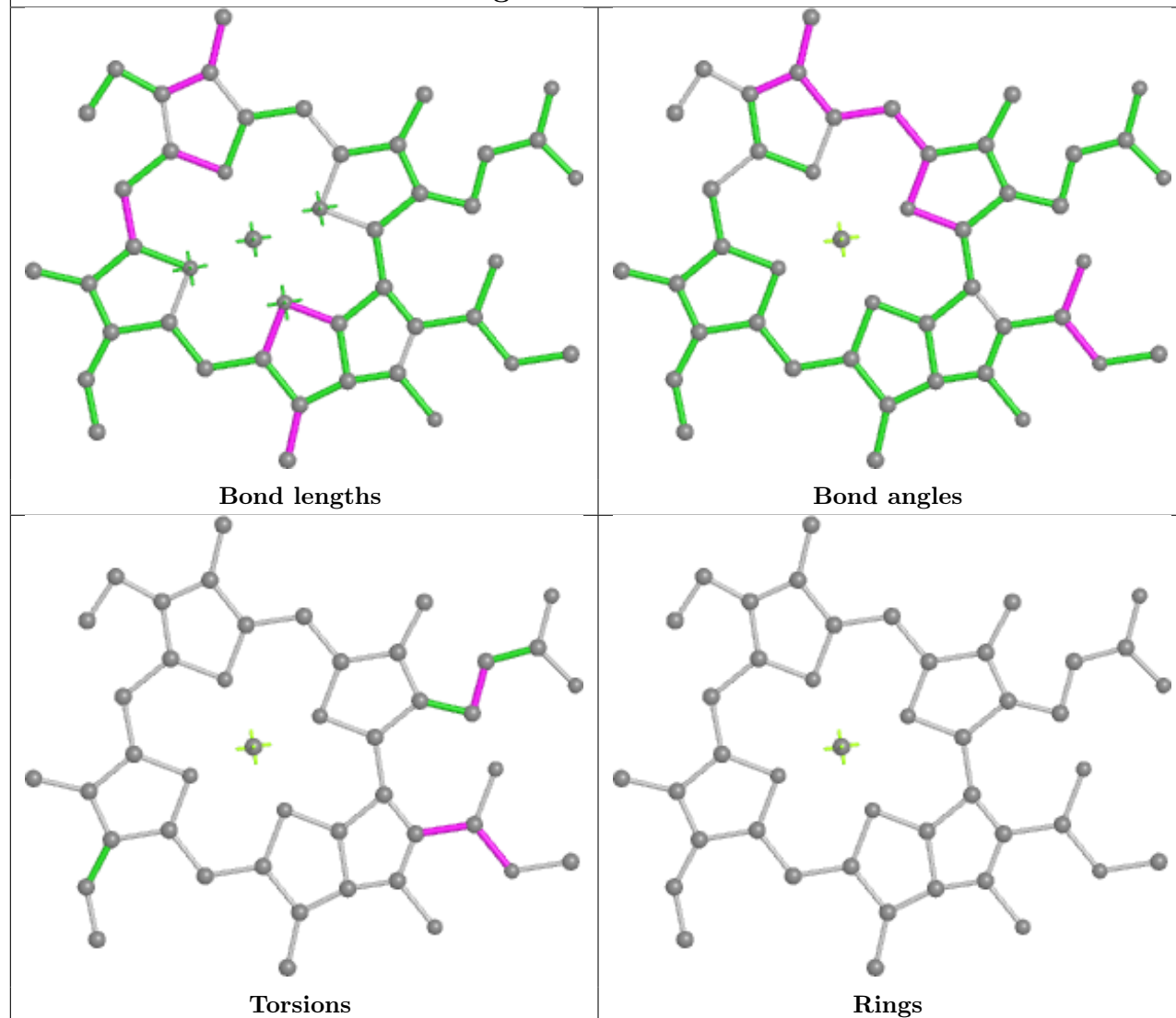




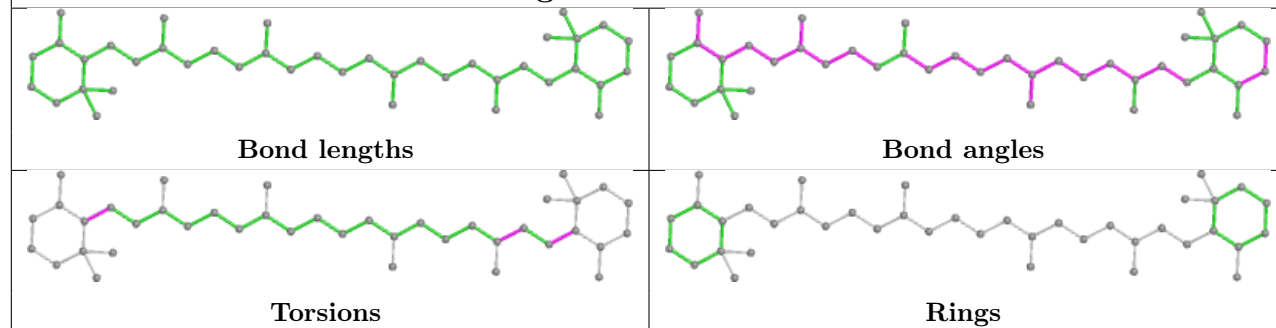
Ligand CLA u 505

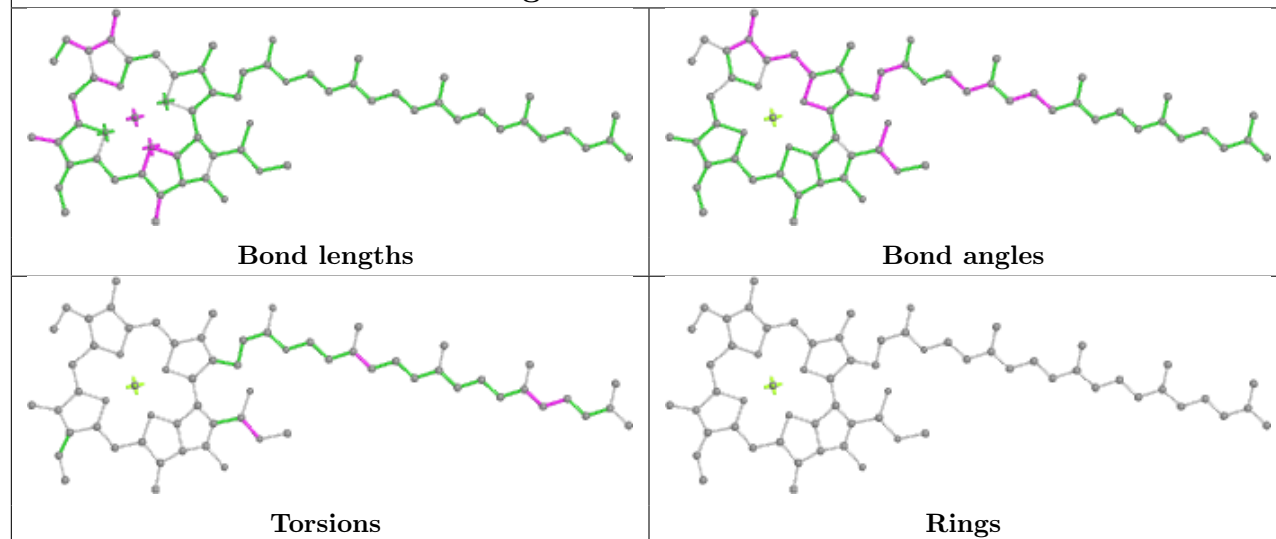
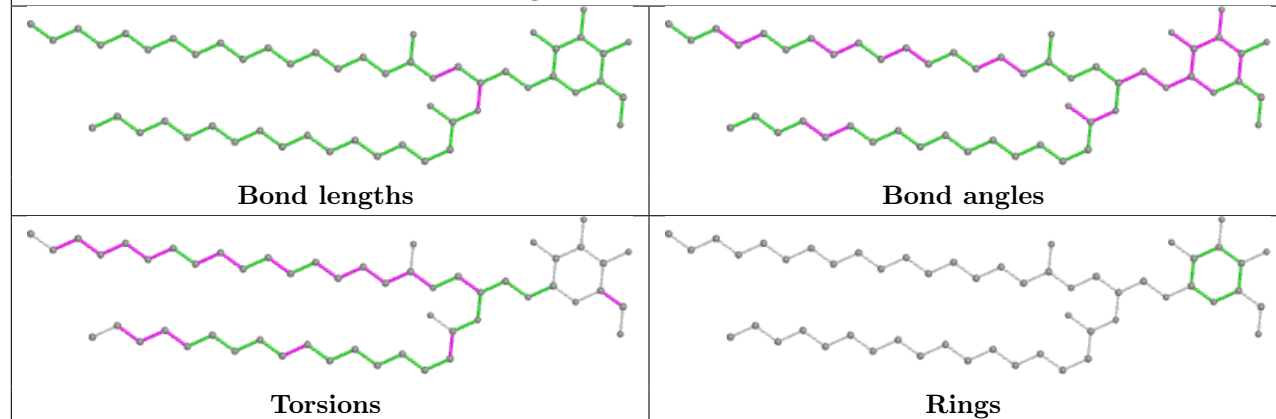


Ligand CLA d 503

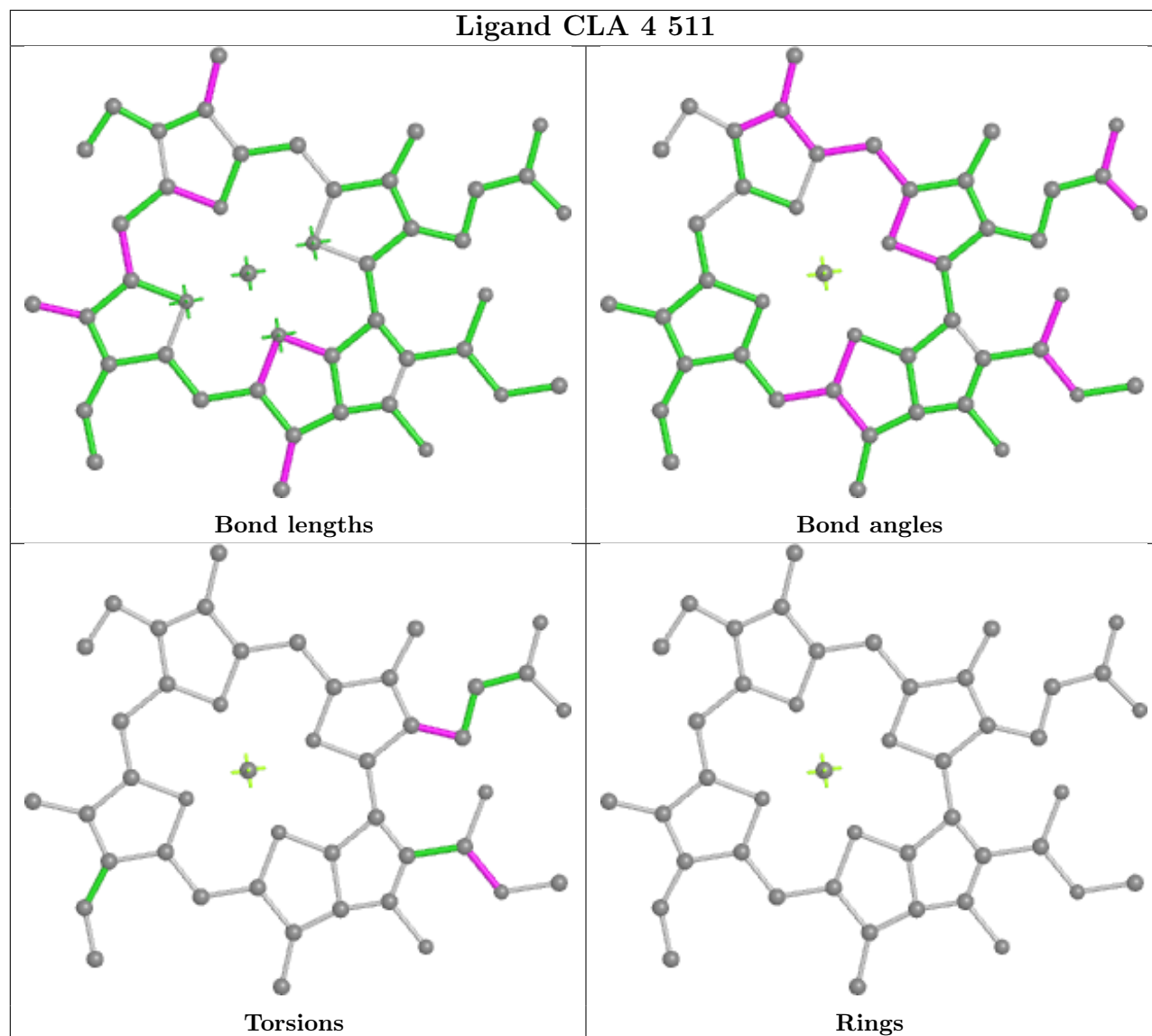


Ligand BCR t 523

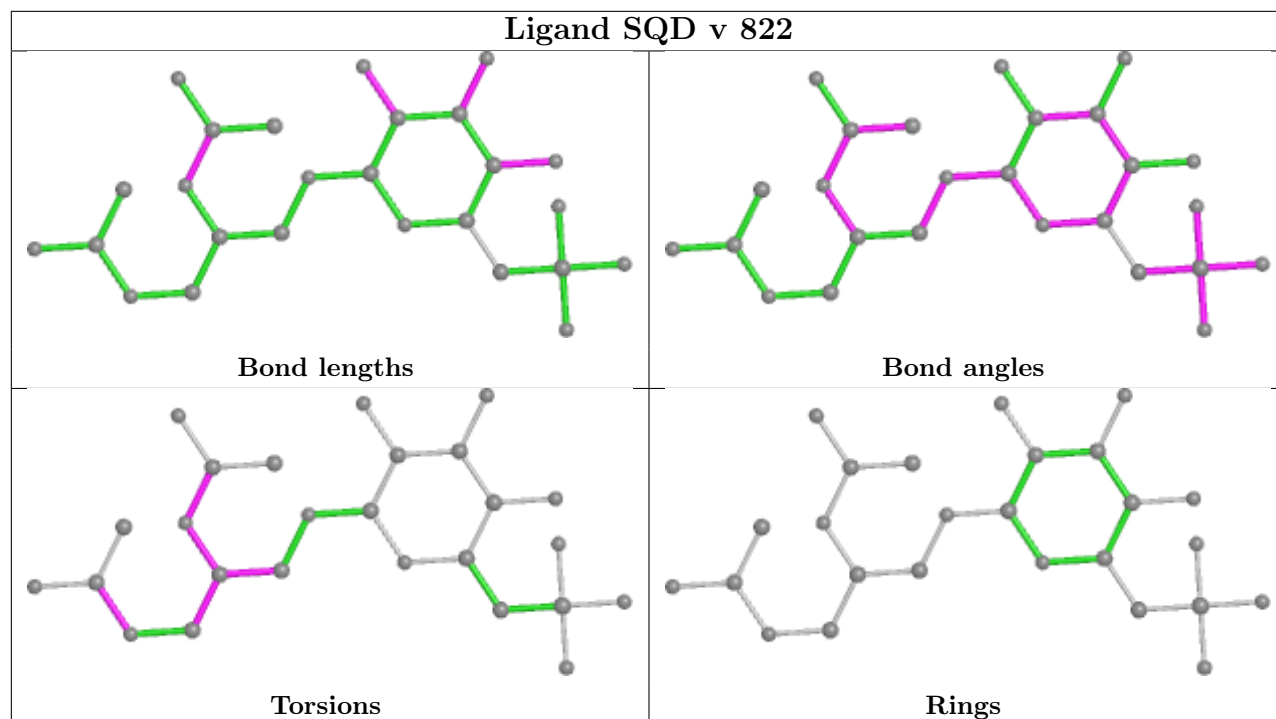


Ligand CLA A 1131**Ligand LMG f 5002**

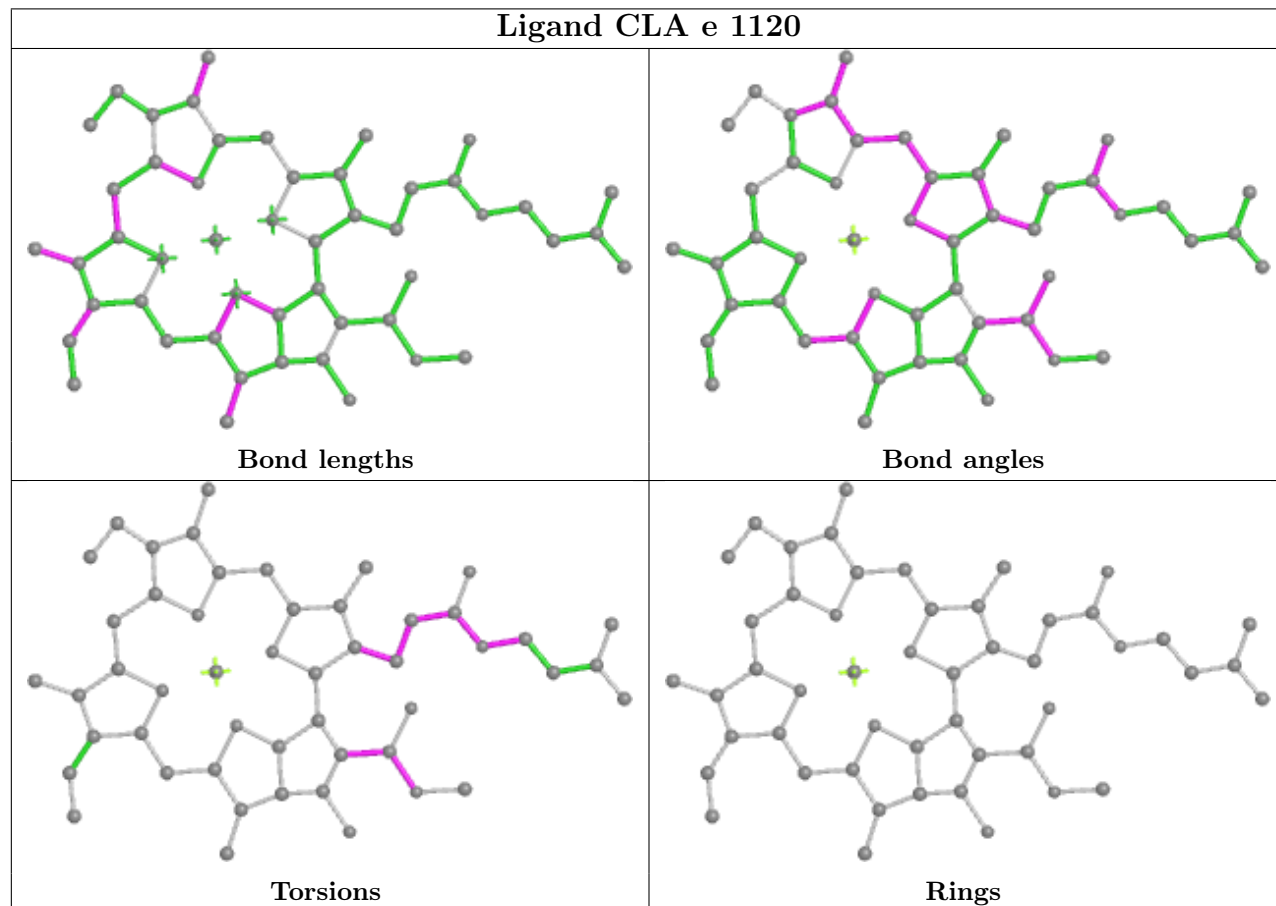
Ligand CLA 4 511

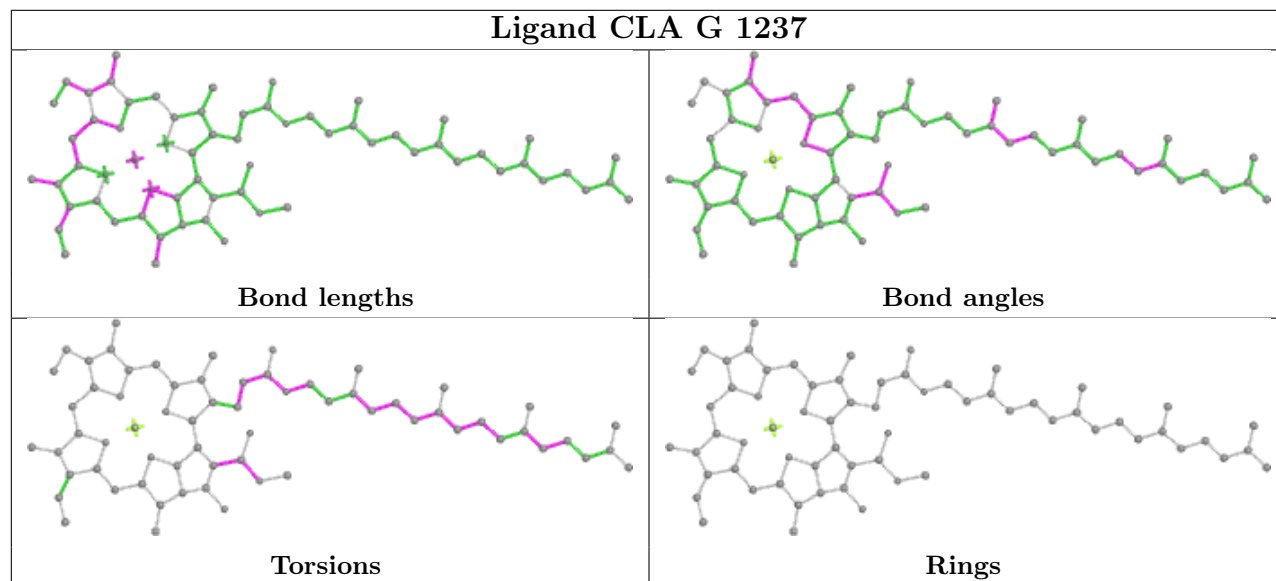
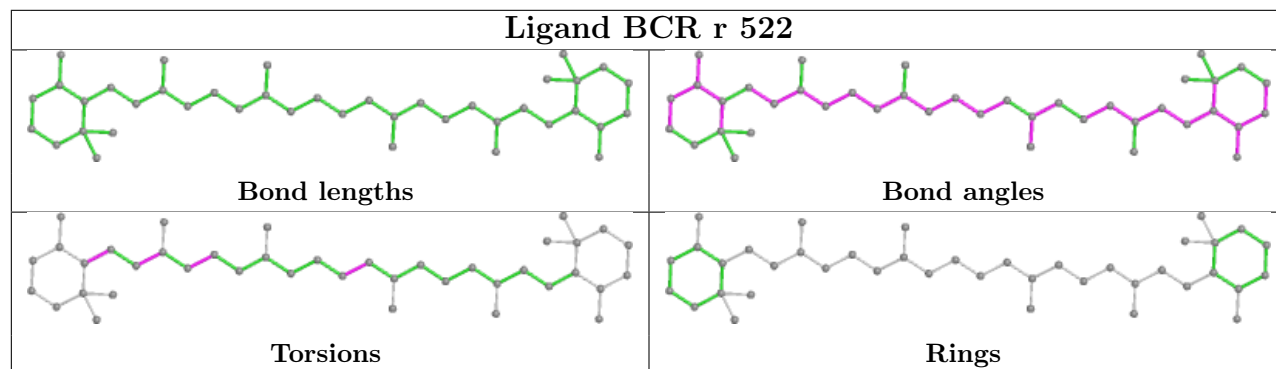
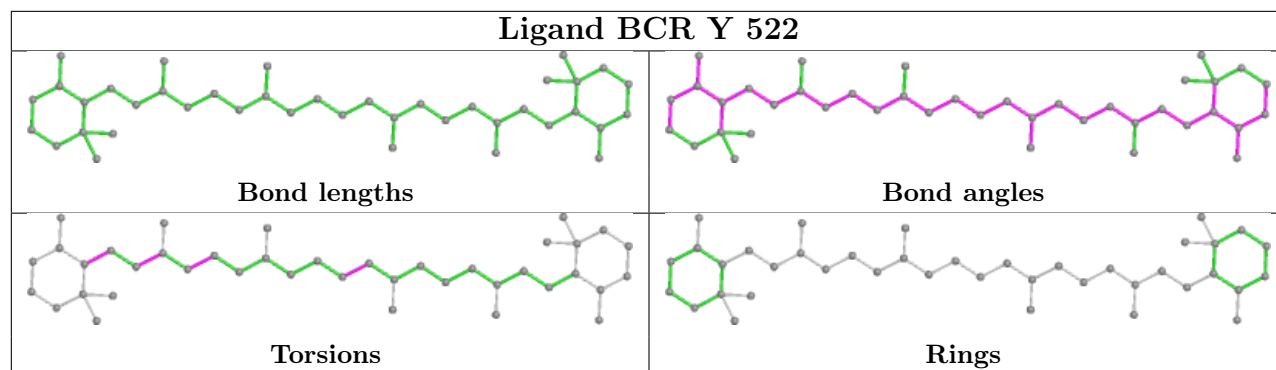
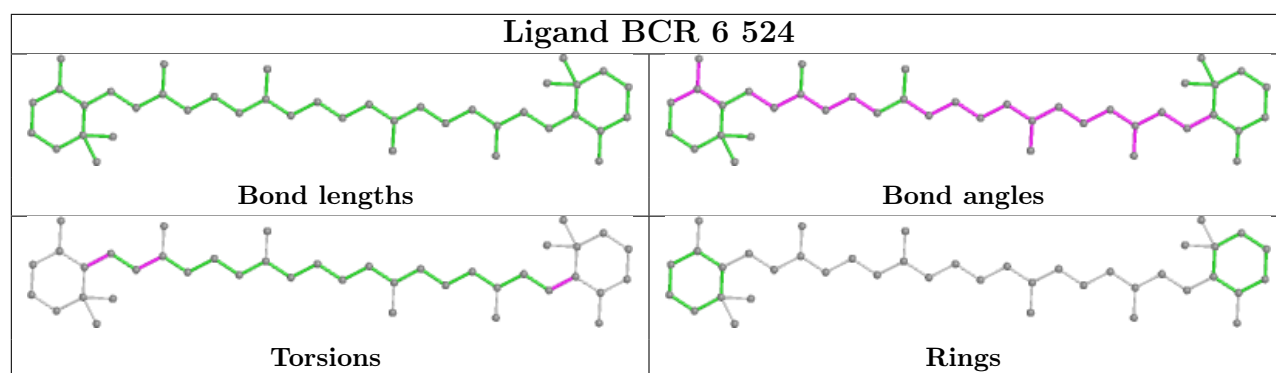


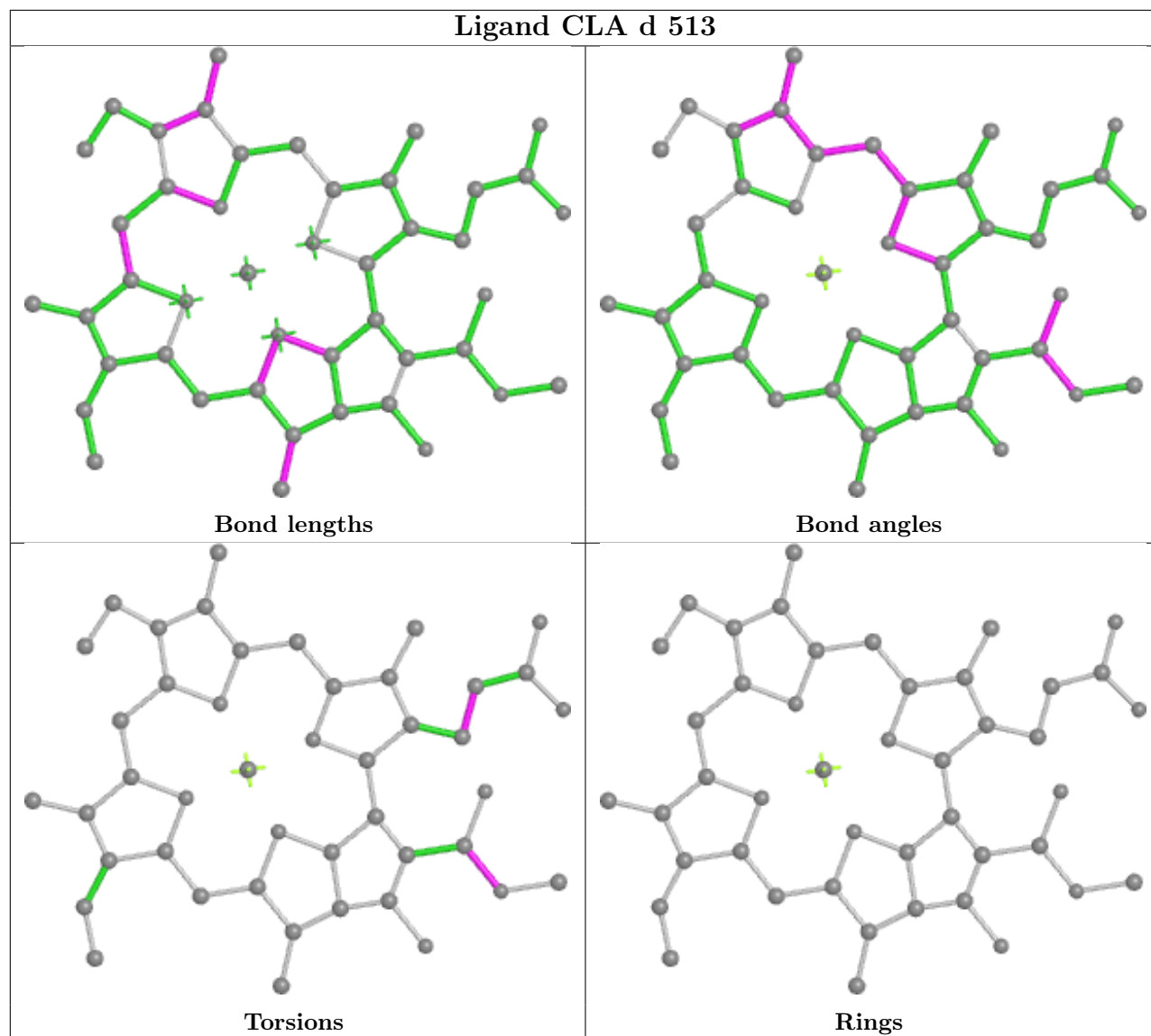
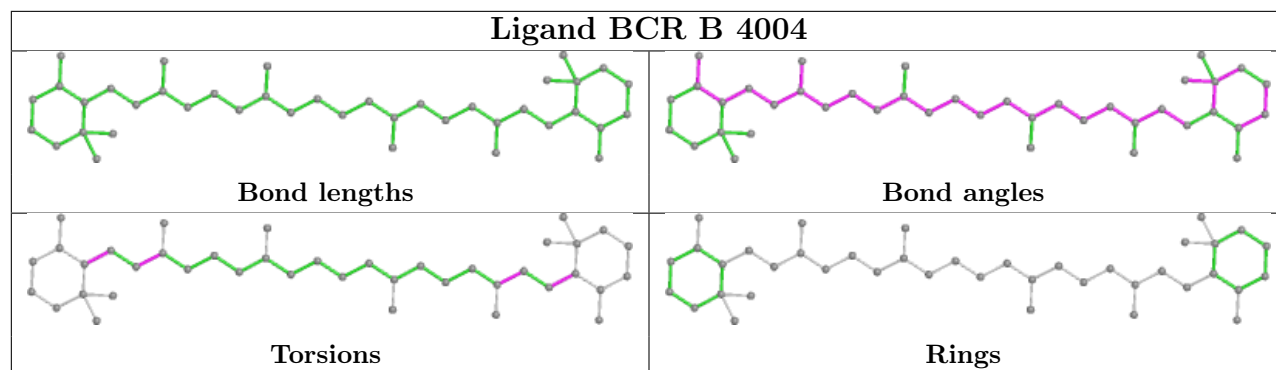
Ligand SQD v 822

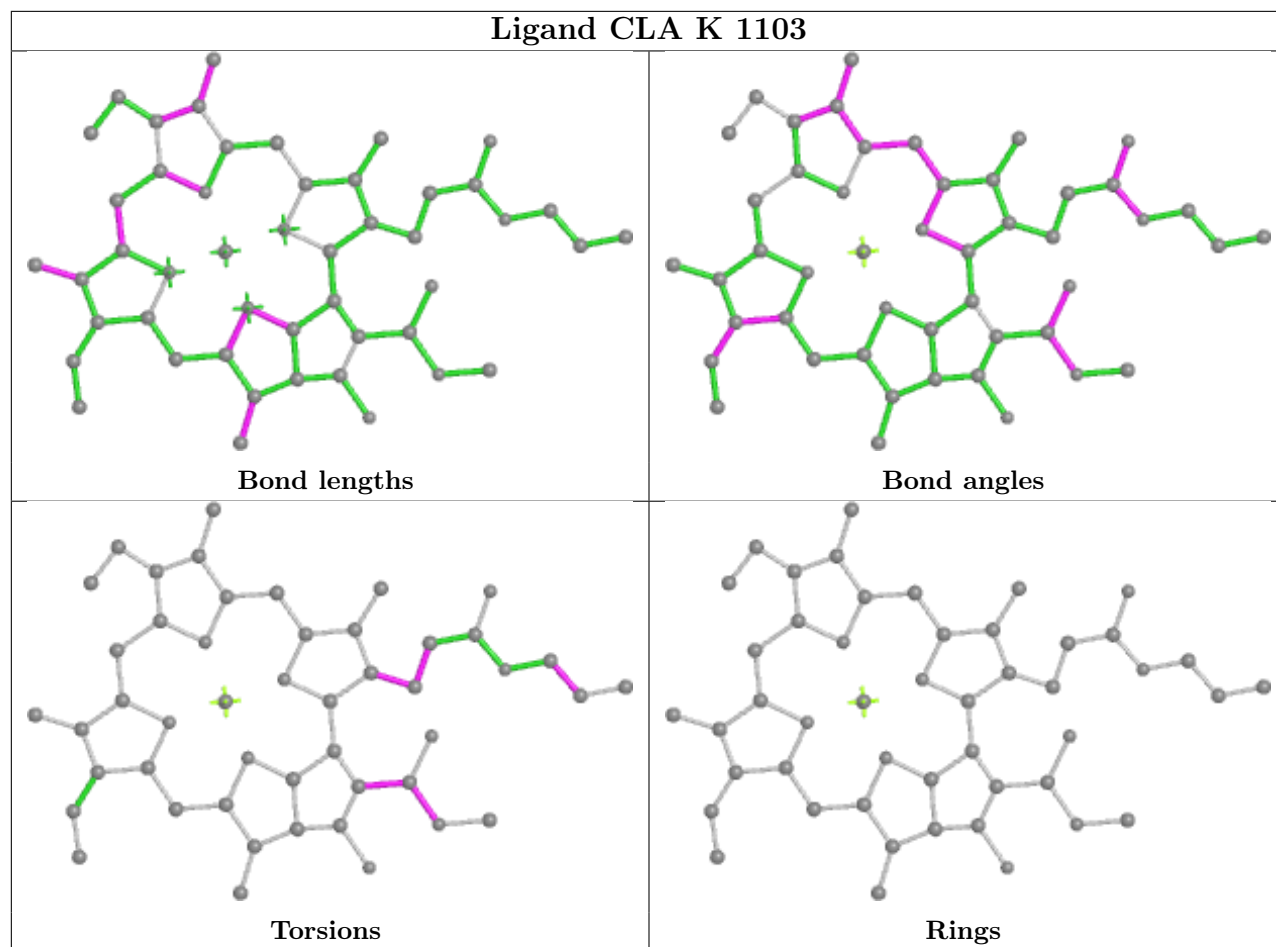


Ligand CLA e 1120

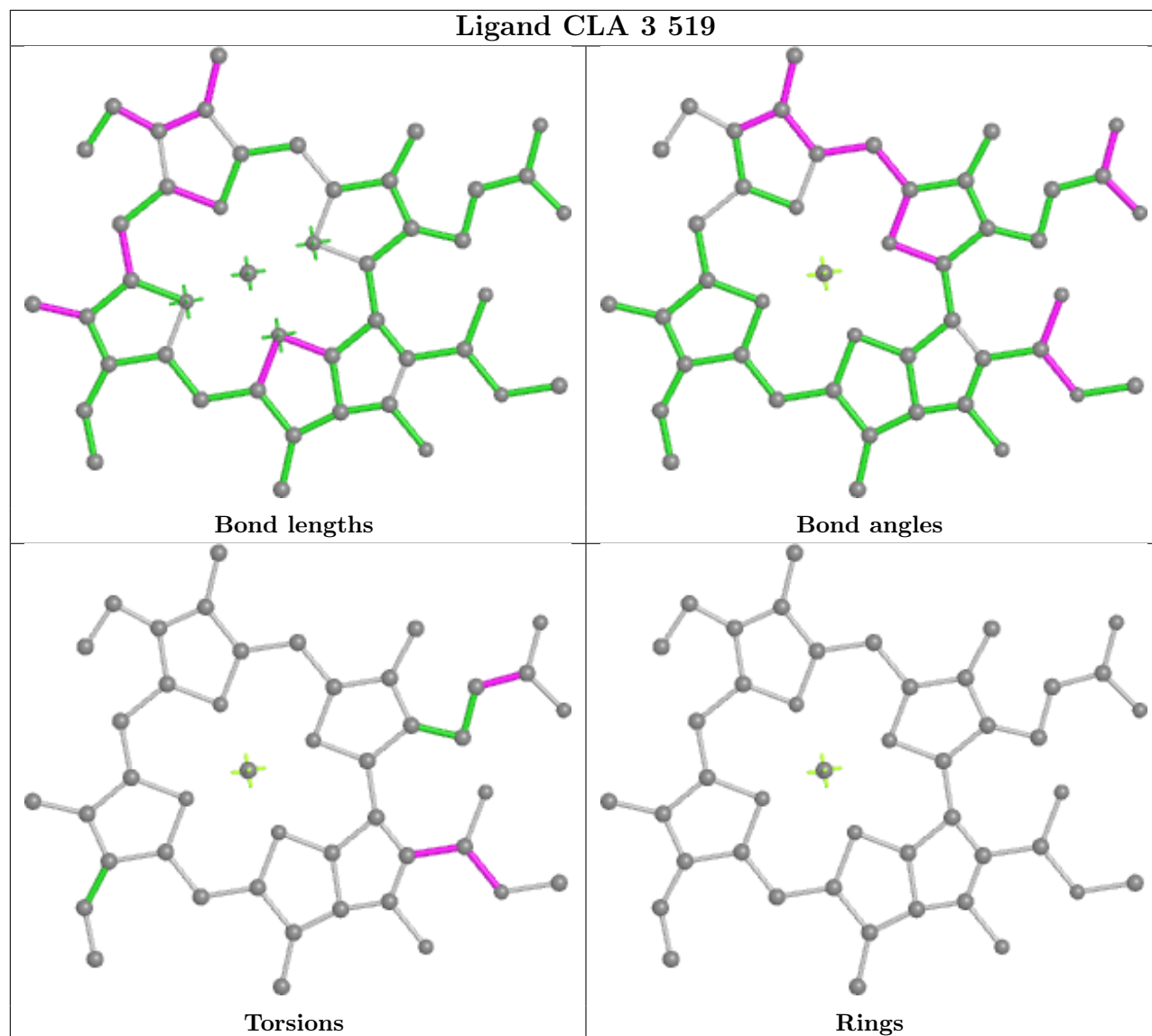




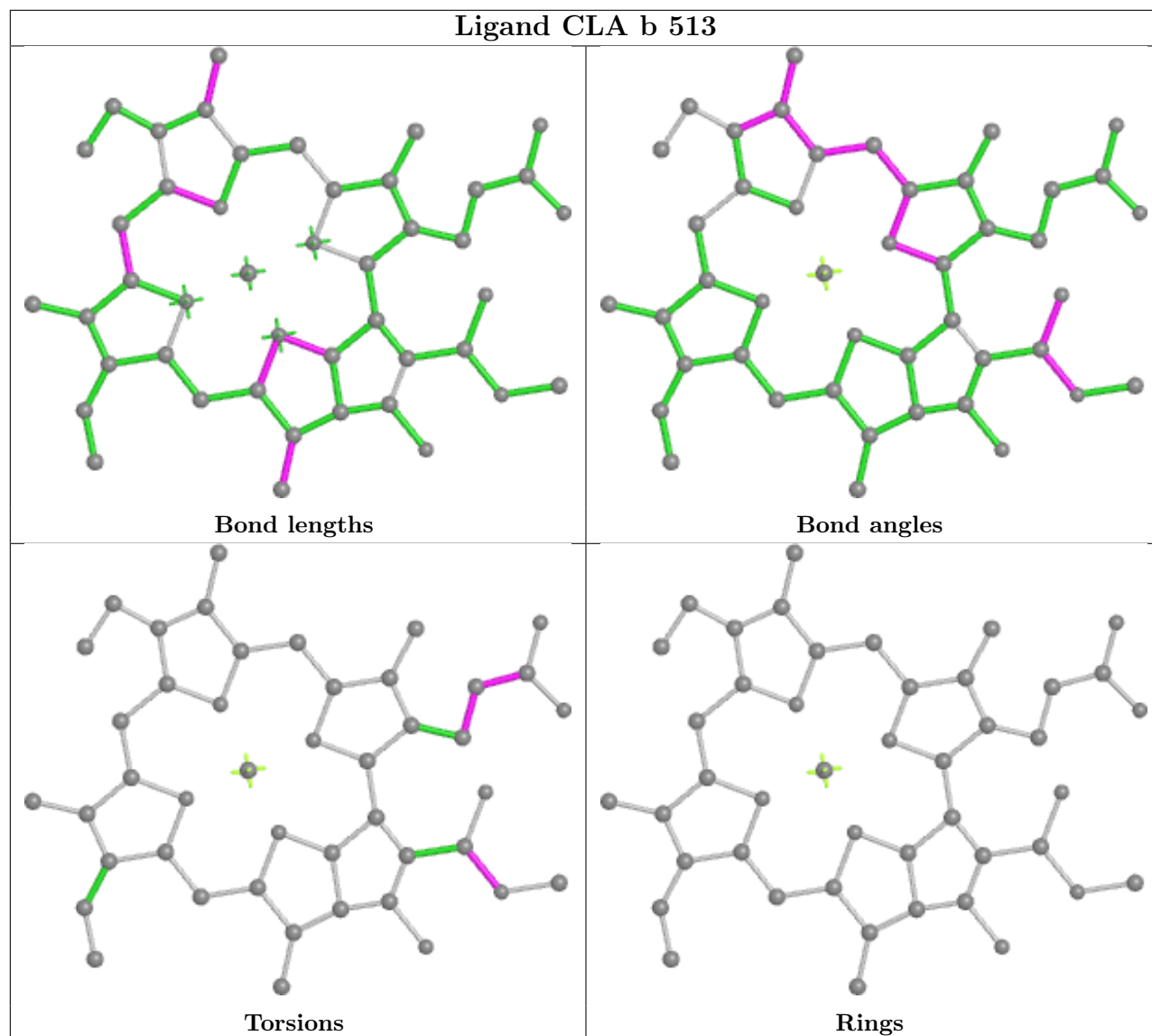




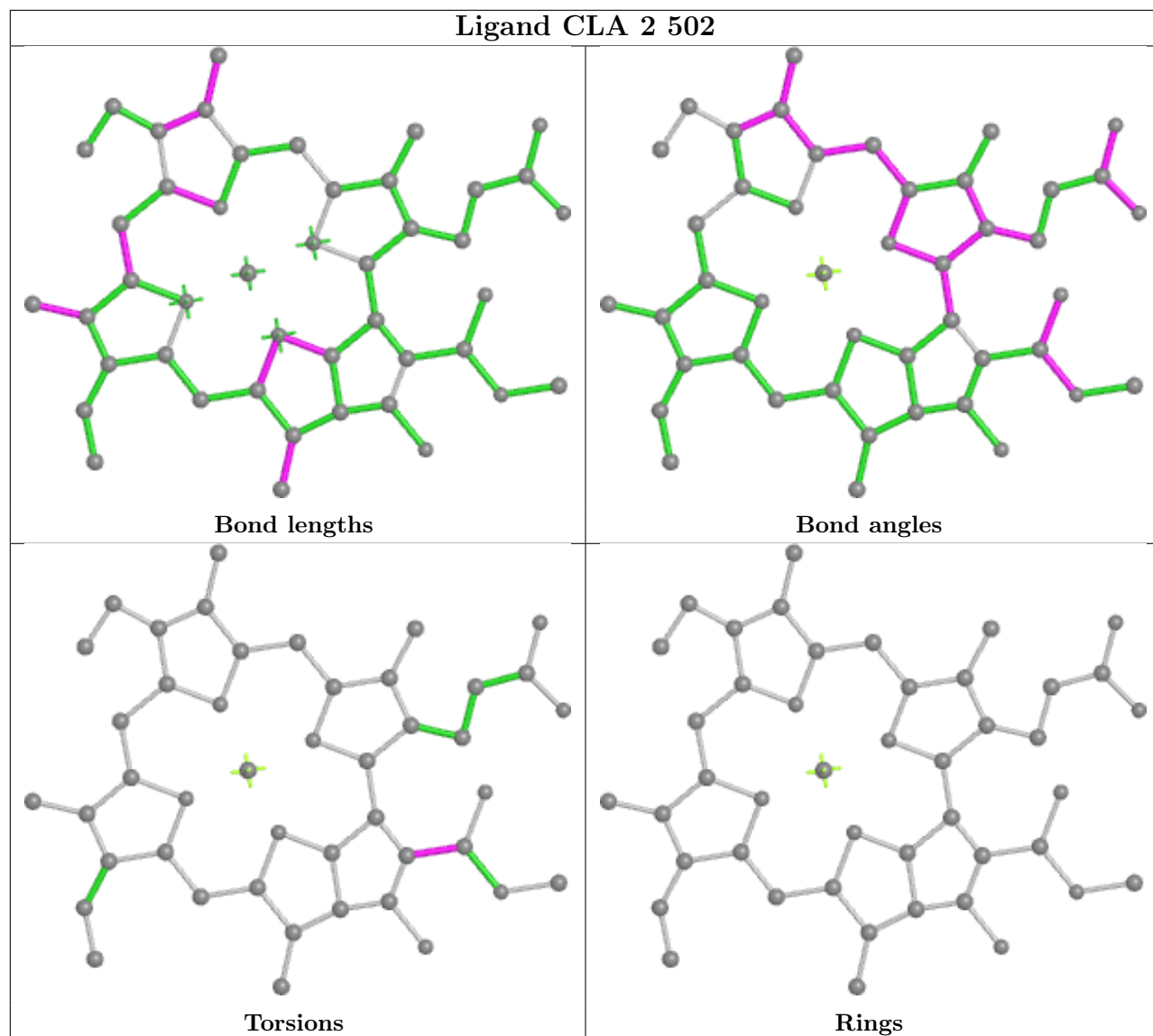
Ligand CLA 3 519



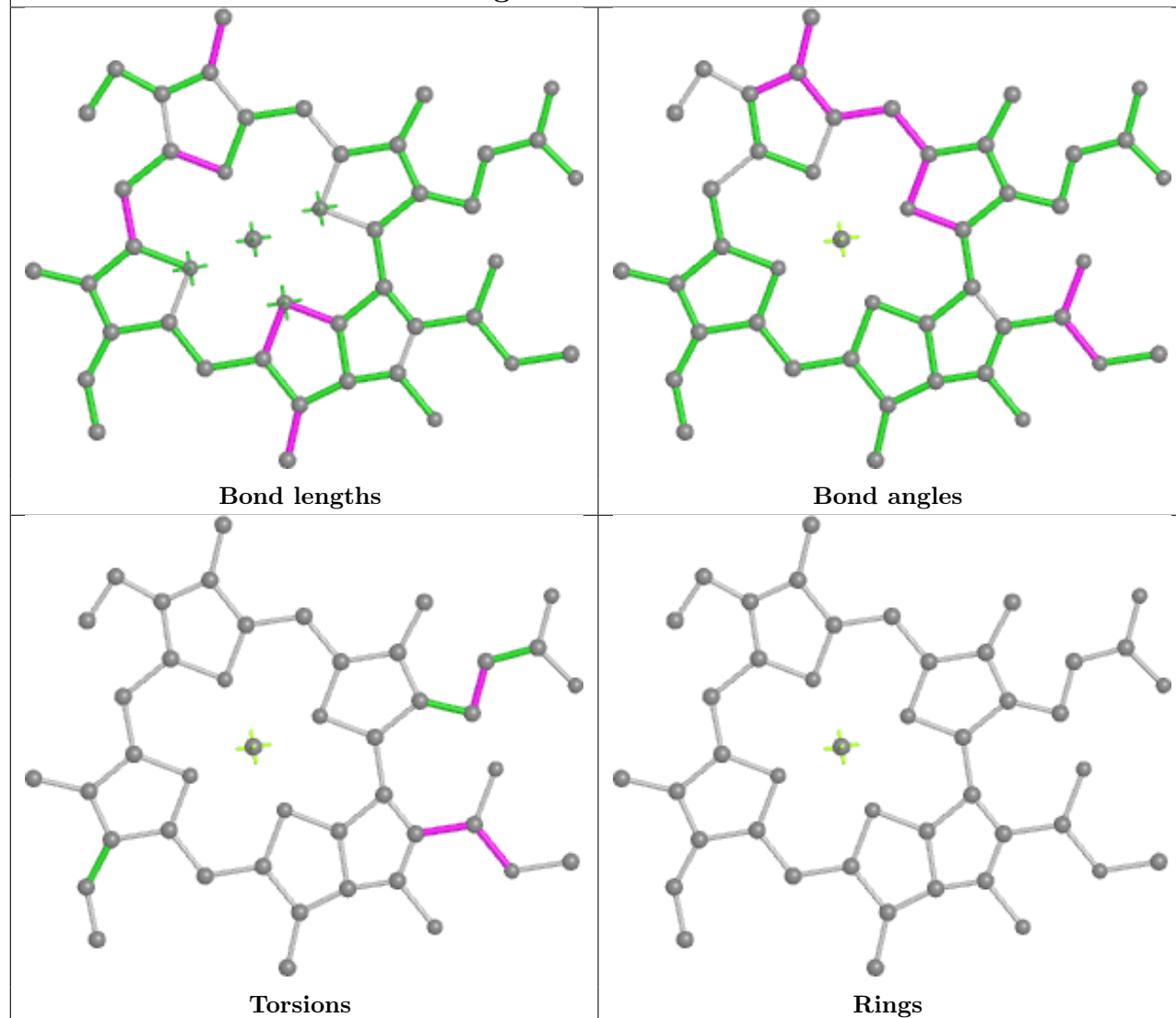
Ligand CLA b 513



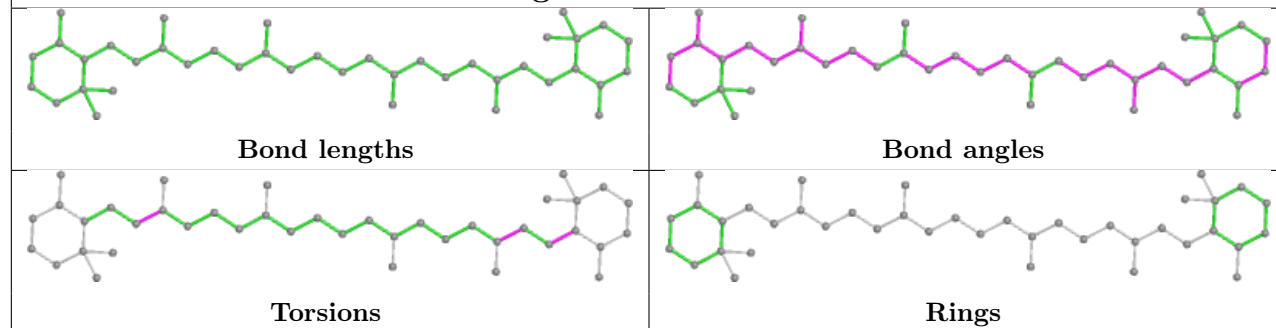
Ligand CLA 2 502

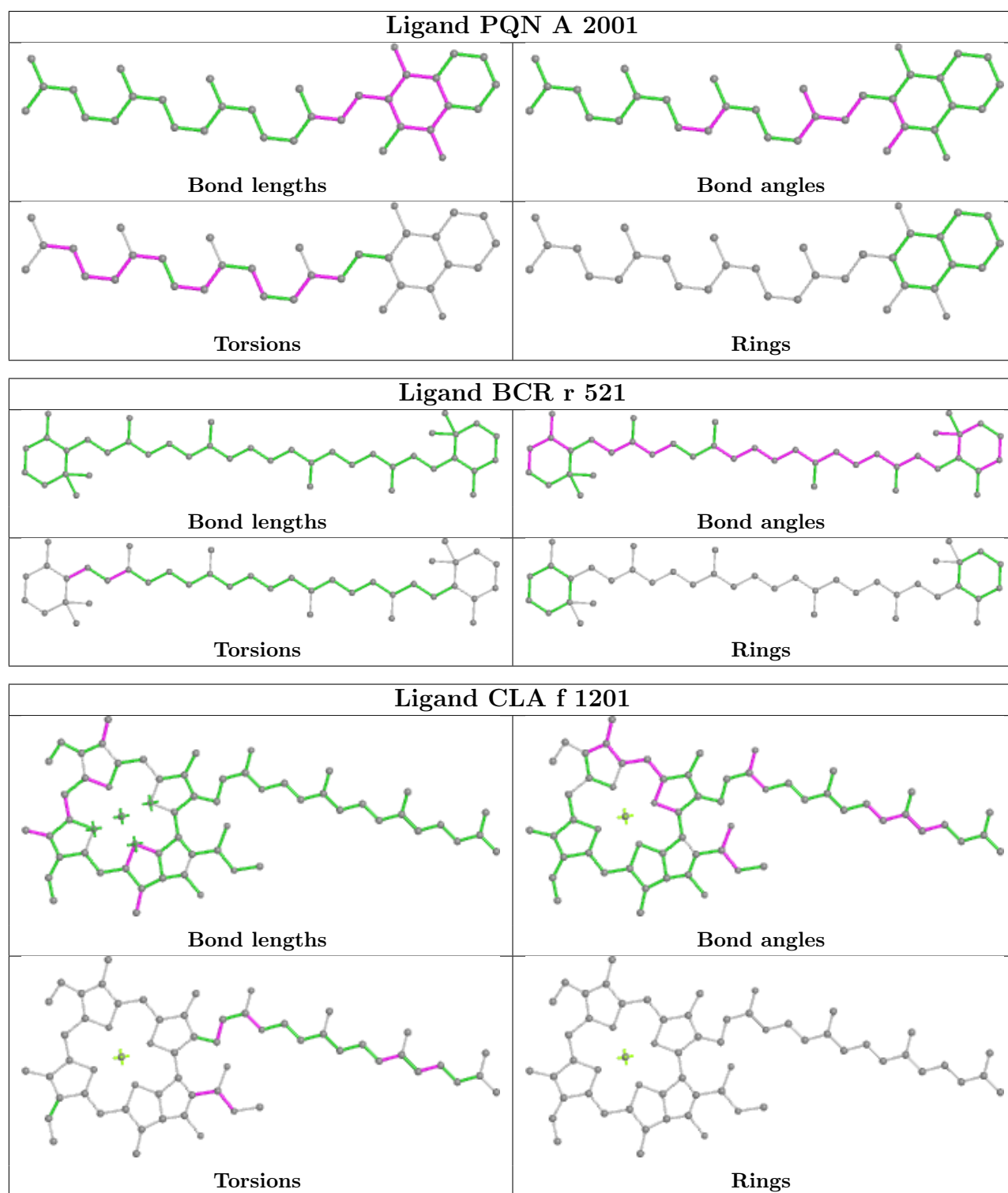


Ligand CLA v 503

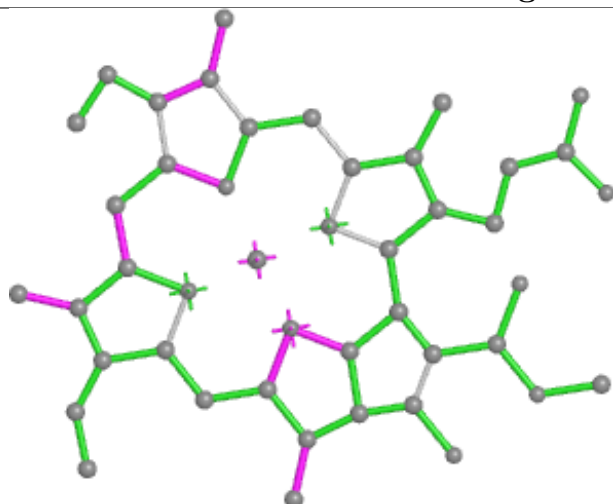


Ligand BCR Z 523

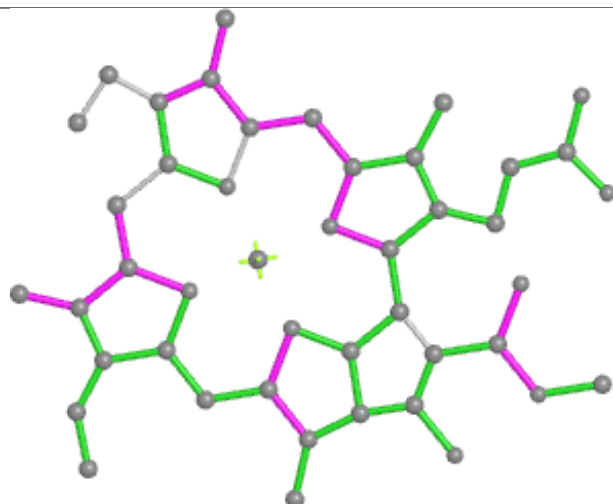




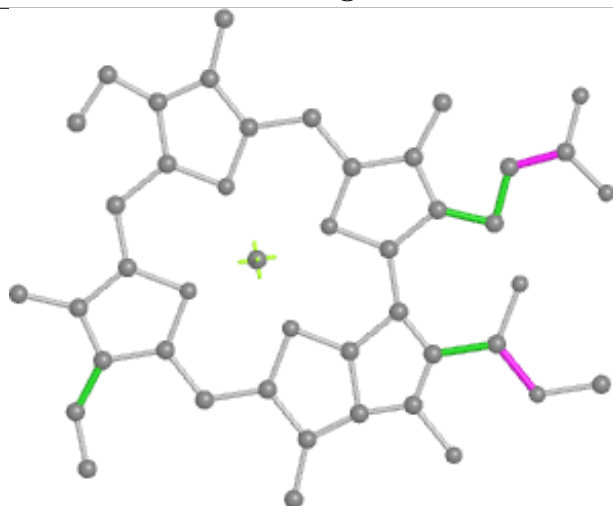
Ligand CLA 4 508



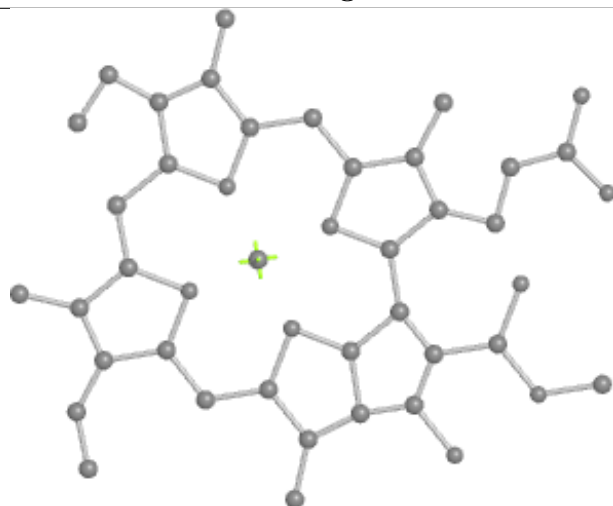
Bond lengths



Bond angles

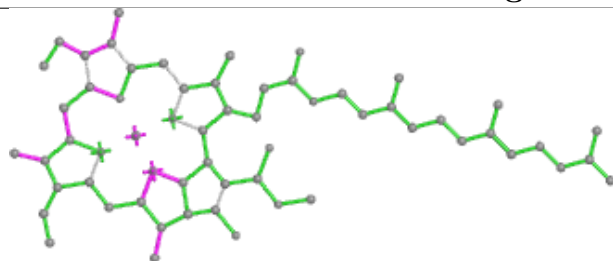


Torsions

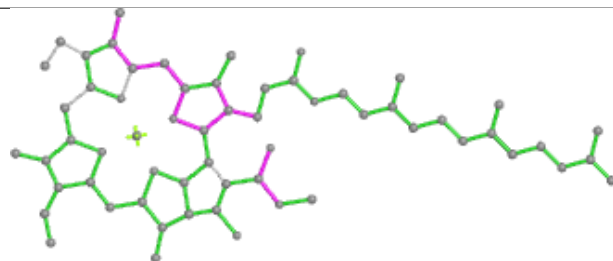


Rings

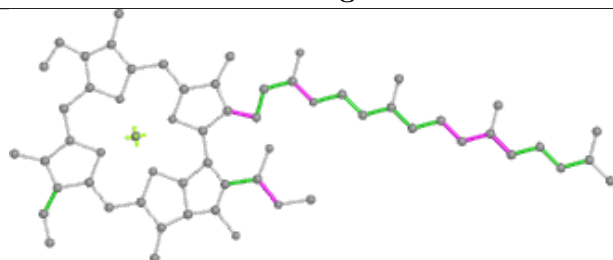
Ligand CLA B 1230



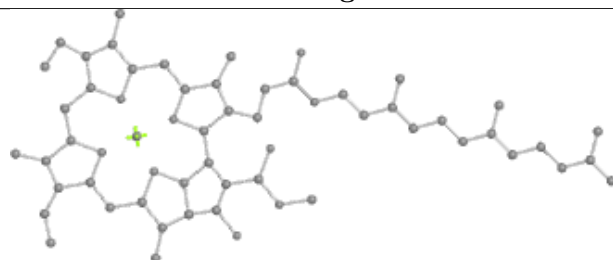
Bond lengths



Bond angles

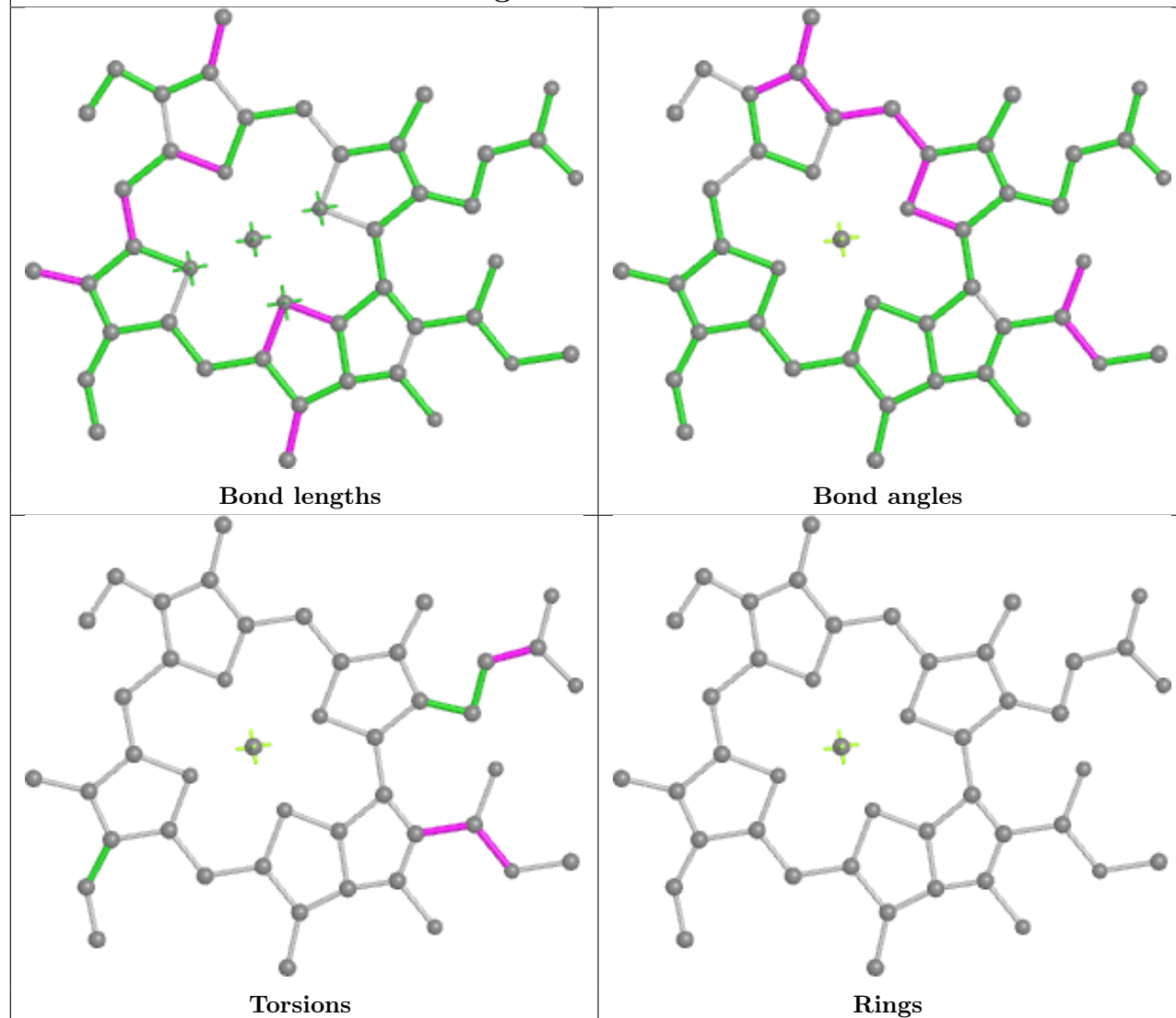


Torsions

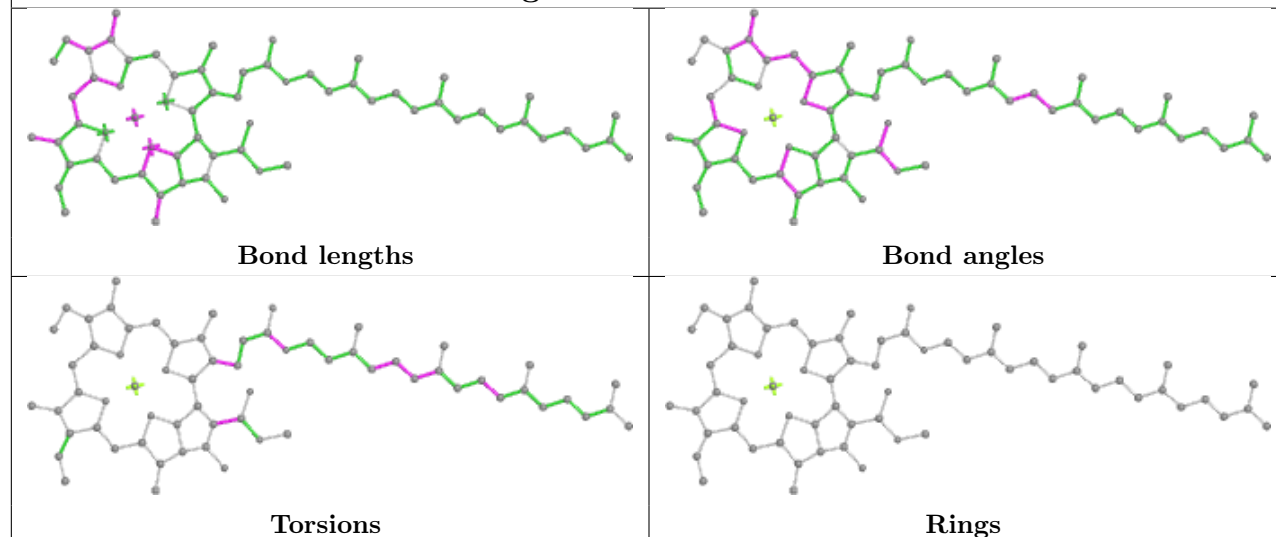


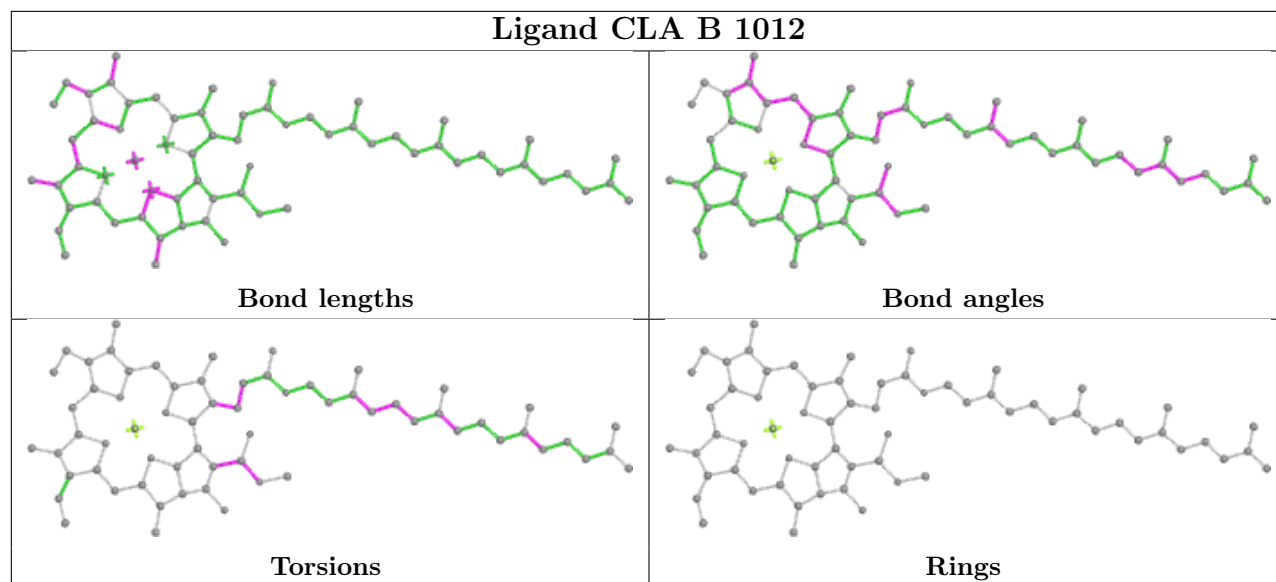
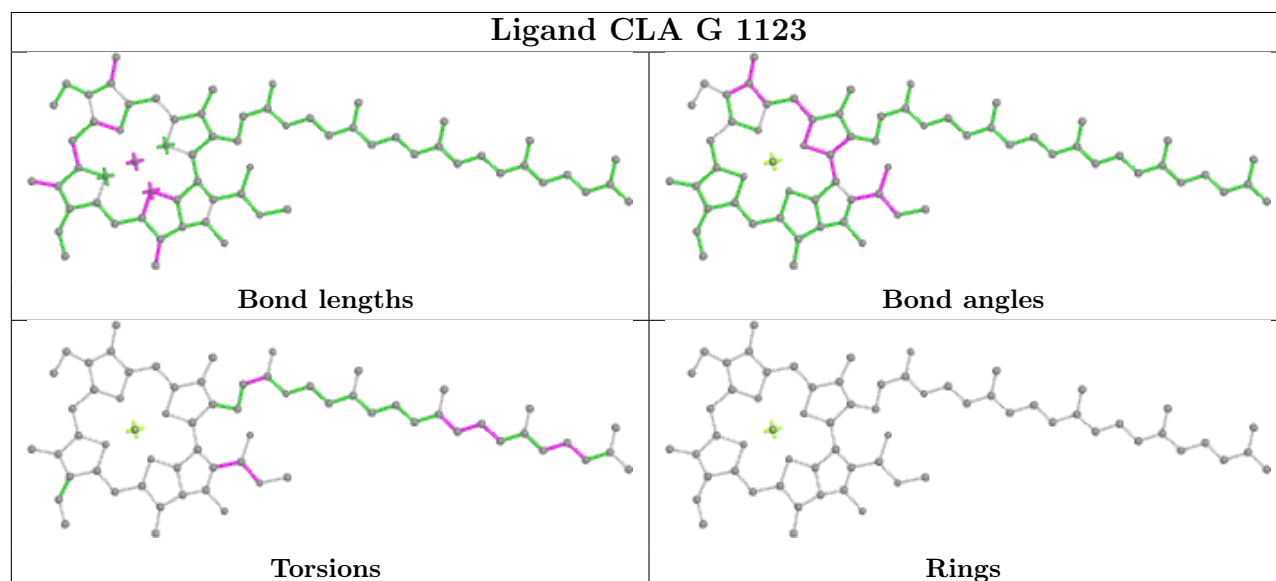
Rings

Ligand CLA 6 510

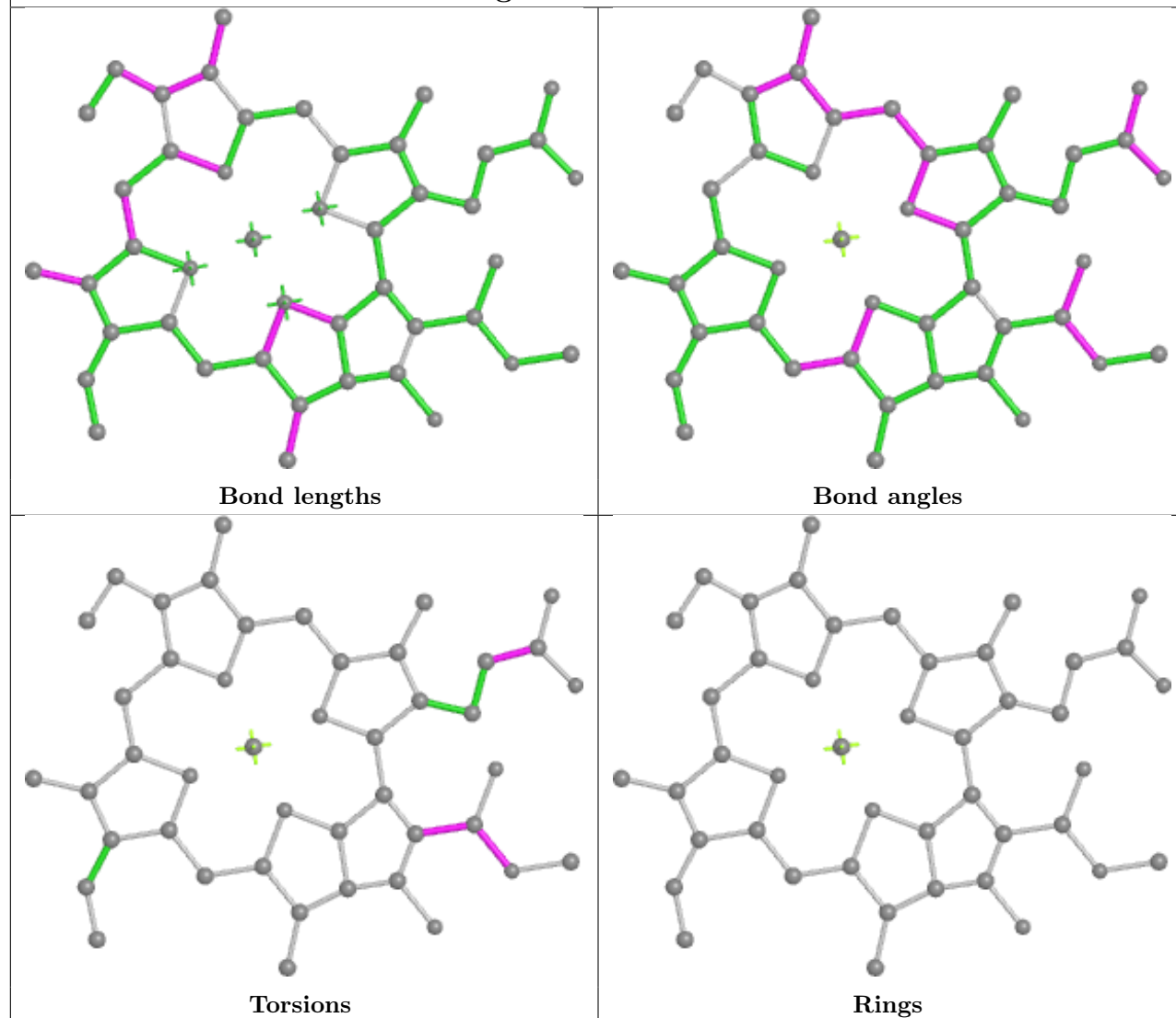


Ligand CLA G 1128

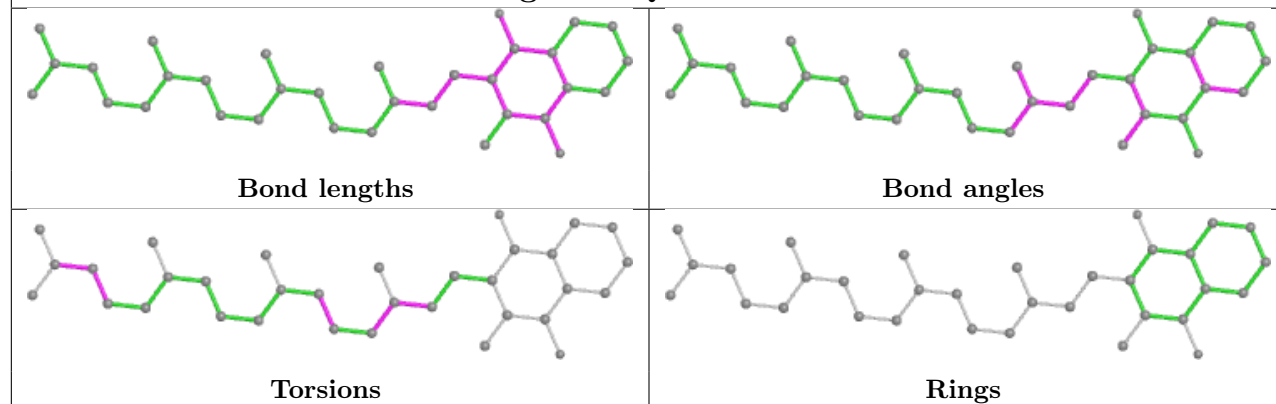


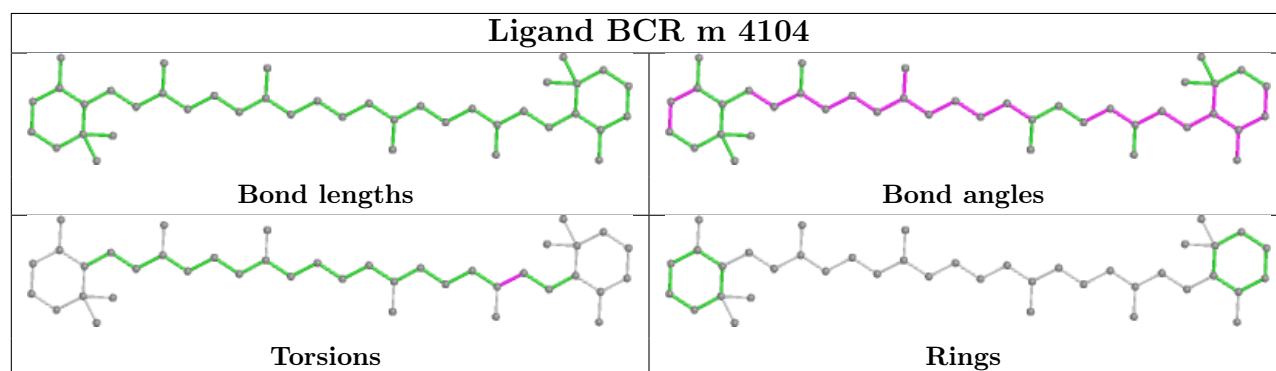
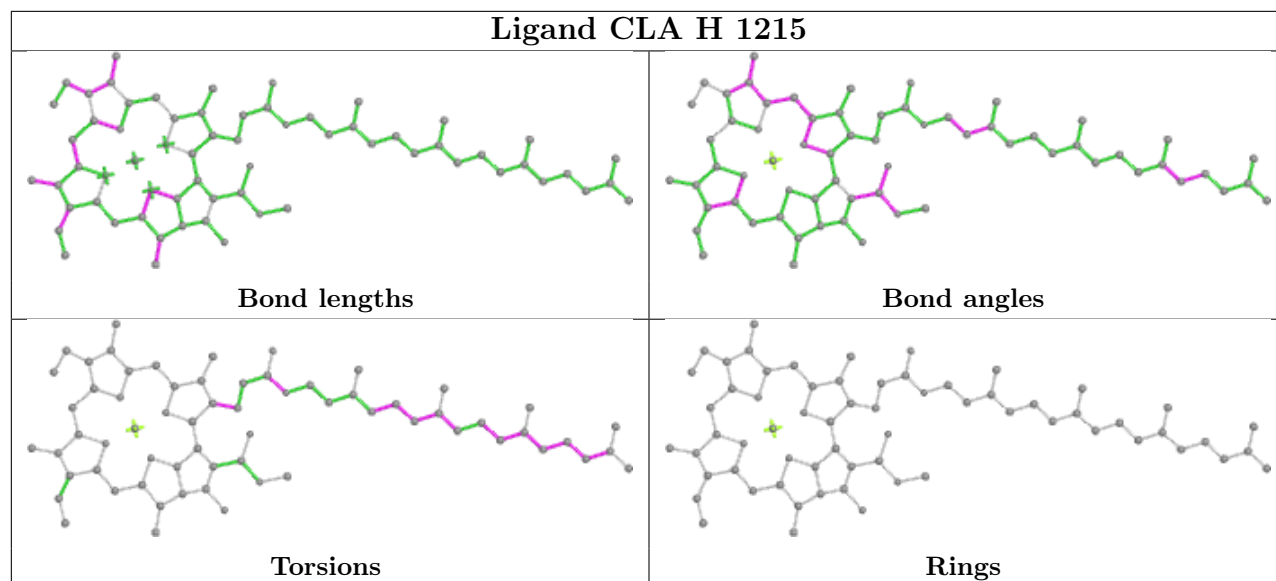
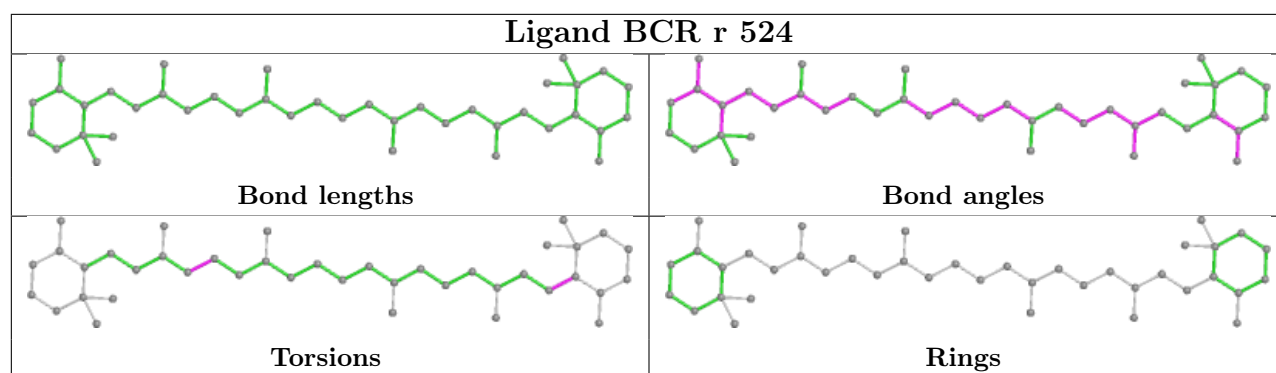
Ligand CLA B 1012**Ligand CLA G 1123**

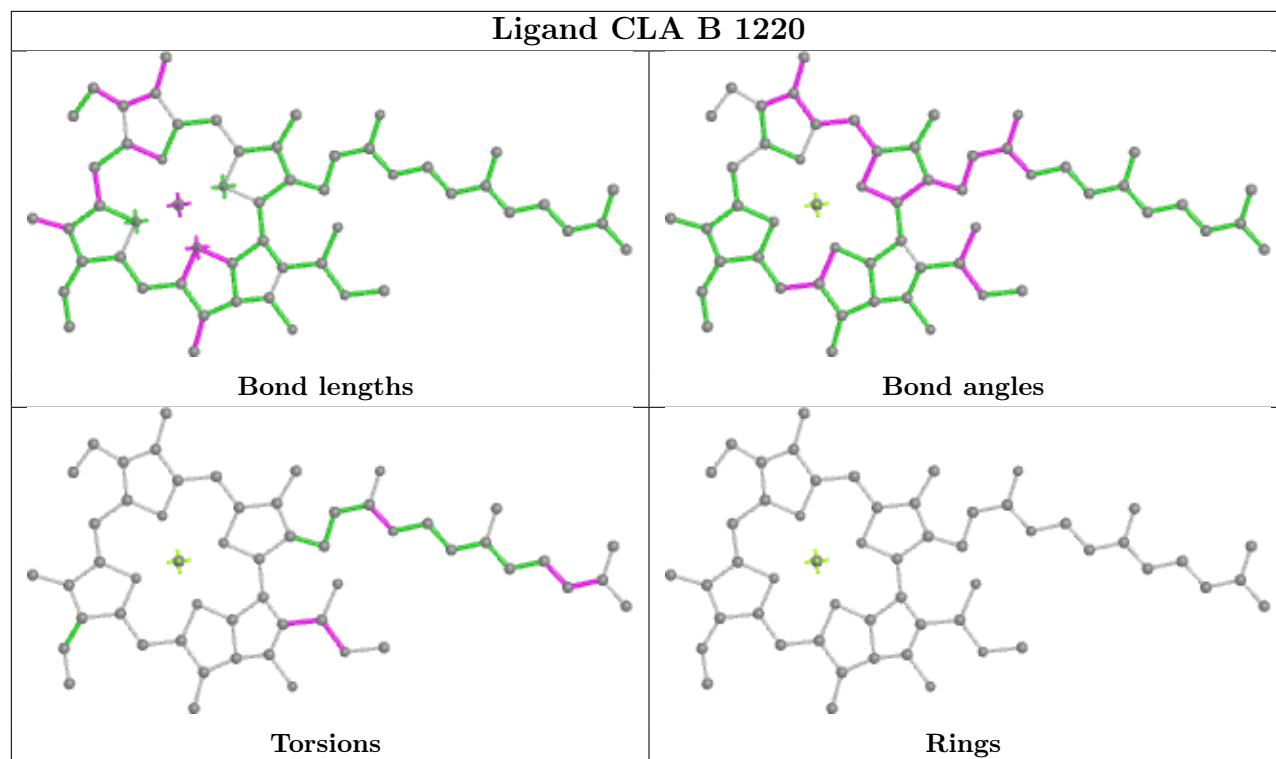
Ligand CLA r 519

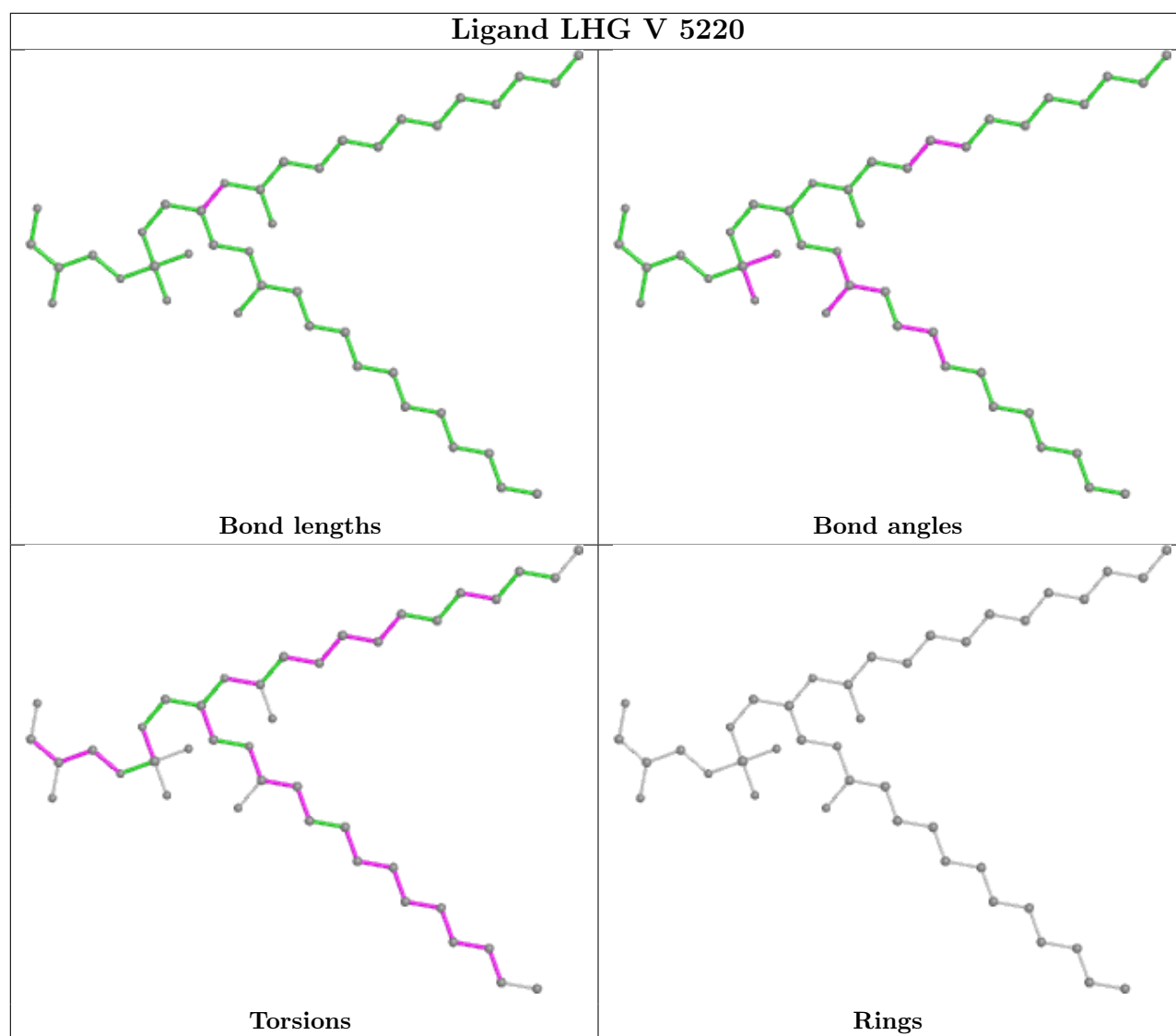


Ligand PQN H 2002

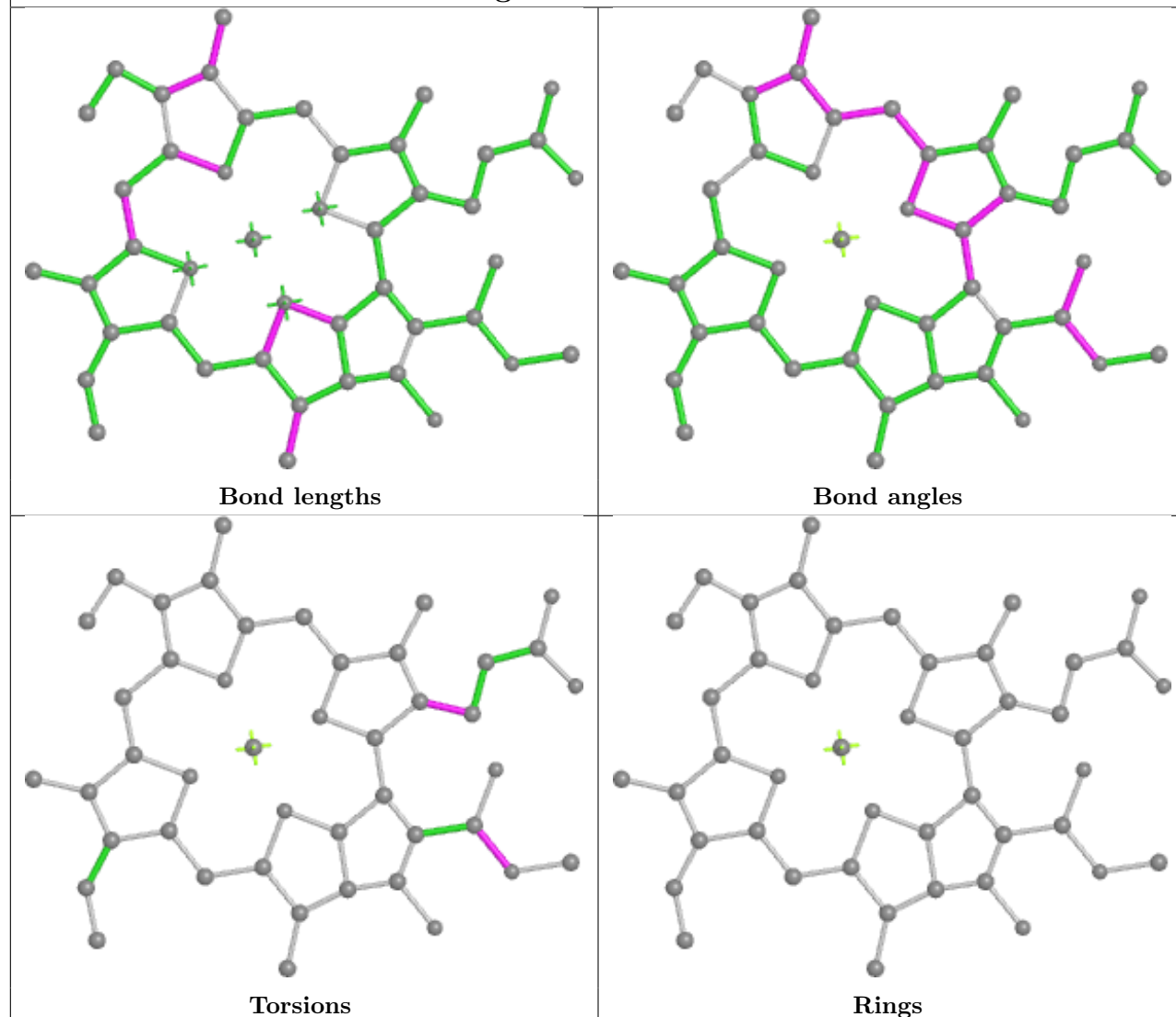




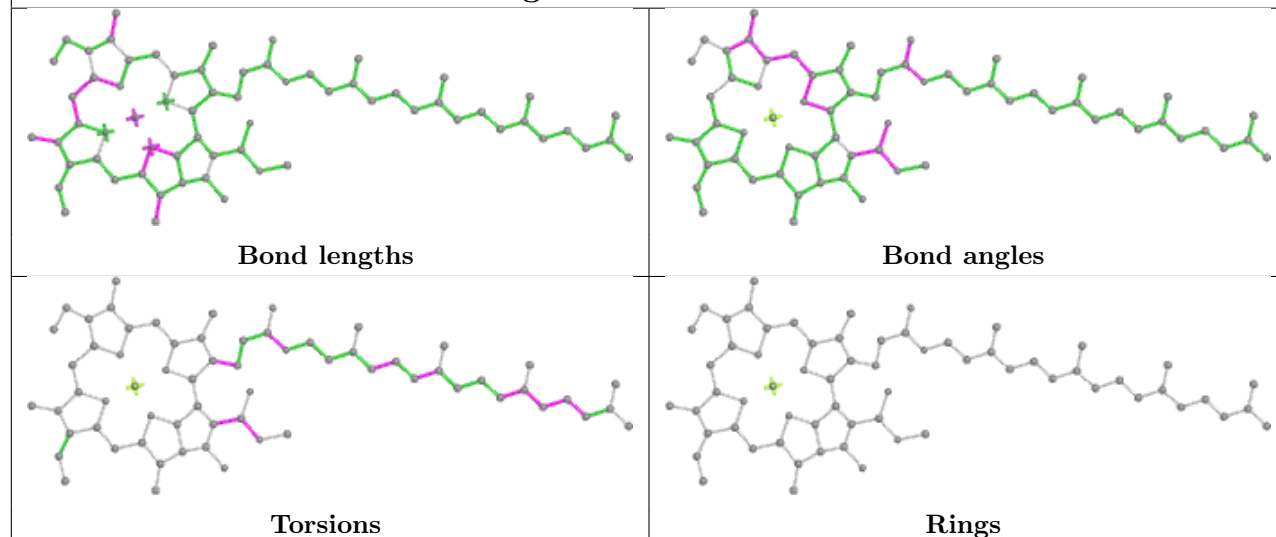




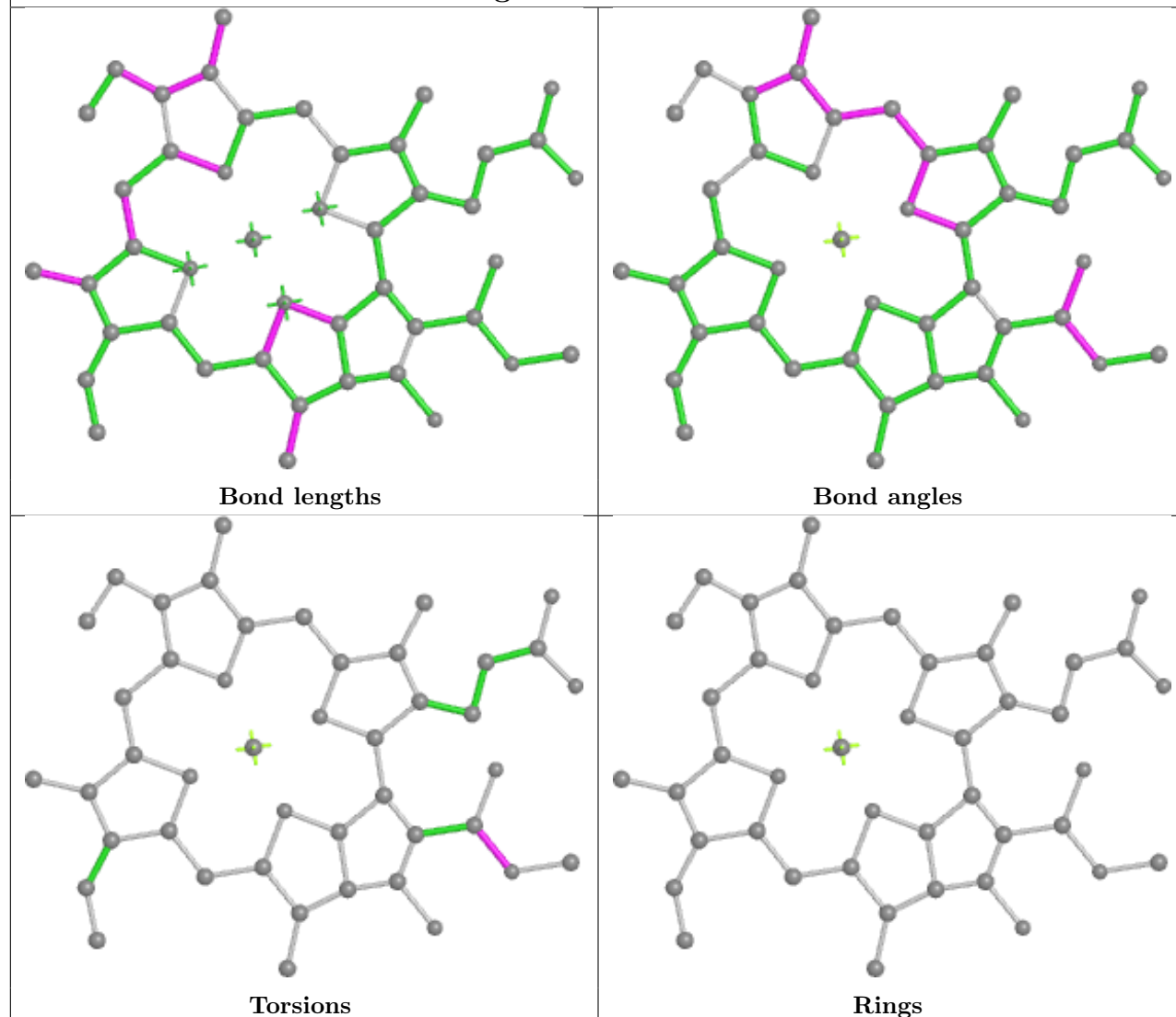
Ligand CLA c 504



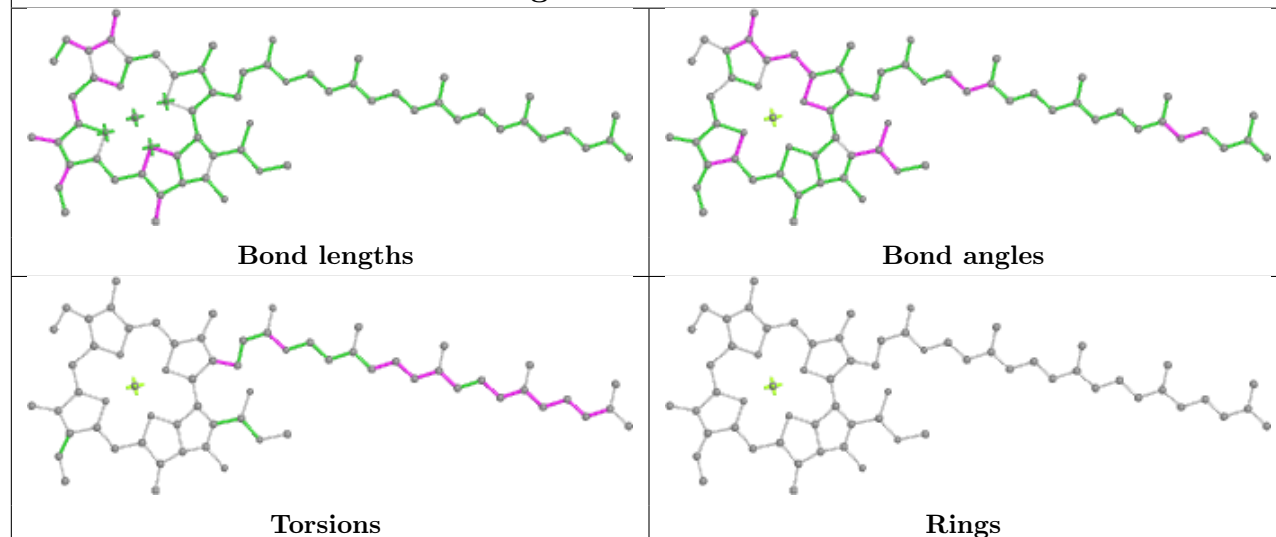
Ligand CLA A 1109



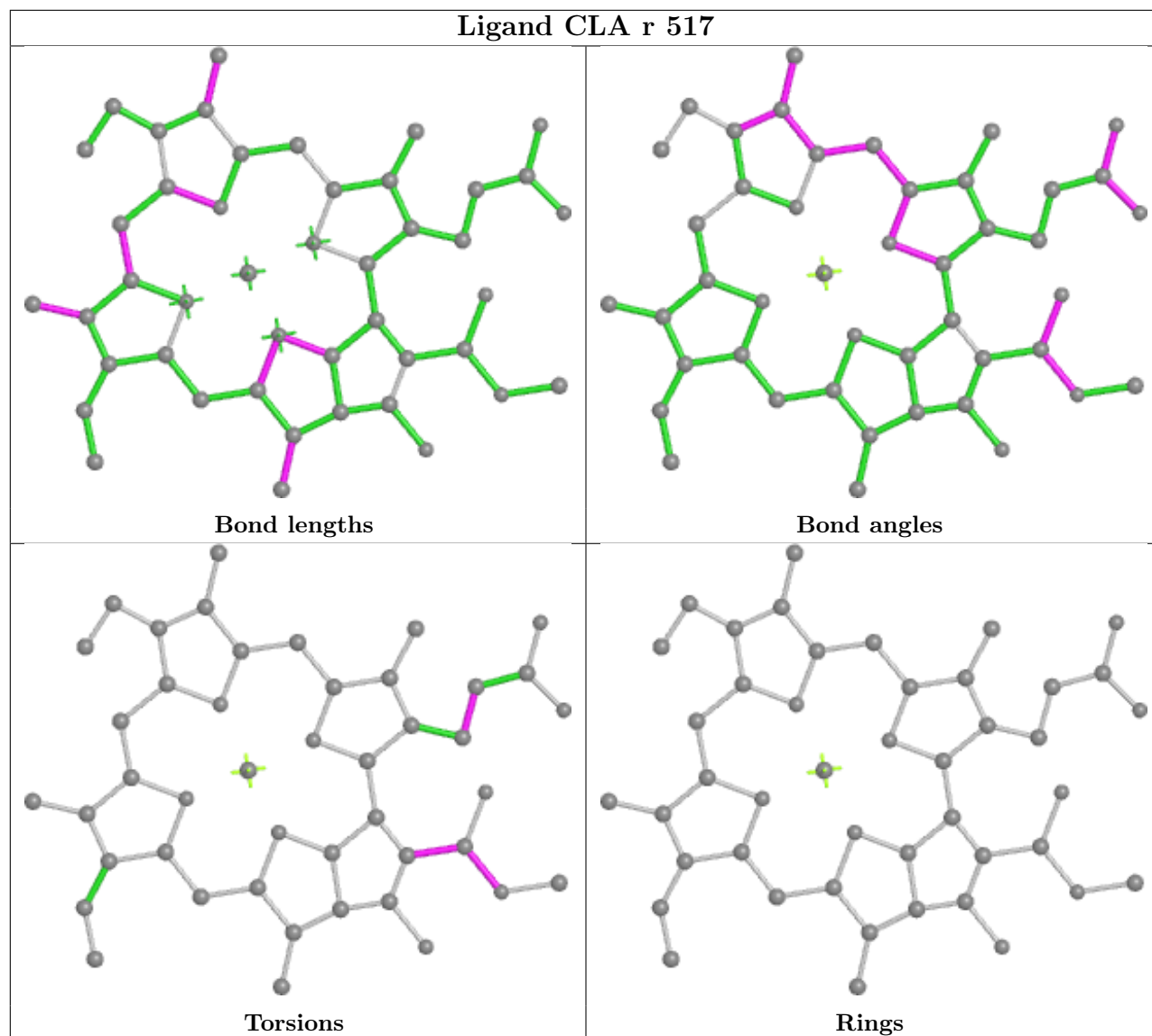
Ligand CLA 2 513



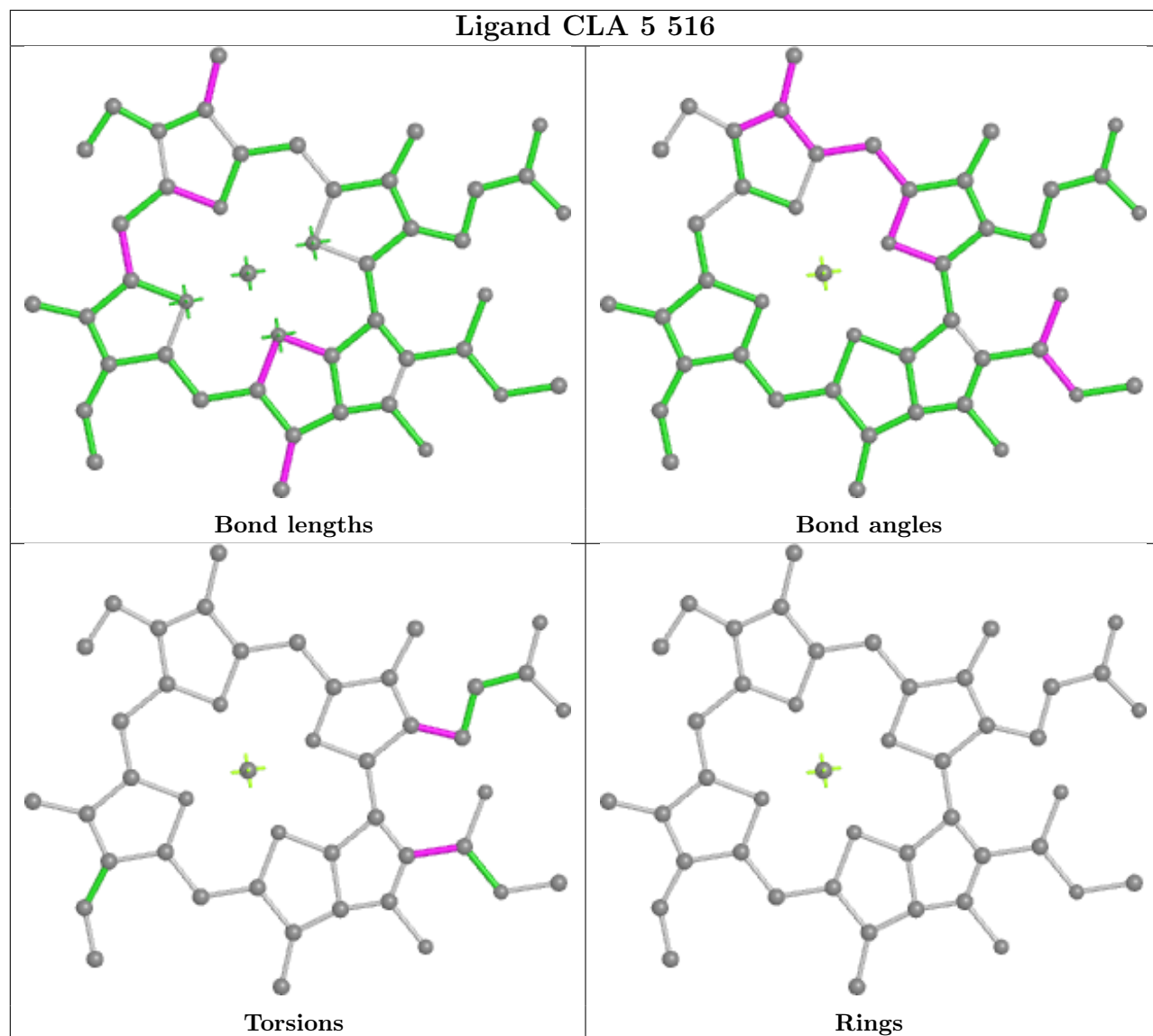
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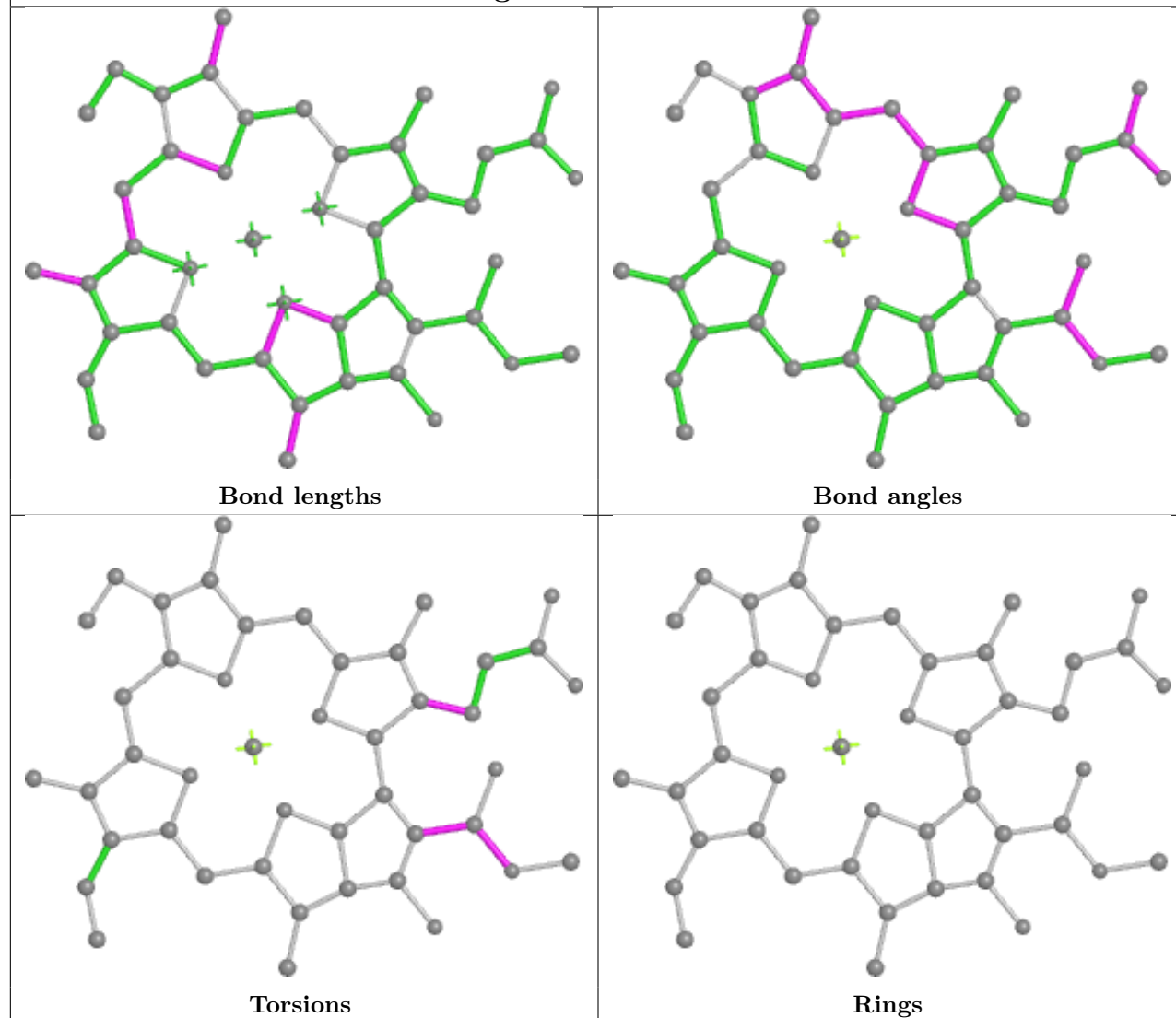
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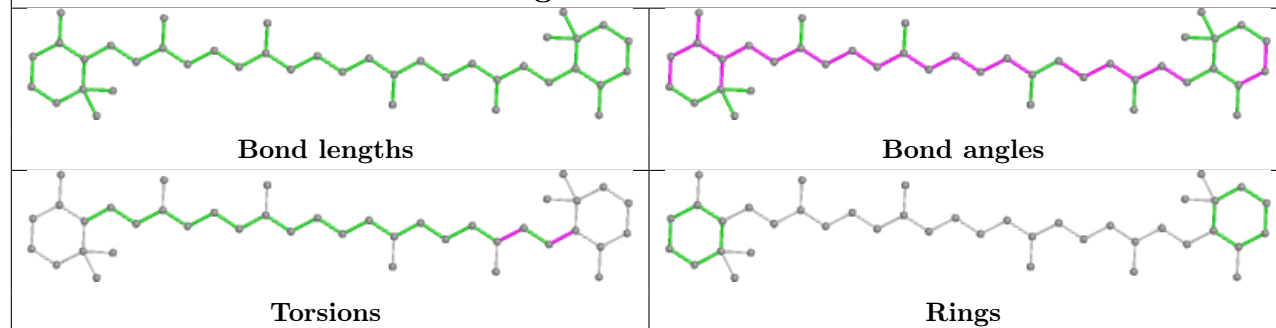
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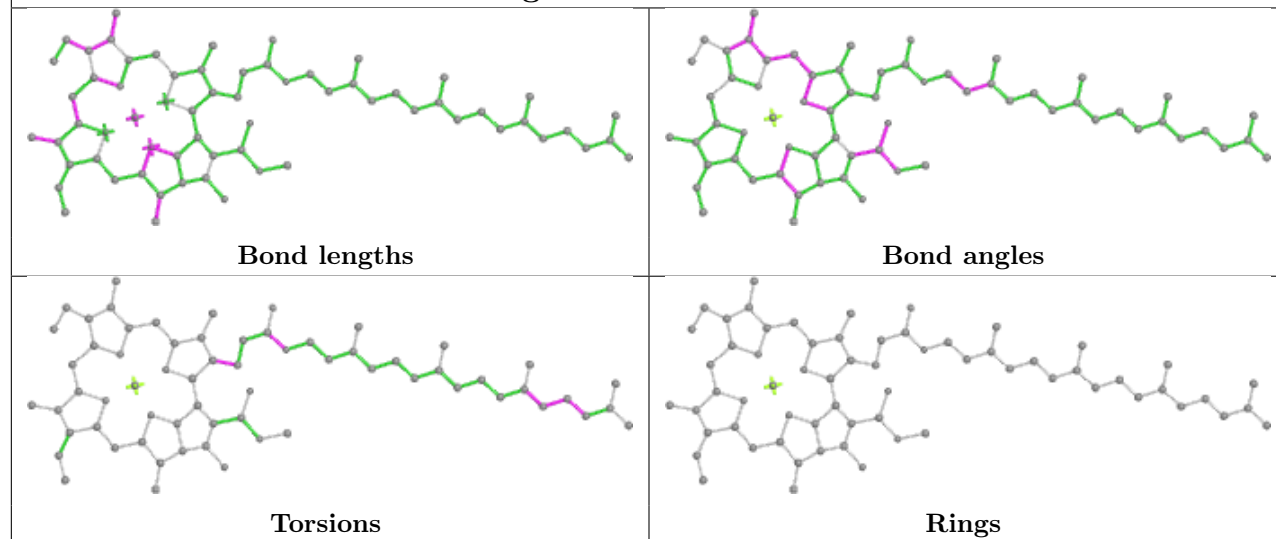
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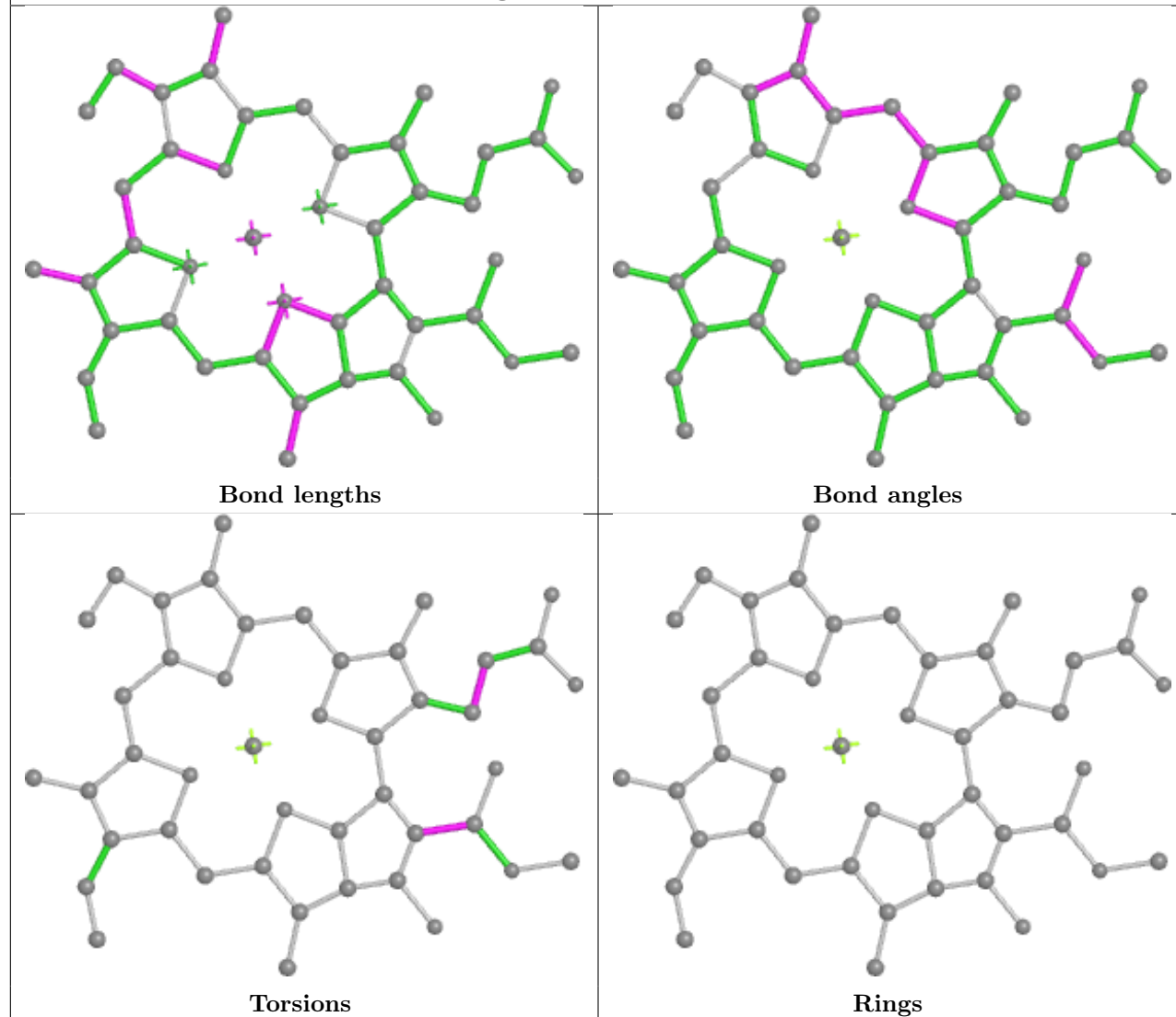
Ligand BCR 3 523

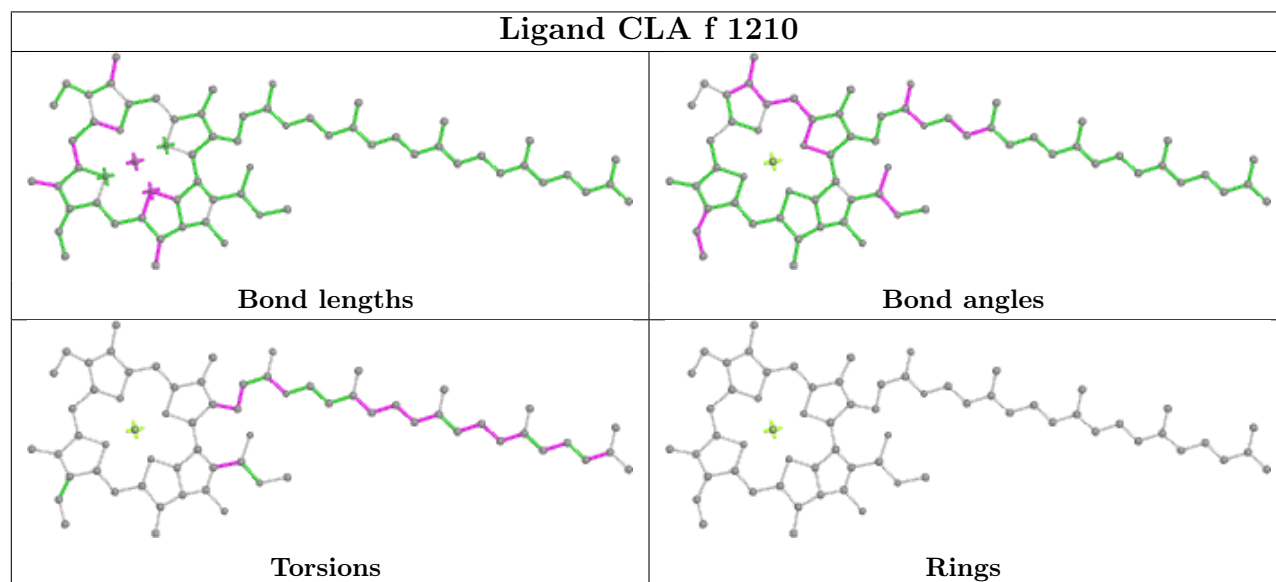
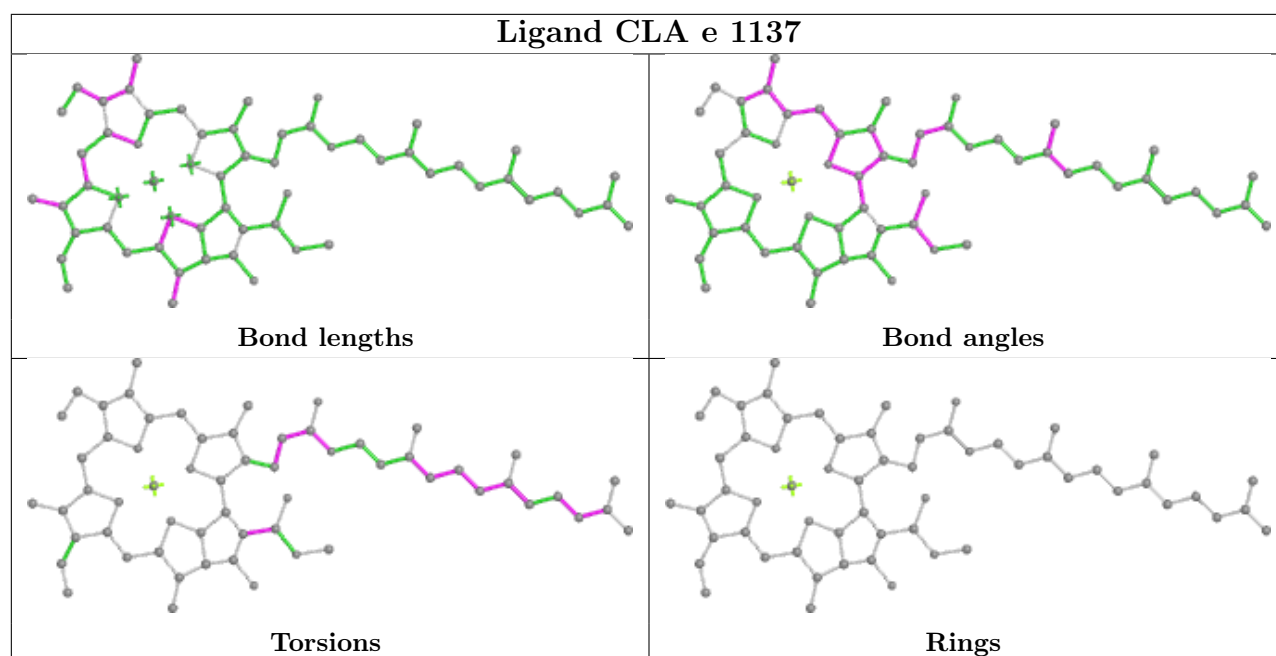


Ligand CLA H 1225

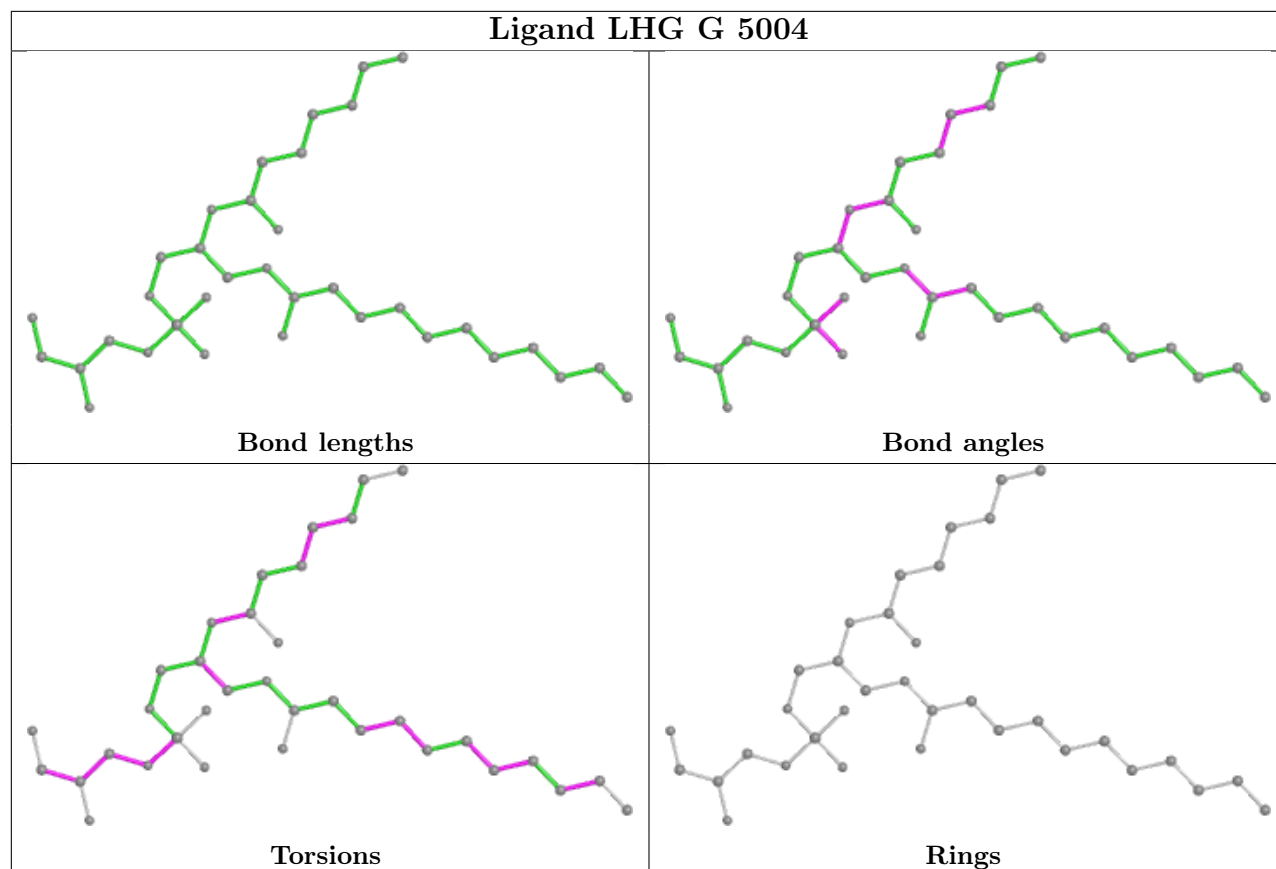


Ligand CLA 4 505

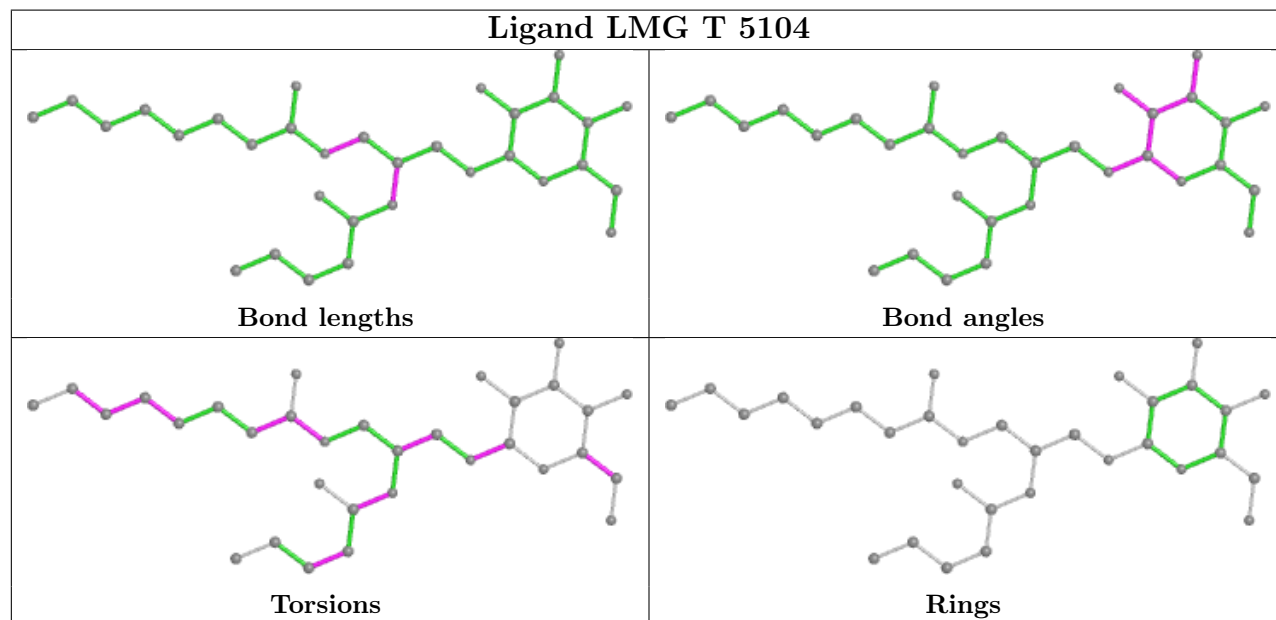


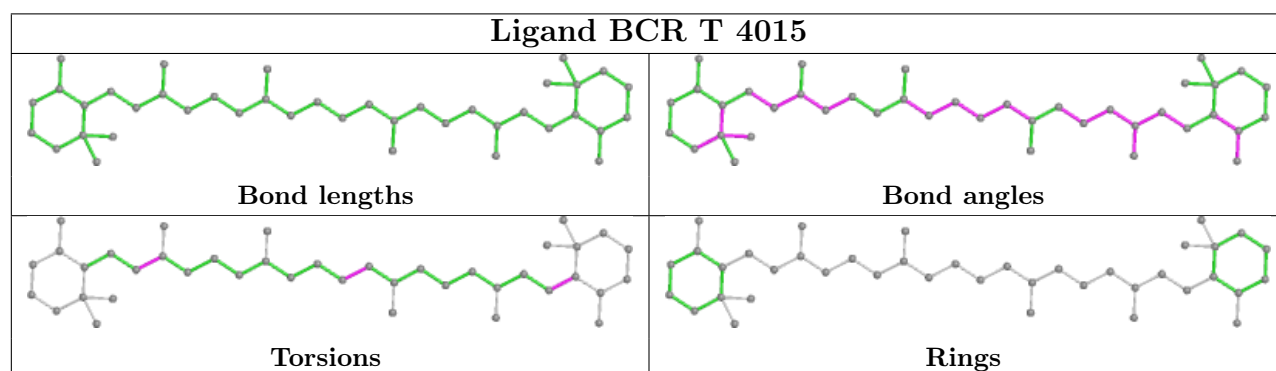
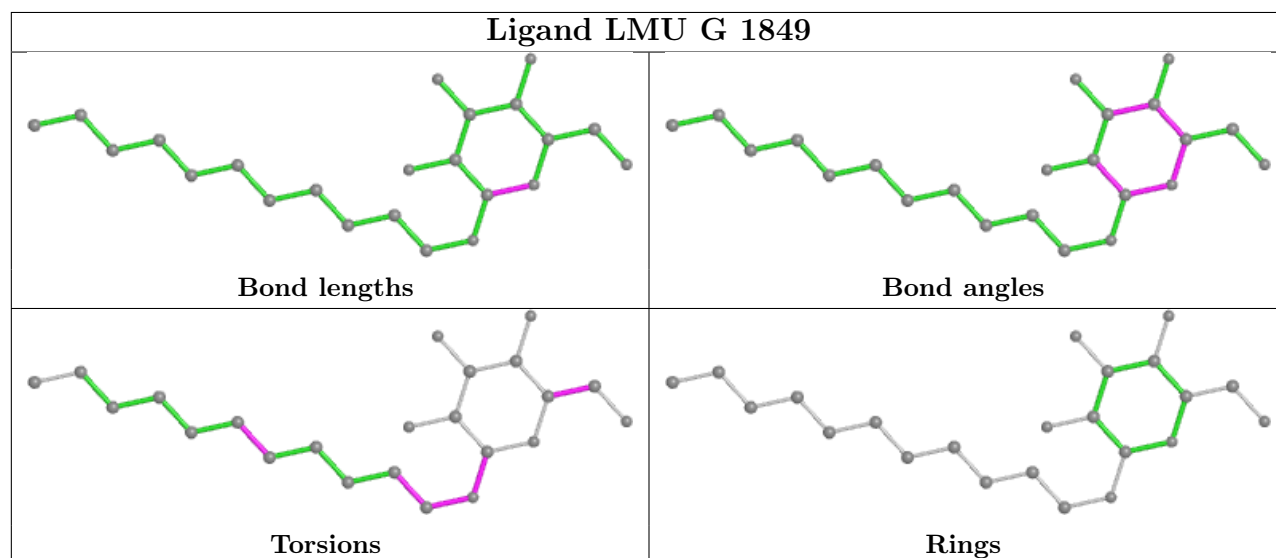
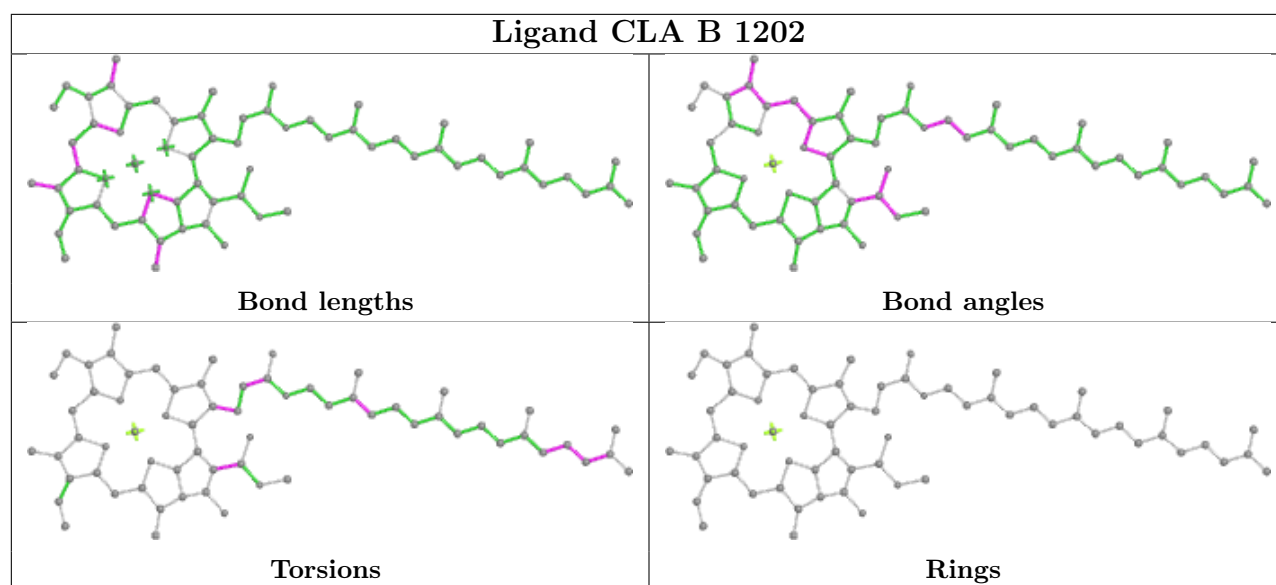


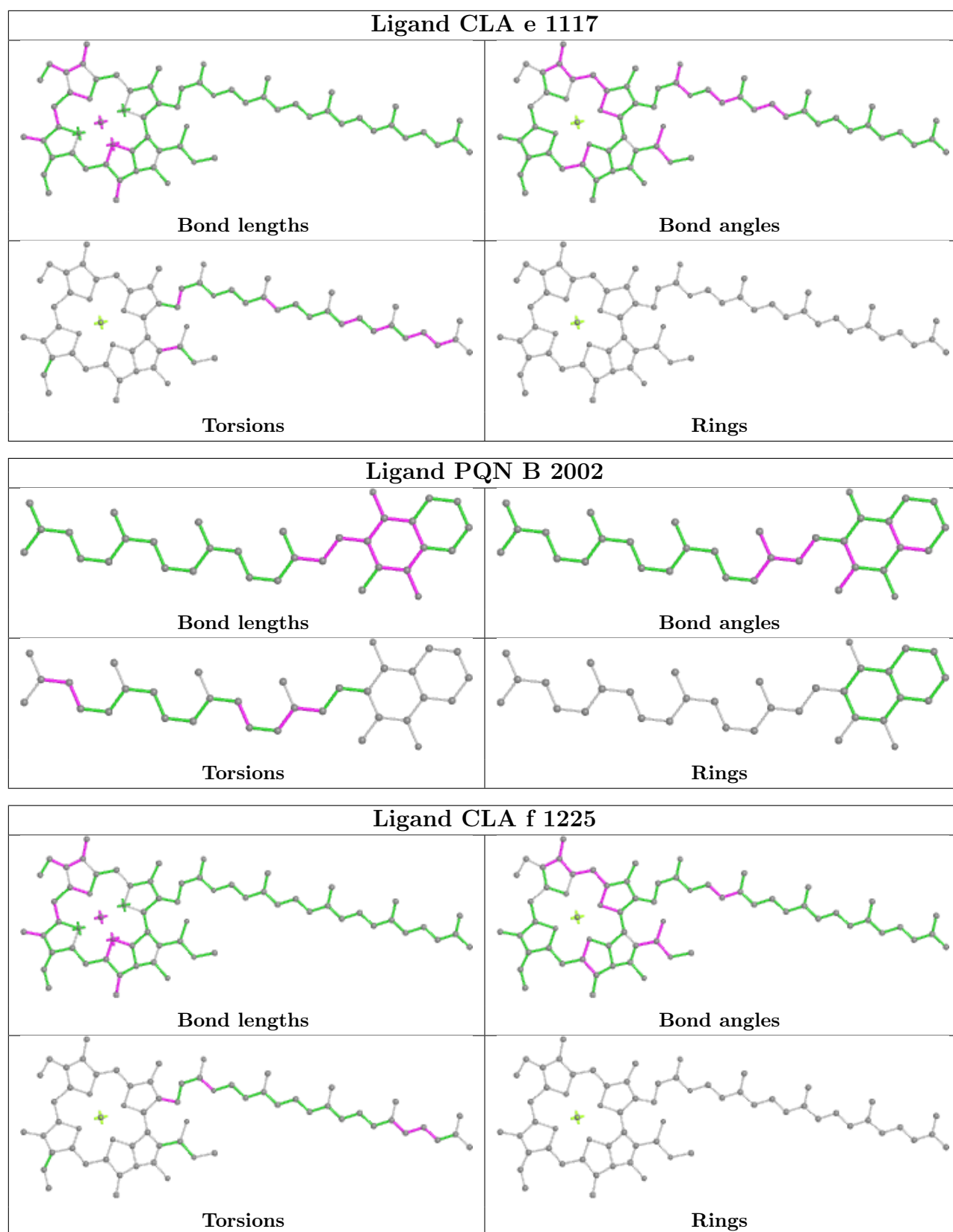
Ligand LHG G 5004



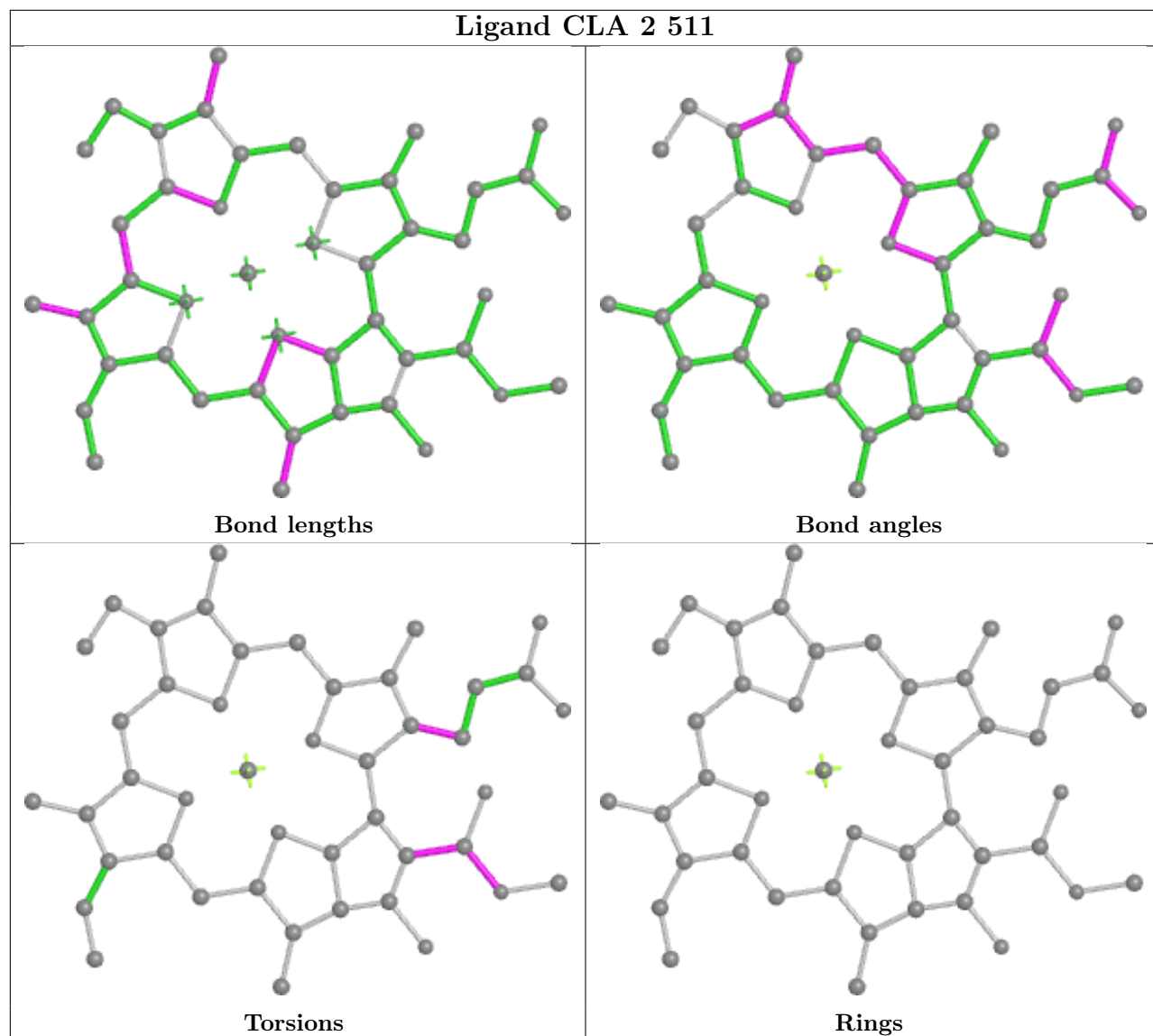
Ligand LMG T 5104



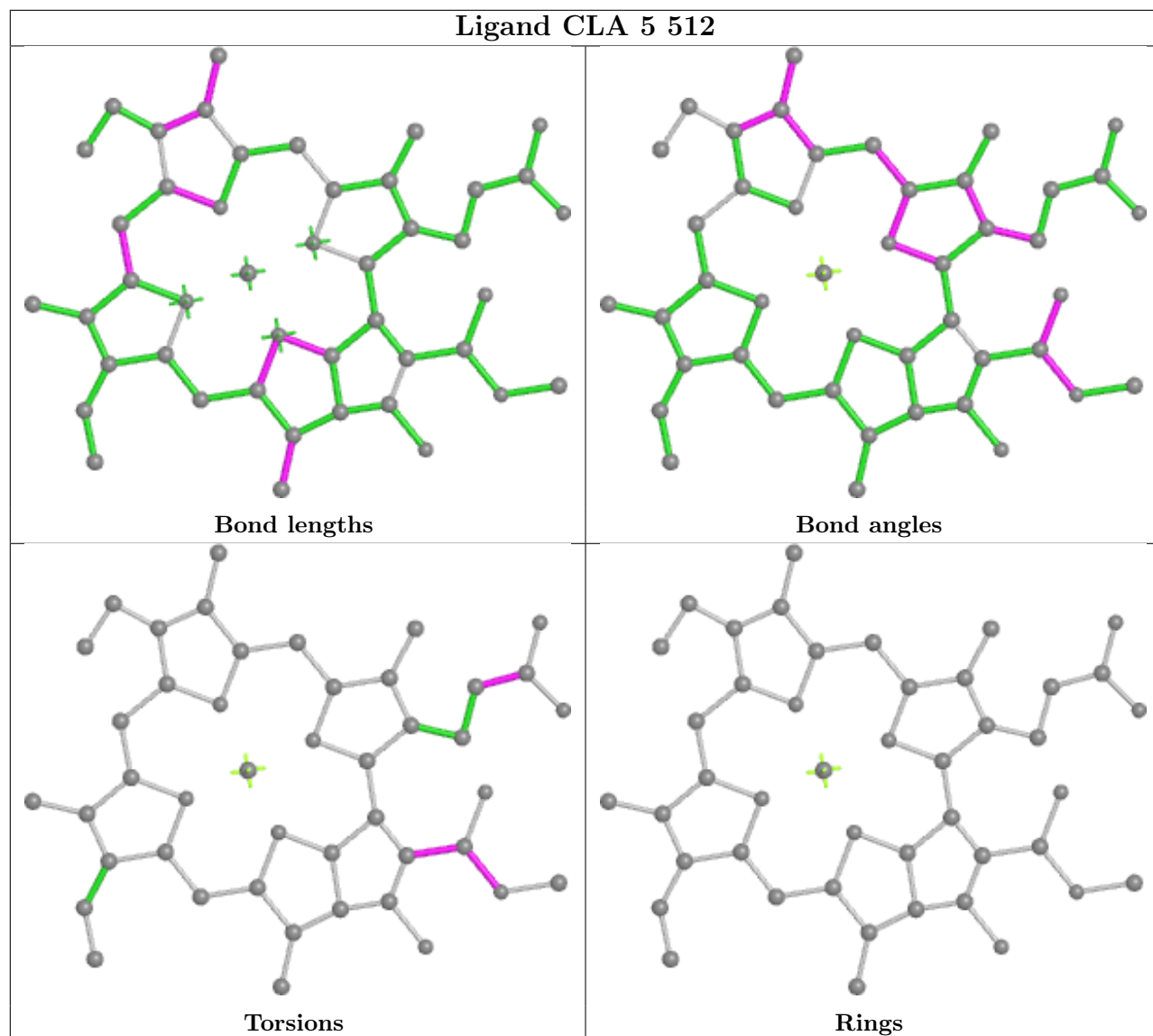




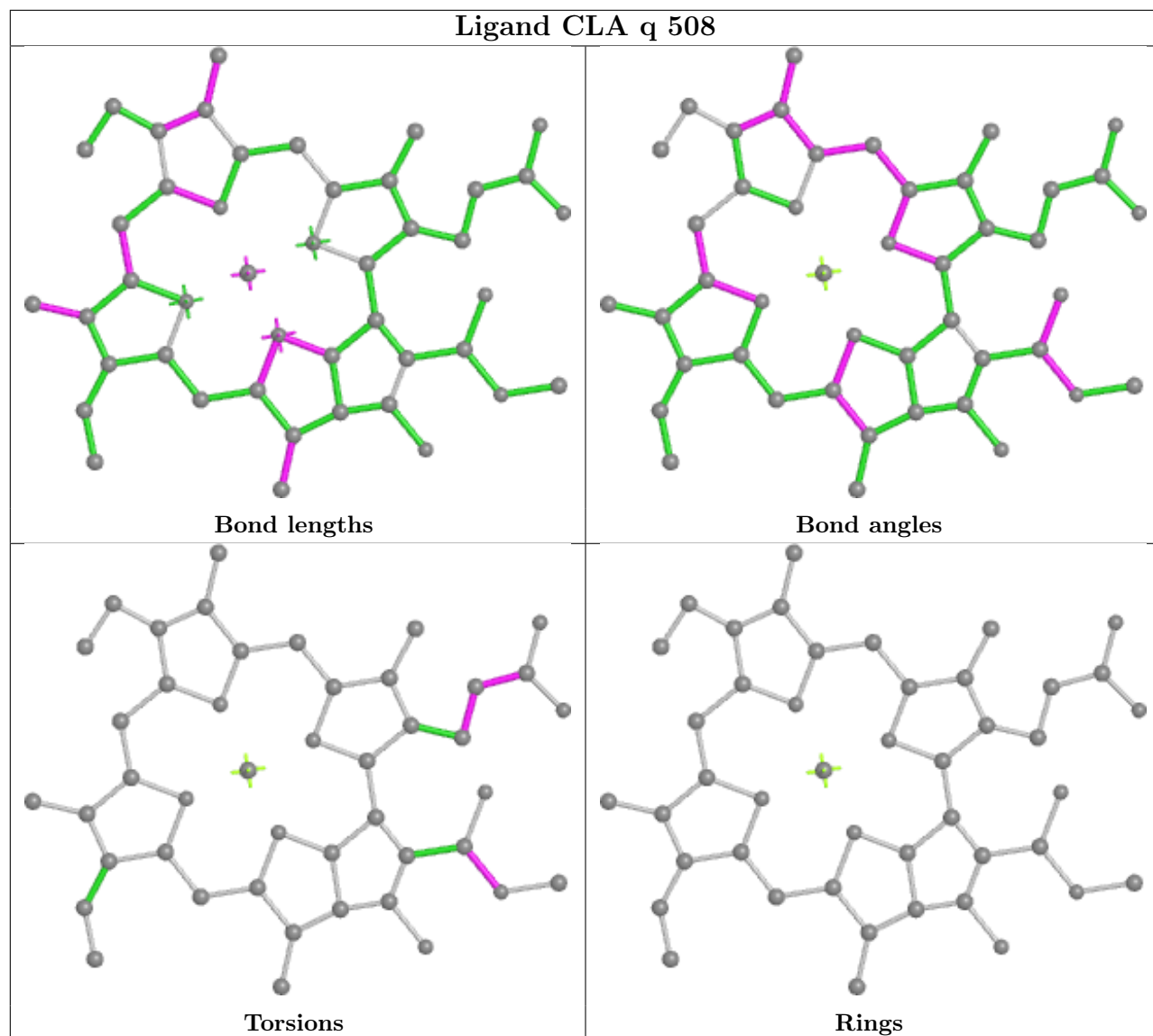
Ligand CLA 2 511



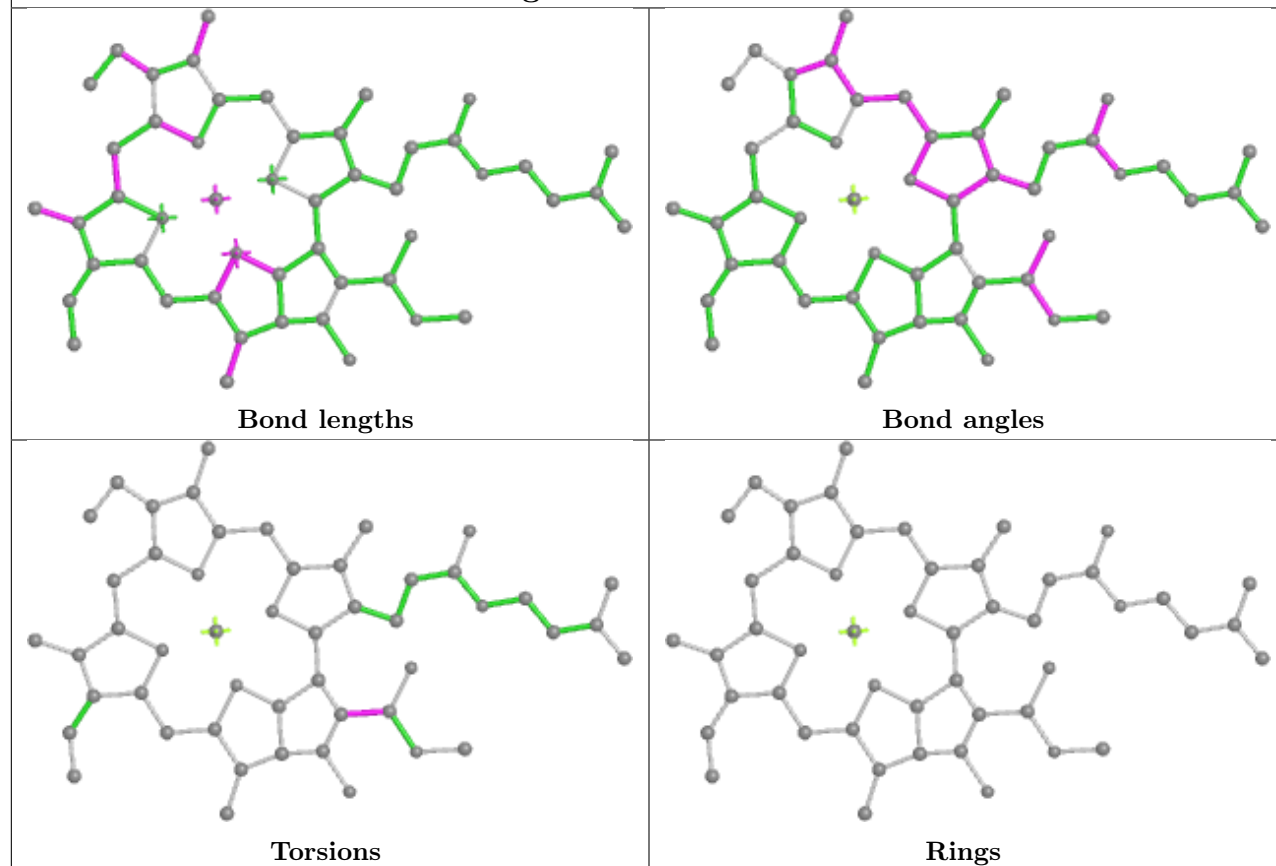
Ligand CLA 5 512



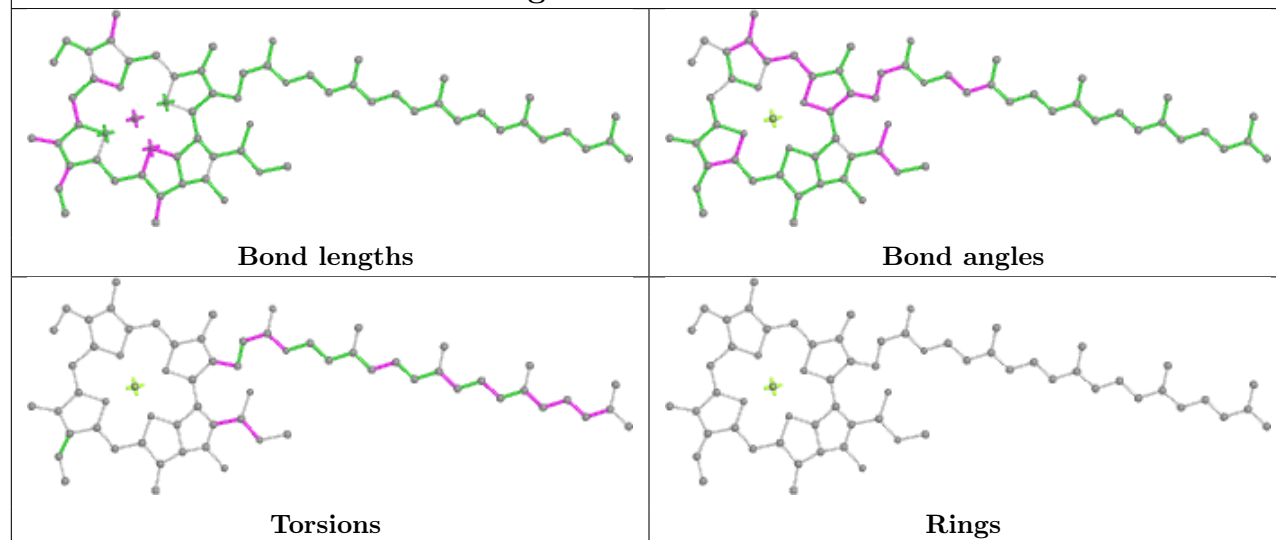
Ligand CLA q 508



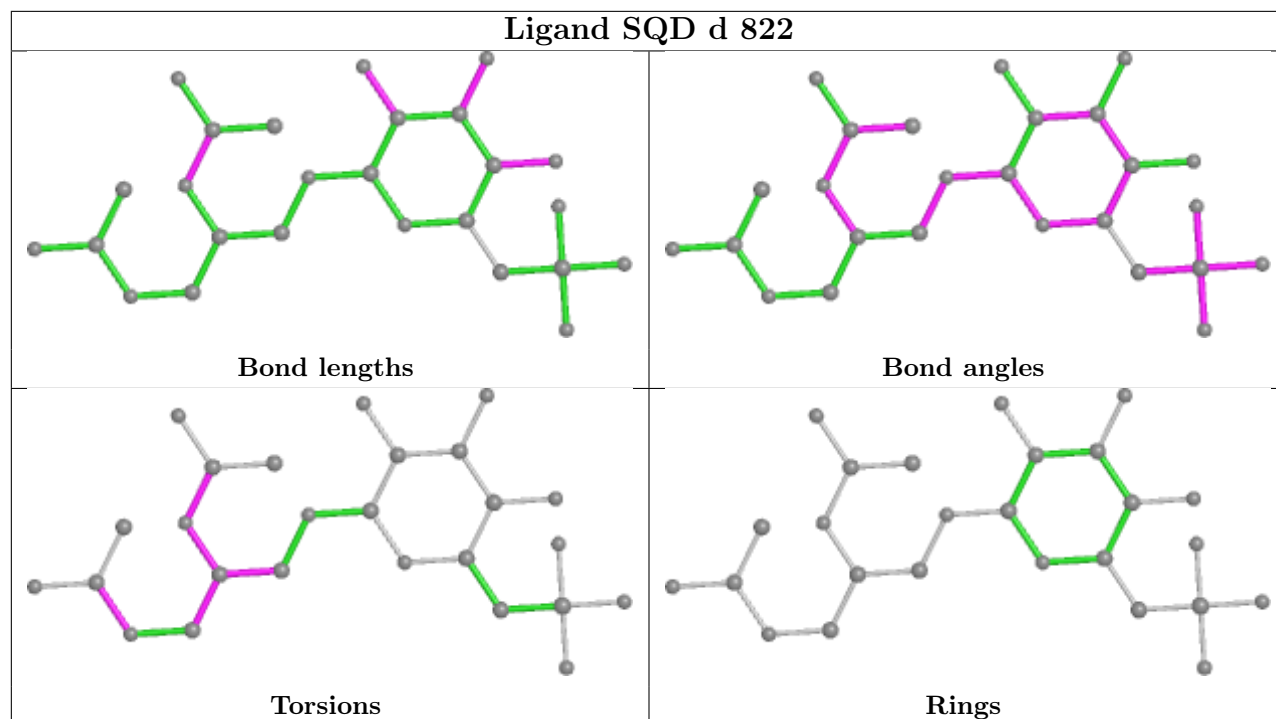
Ligand CLA H 1222



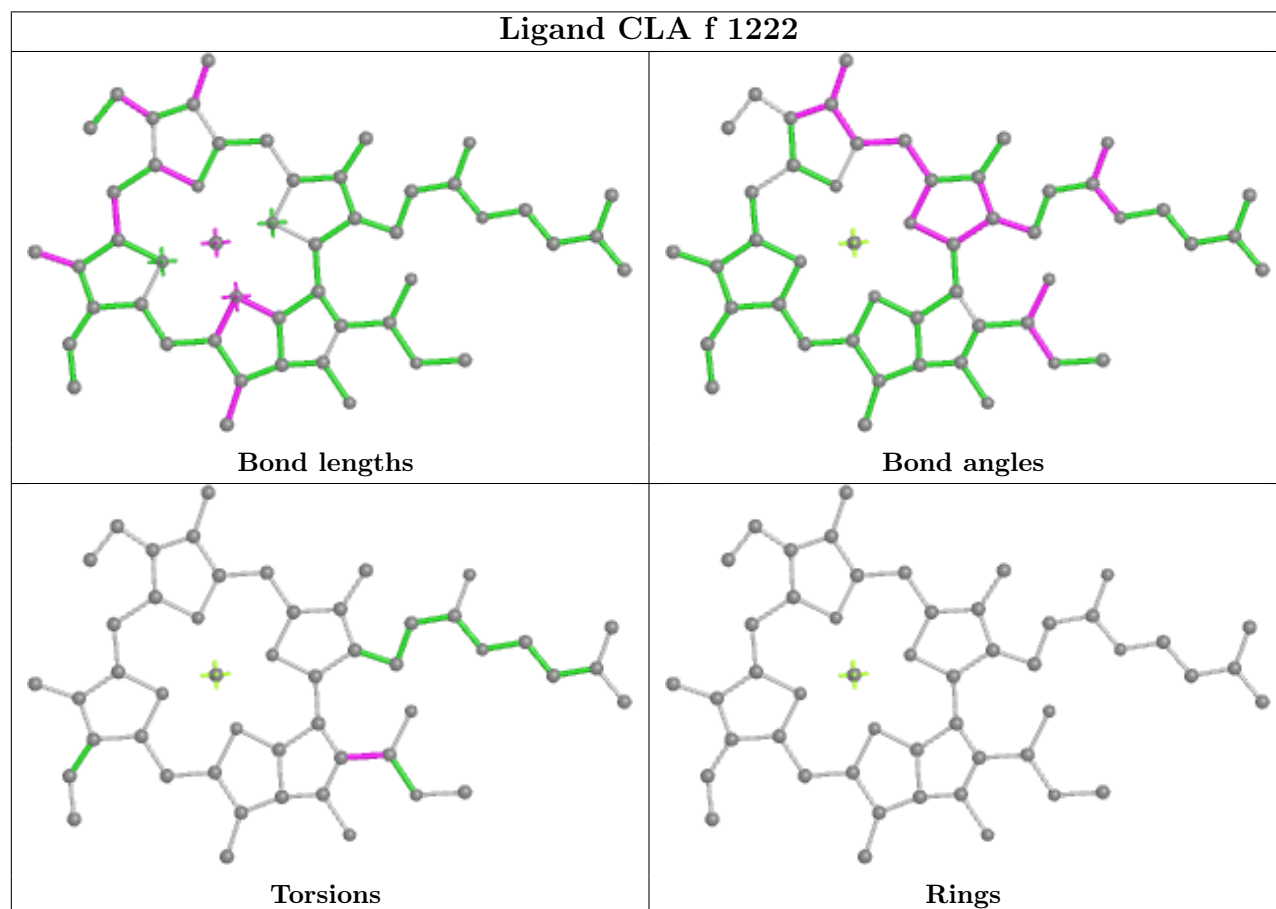
Ligand CLA e 1103



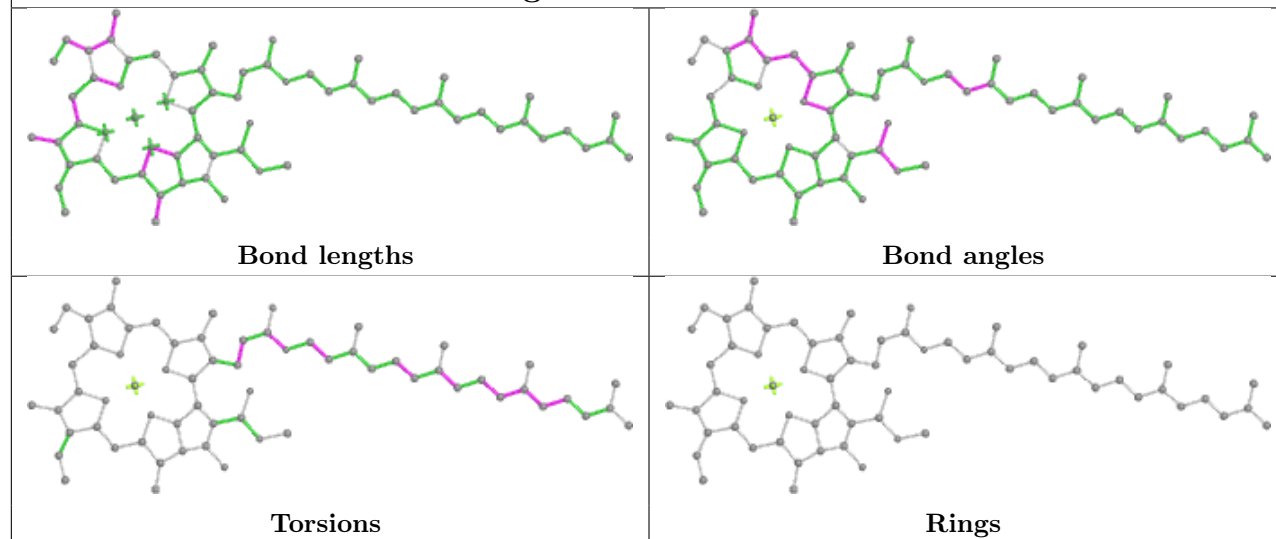
Ligand SQD d 822



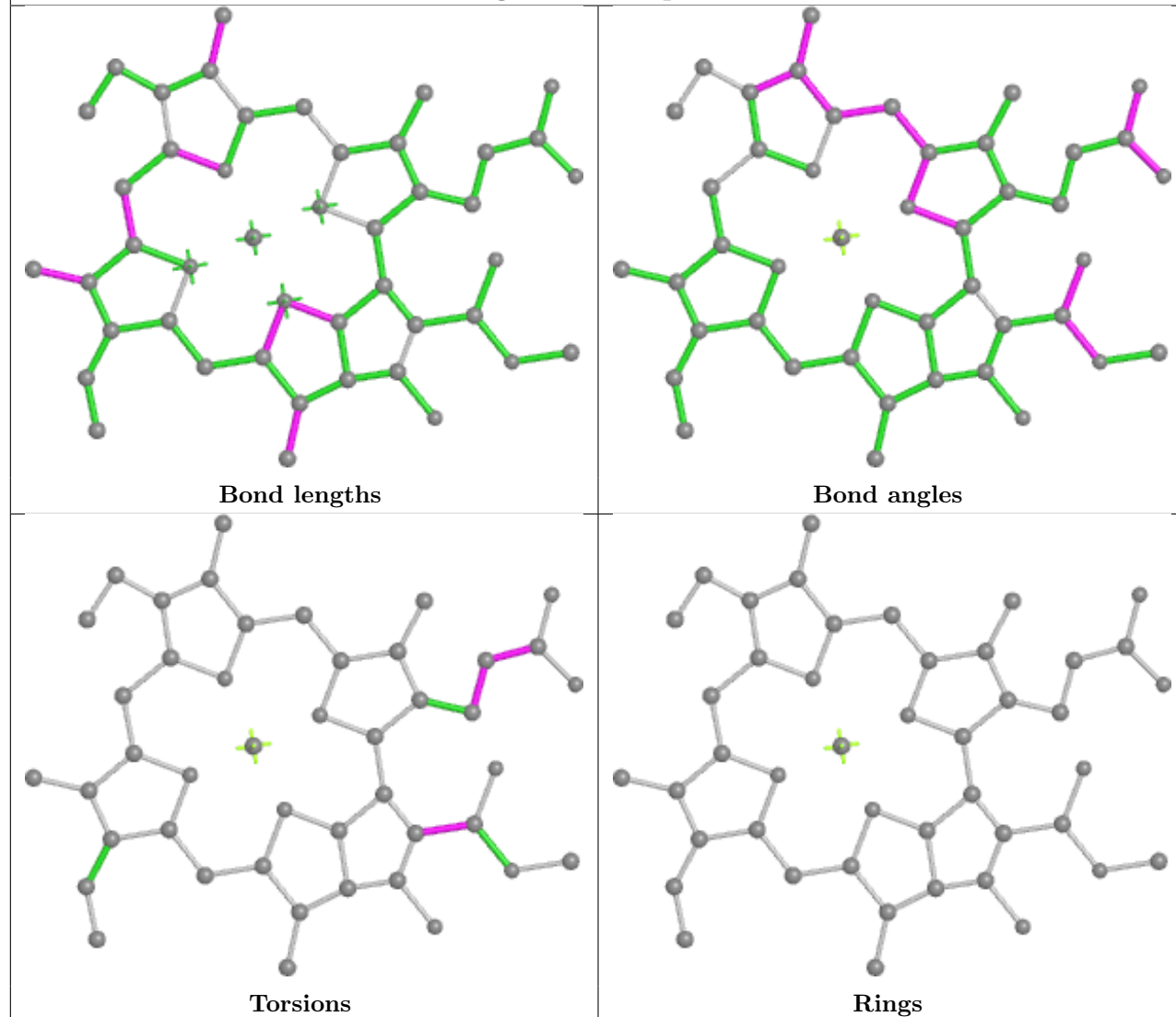
Ligand CLA f 1222



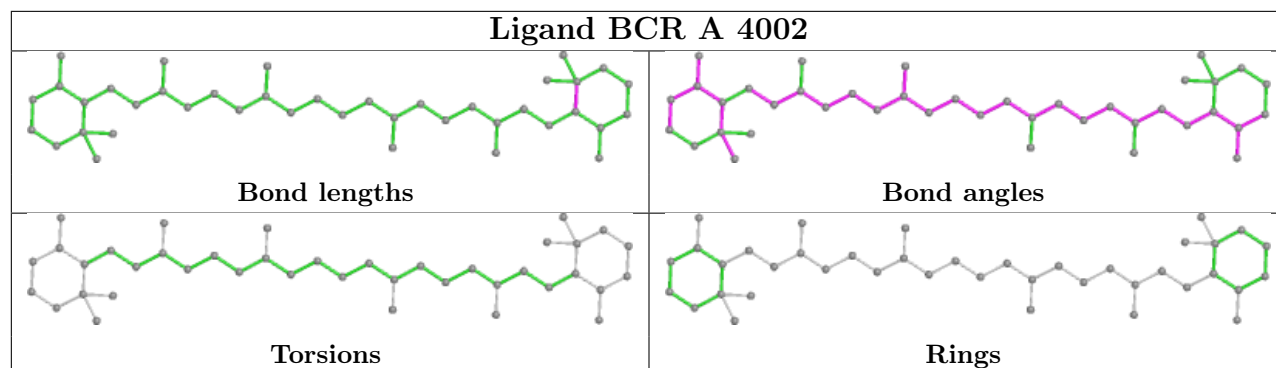
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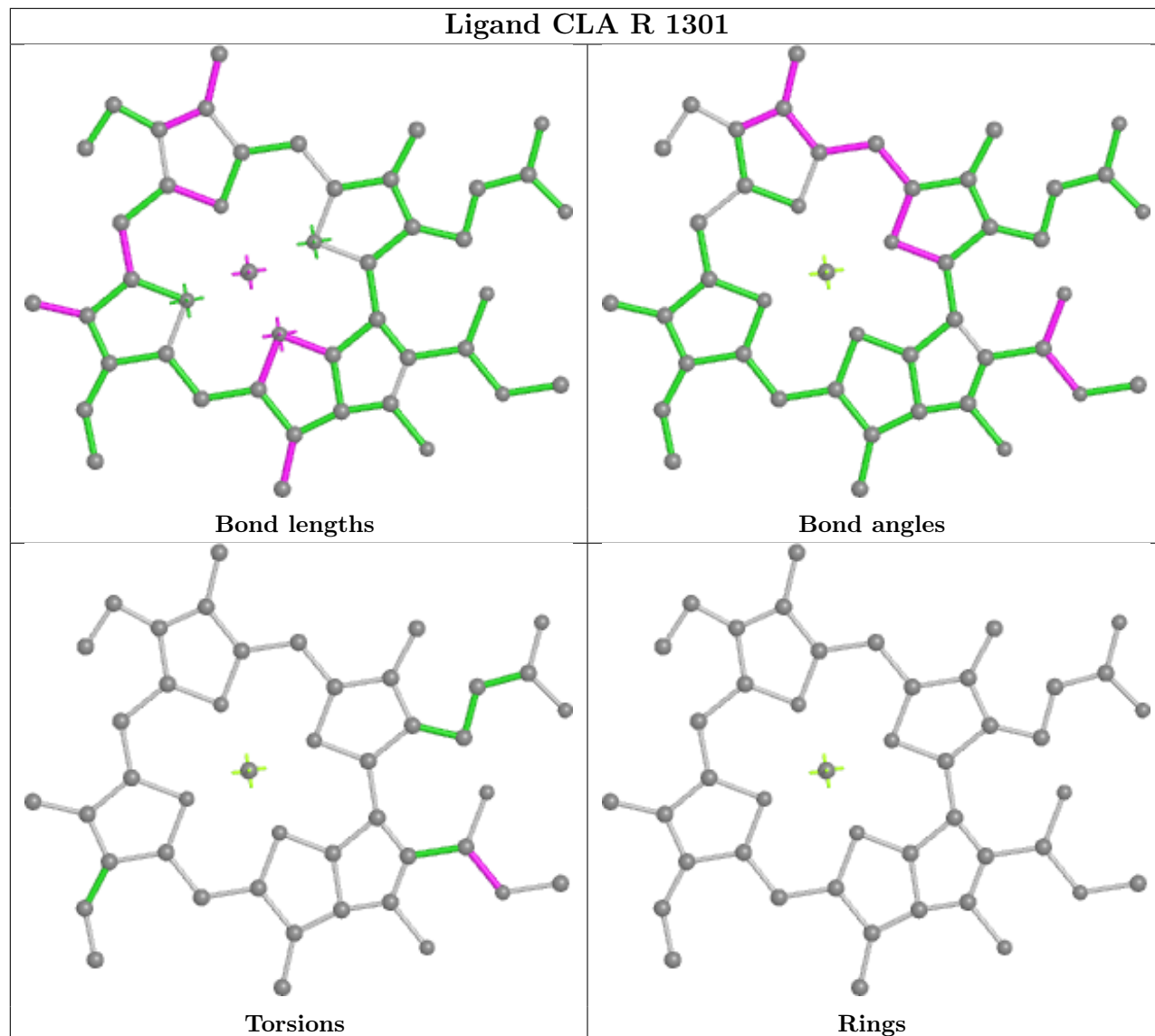
Ligand CLA q 513

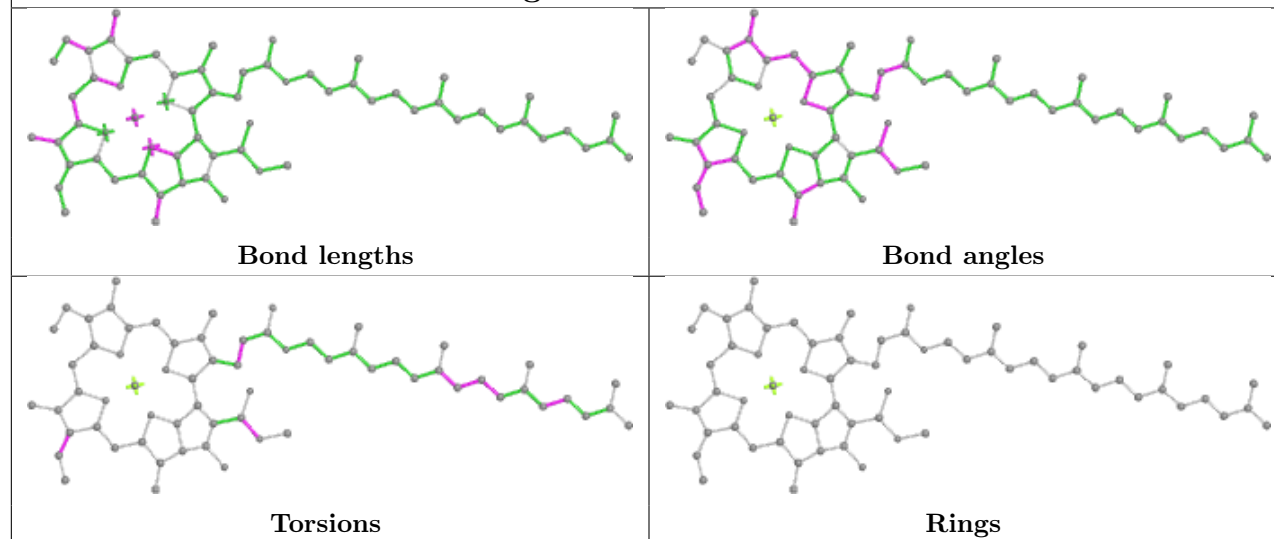
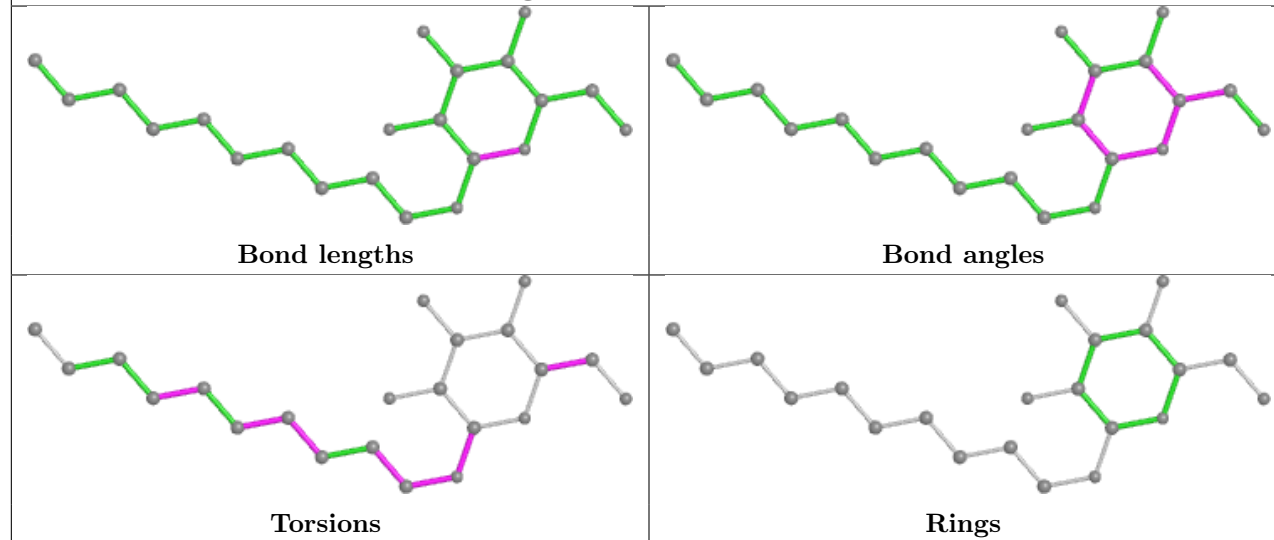


Ligand BCR A 4002

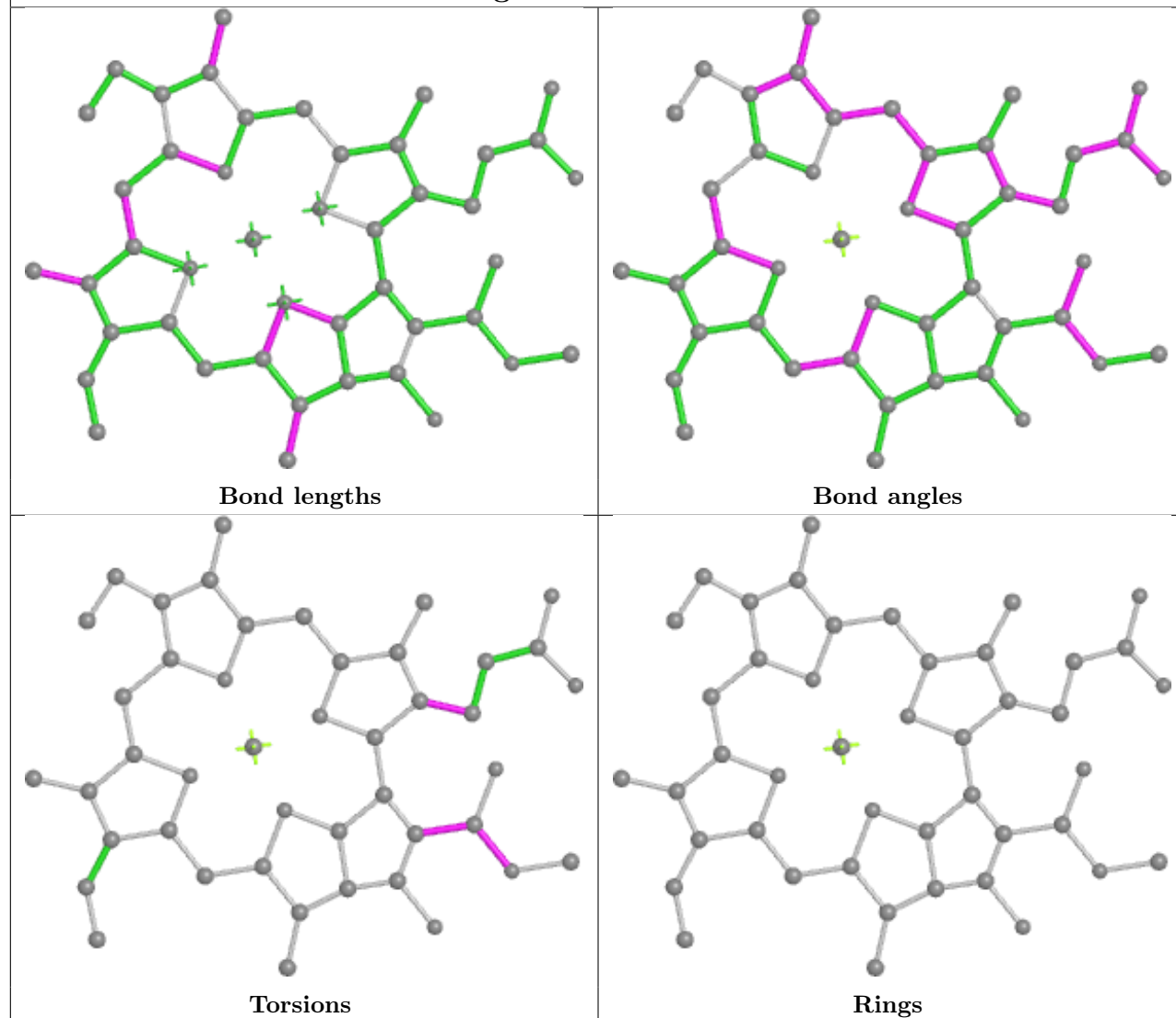


Ligand CLA R 1301

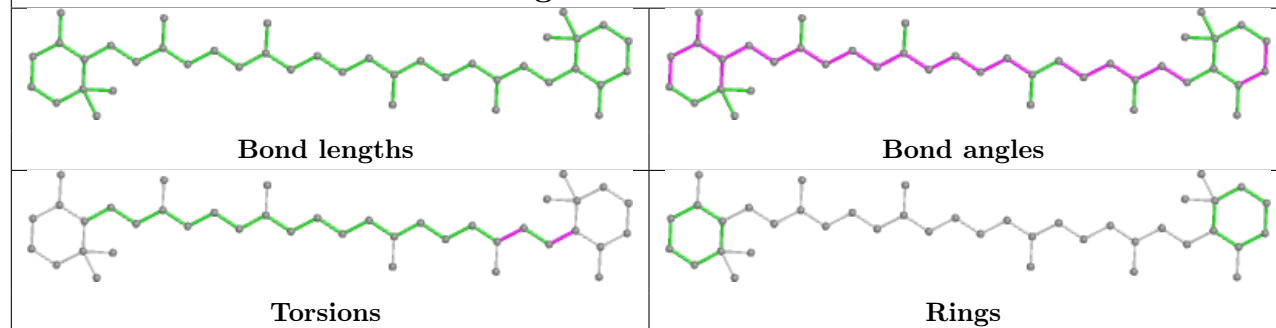


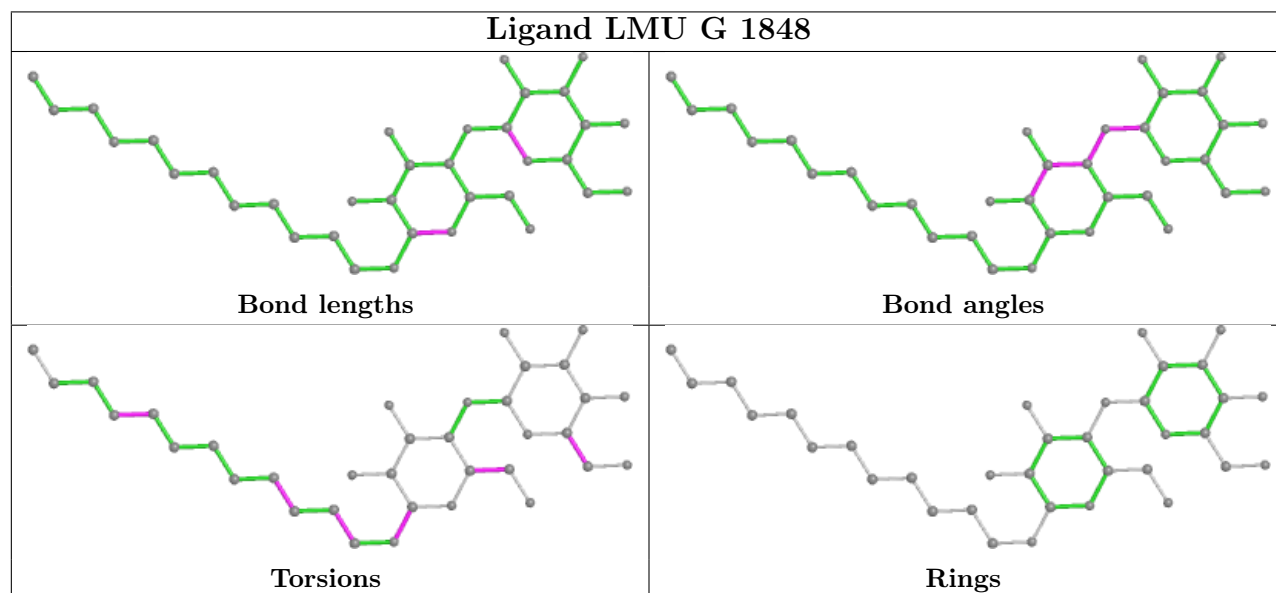
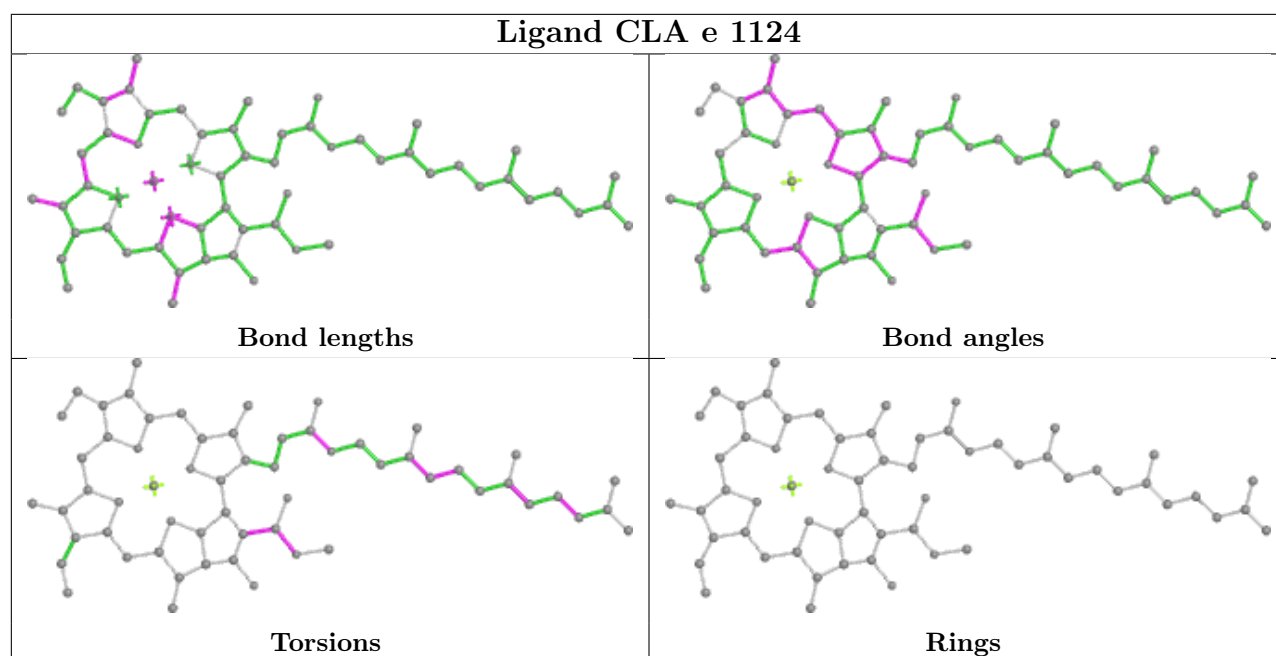
Ligand CLA B 1023**Ligand LMU T 5105**

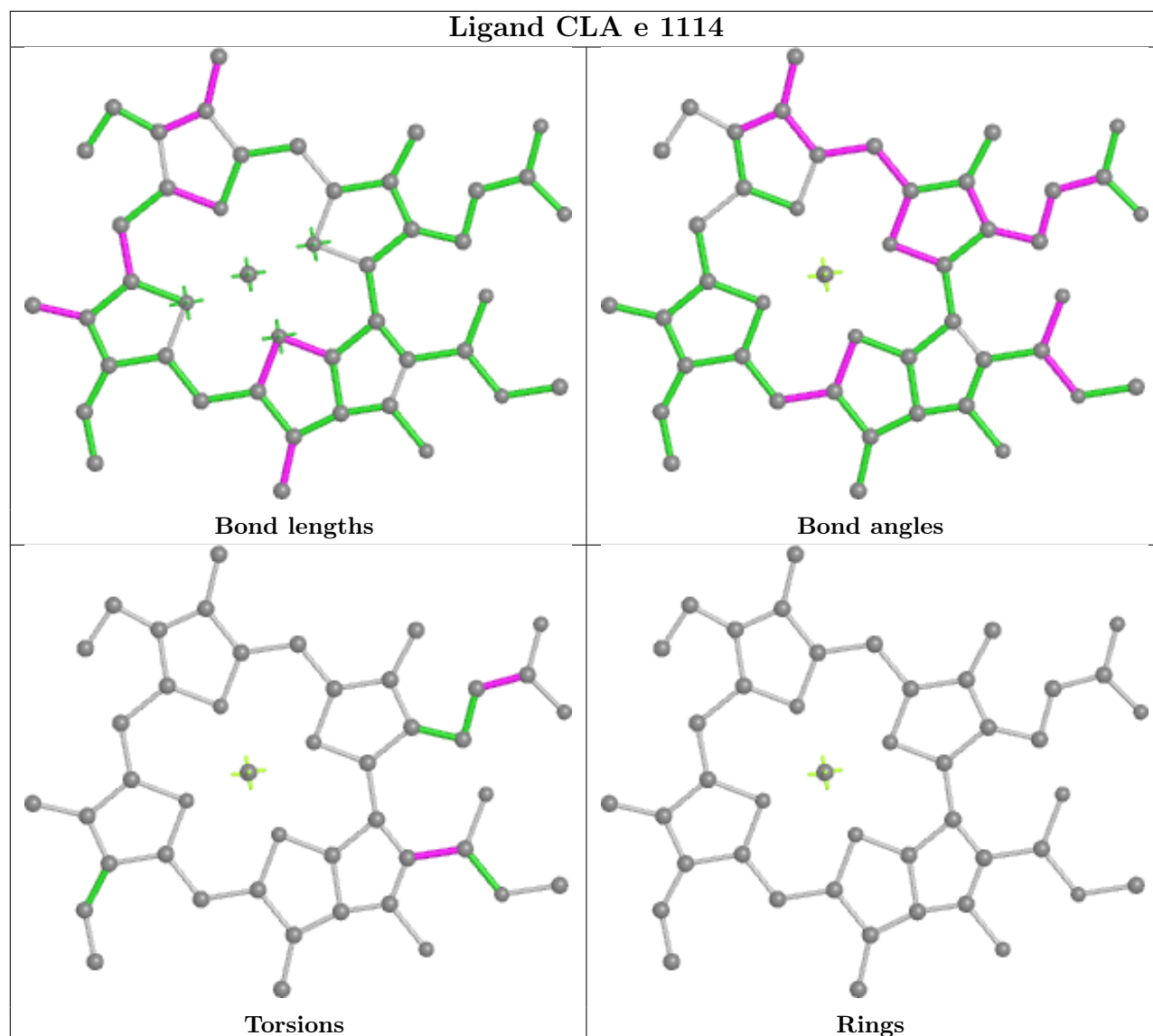
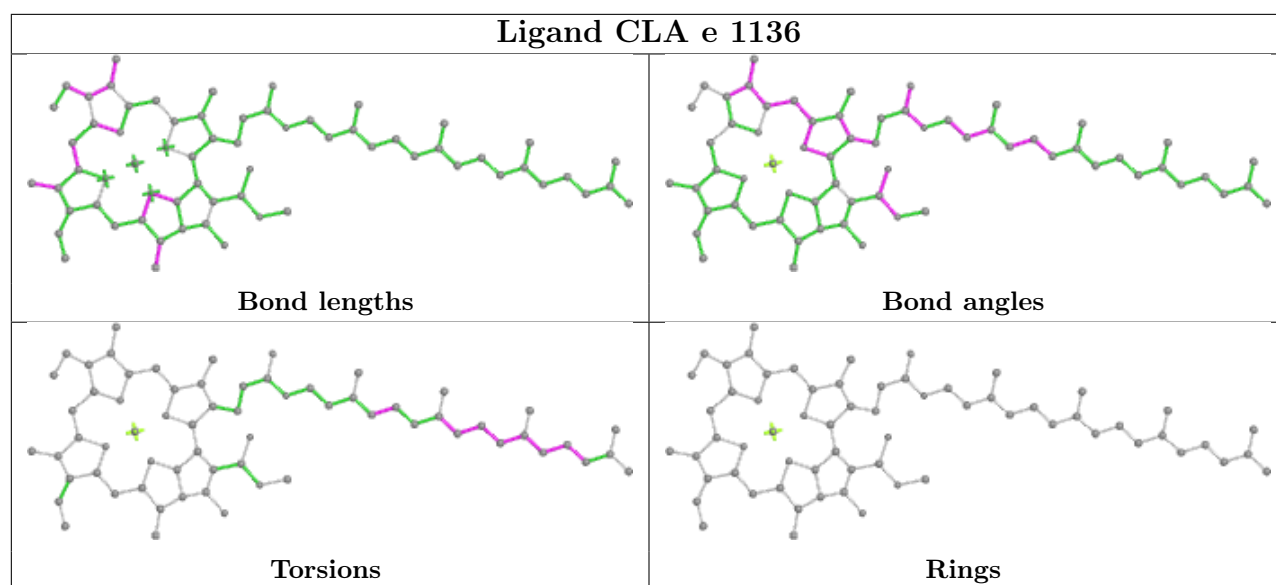
Ligand CLA v 508



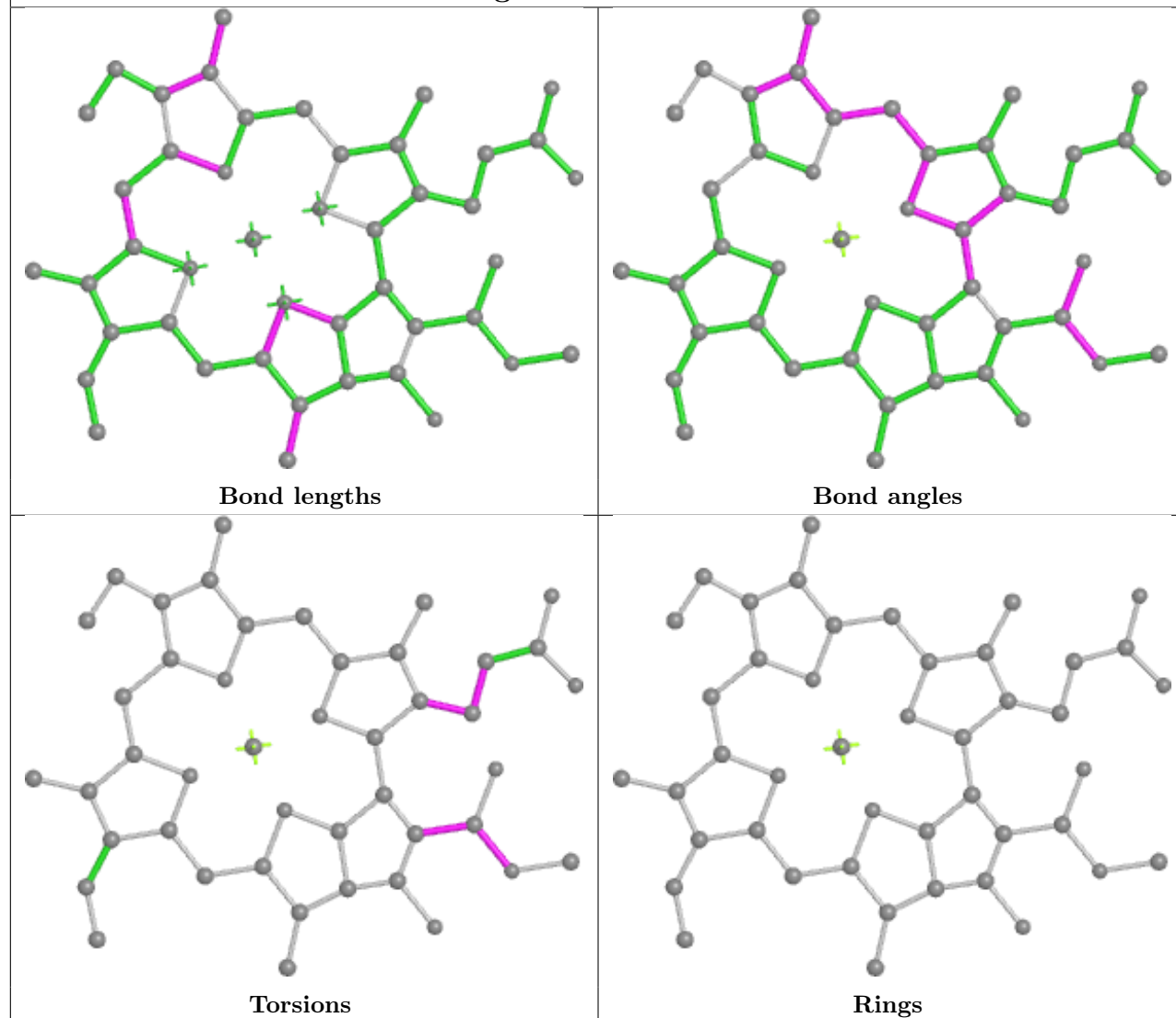
Ligand BCR a 523



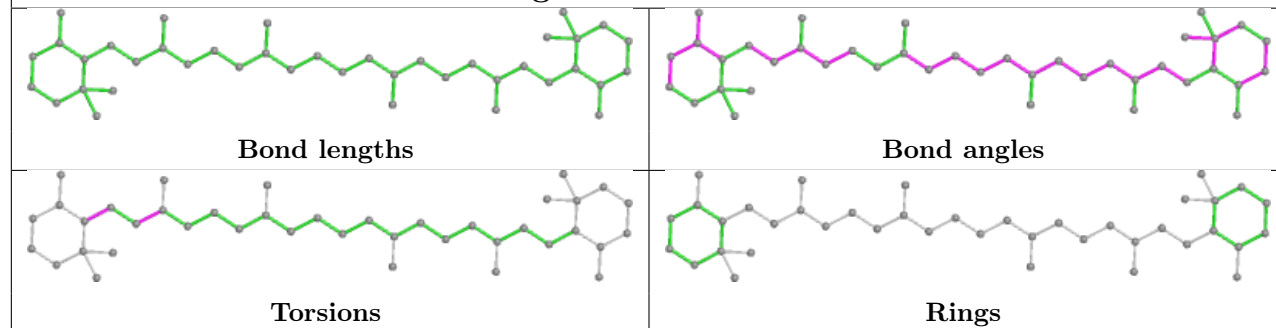




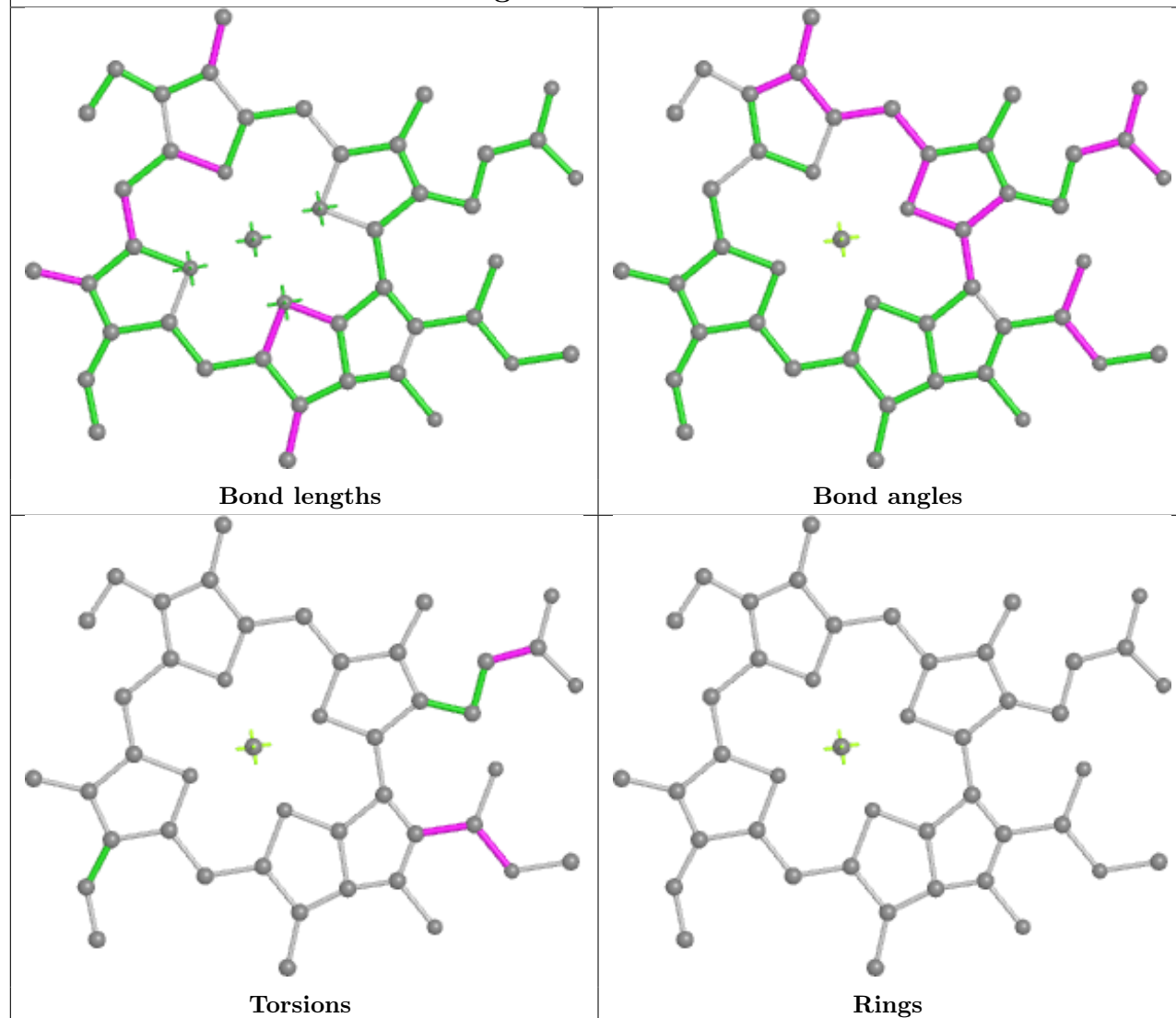
Ligand CLA 5 502



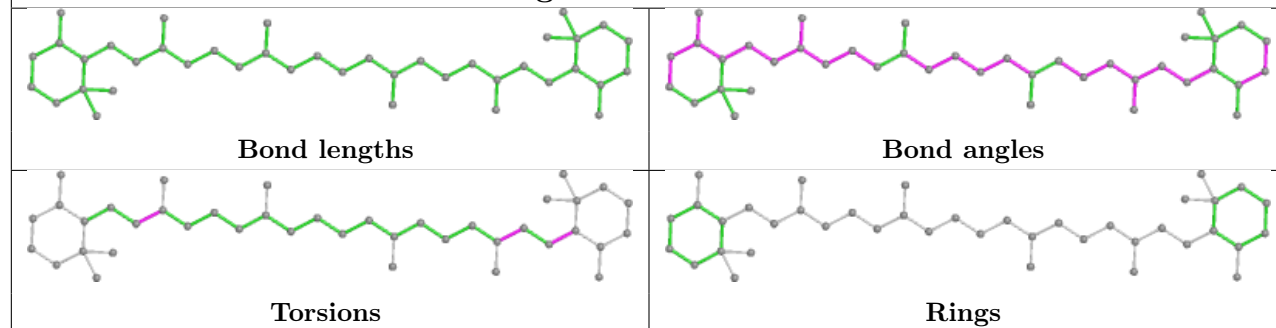
Ligand BCR Z 521

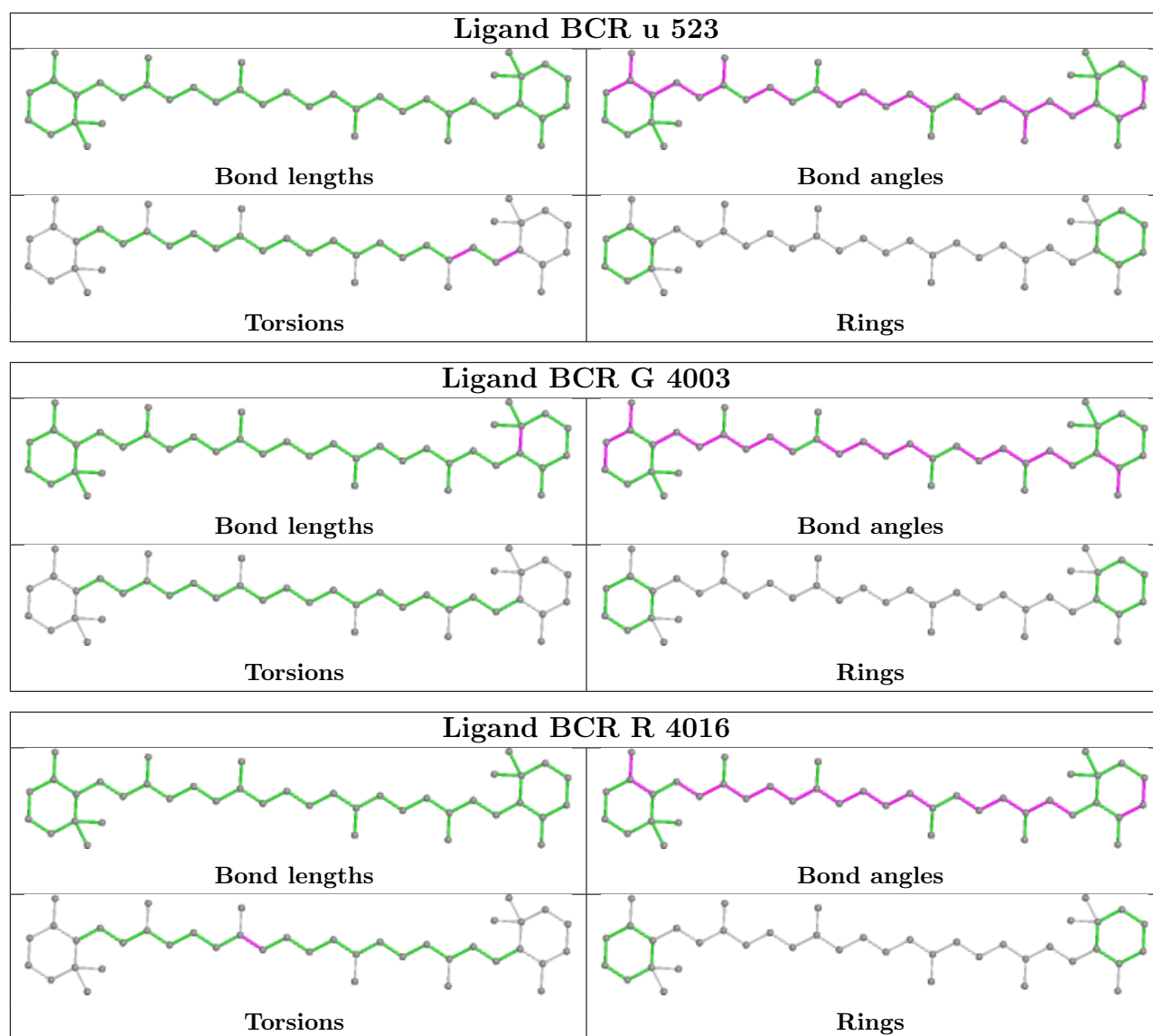


Ligand CLA 4 509

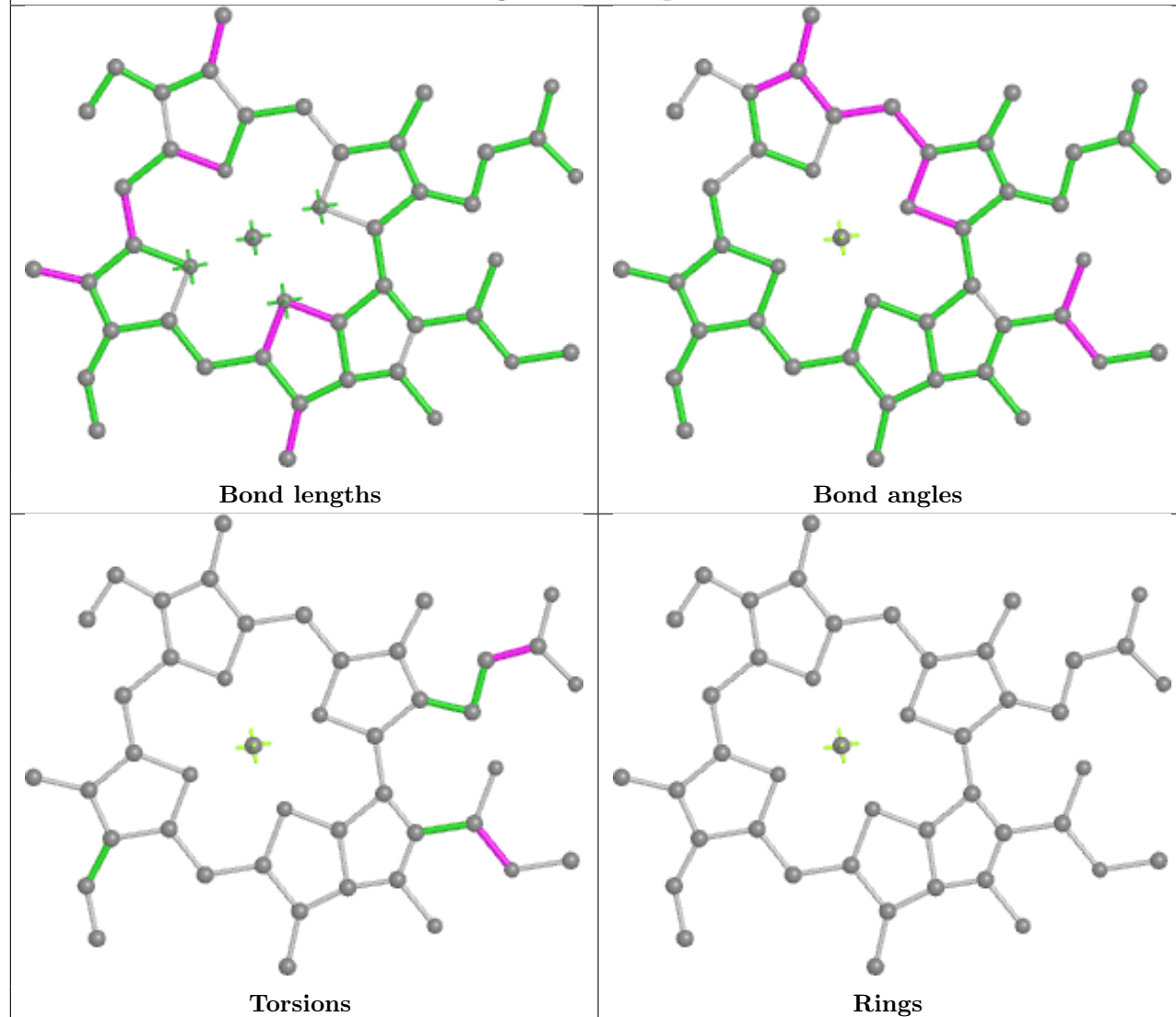


Ligand BCR r 523

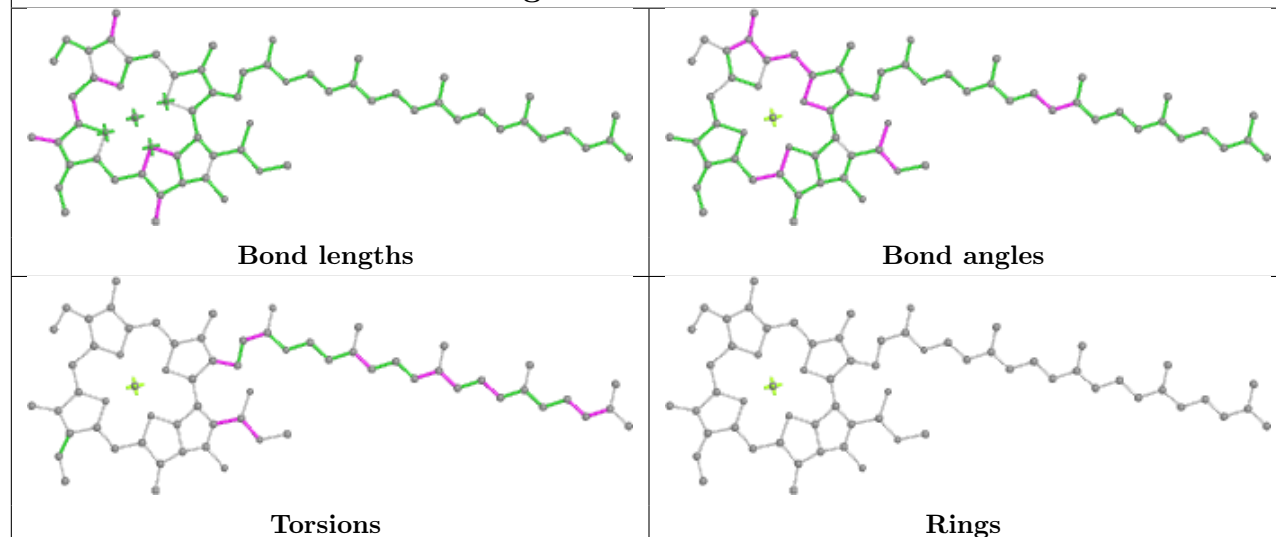


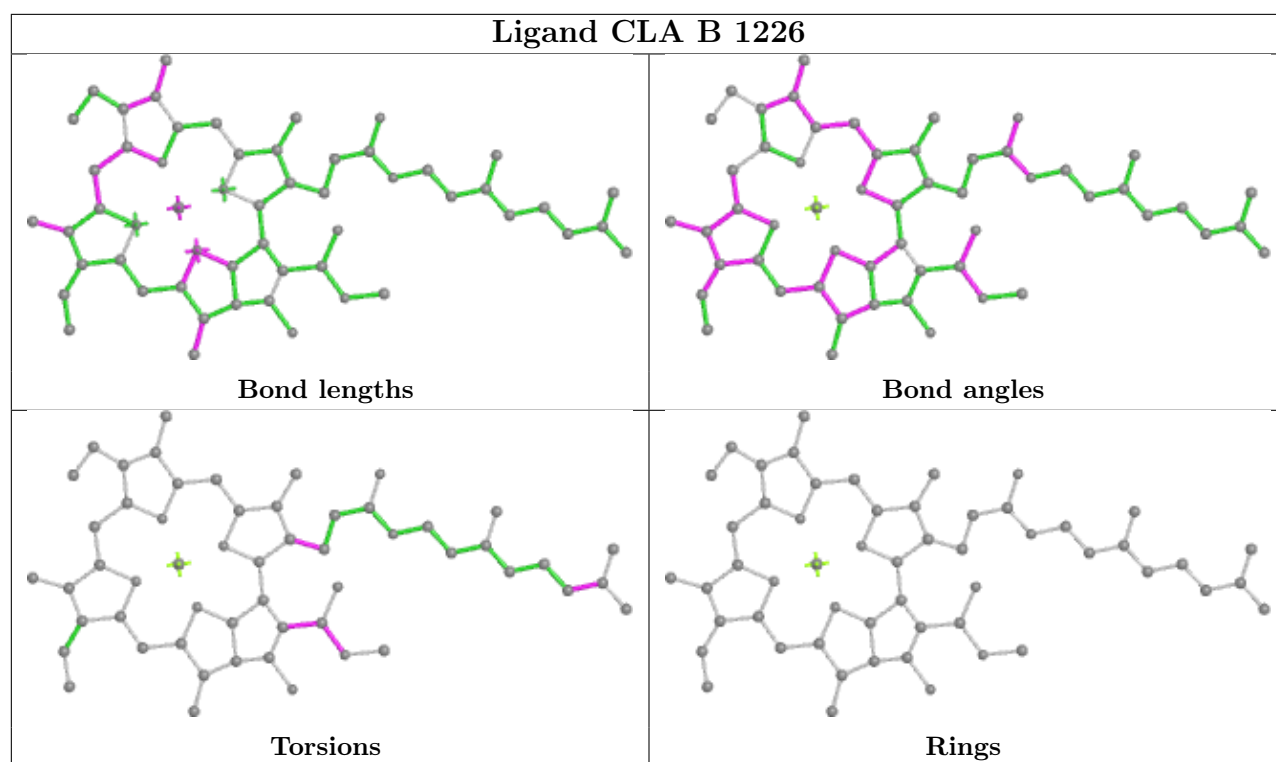


Ligand CLA q 510

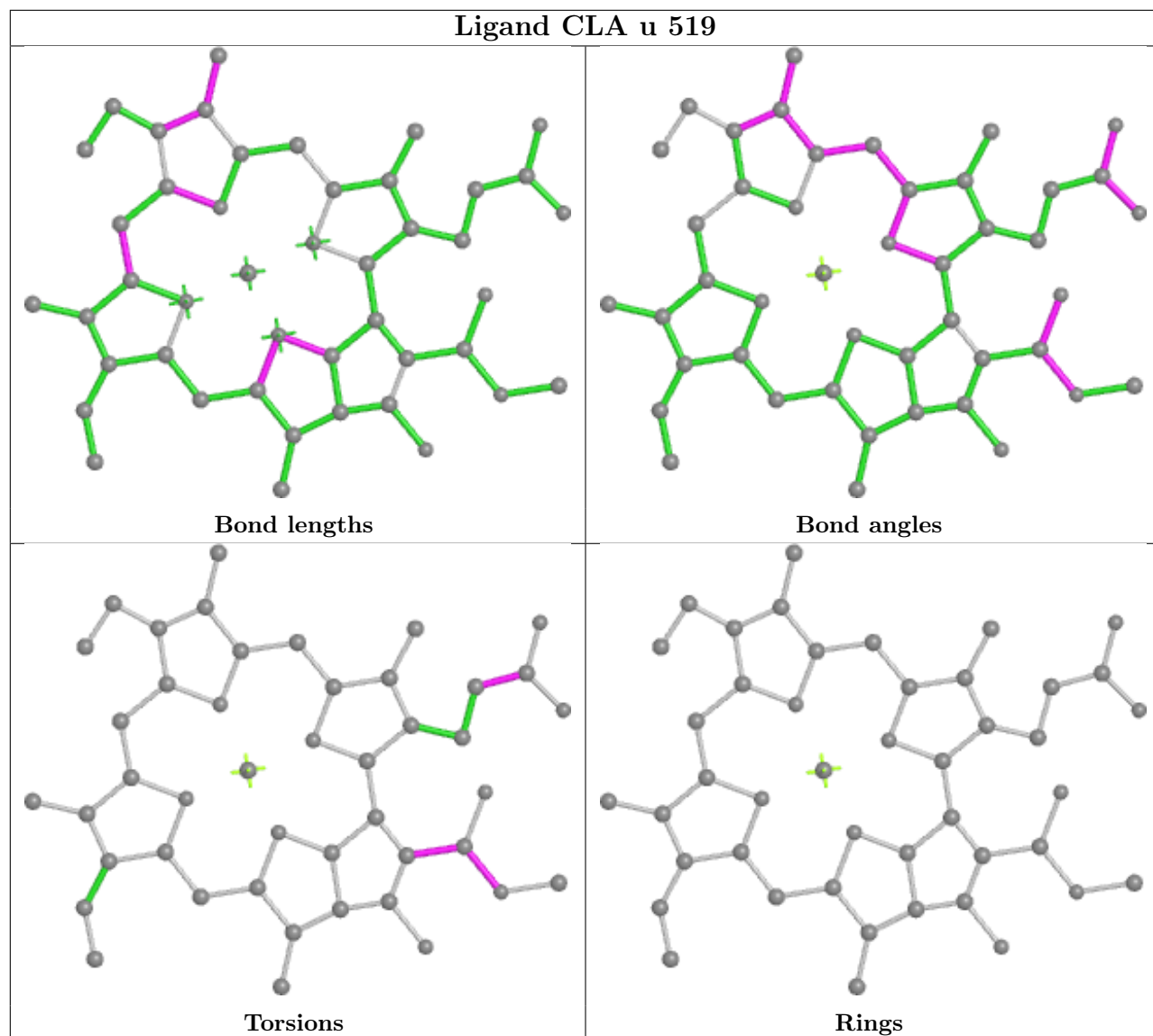


Ligand CLA B 1229

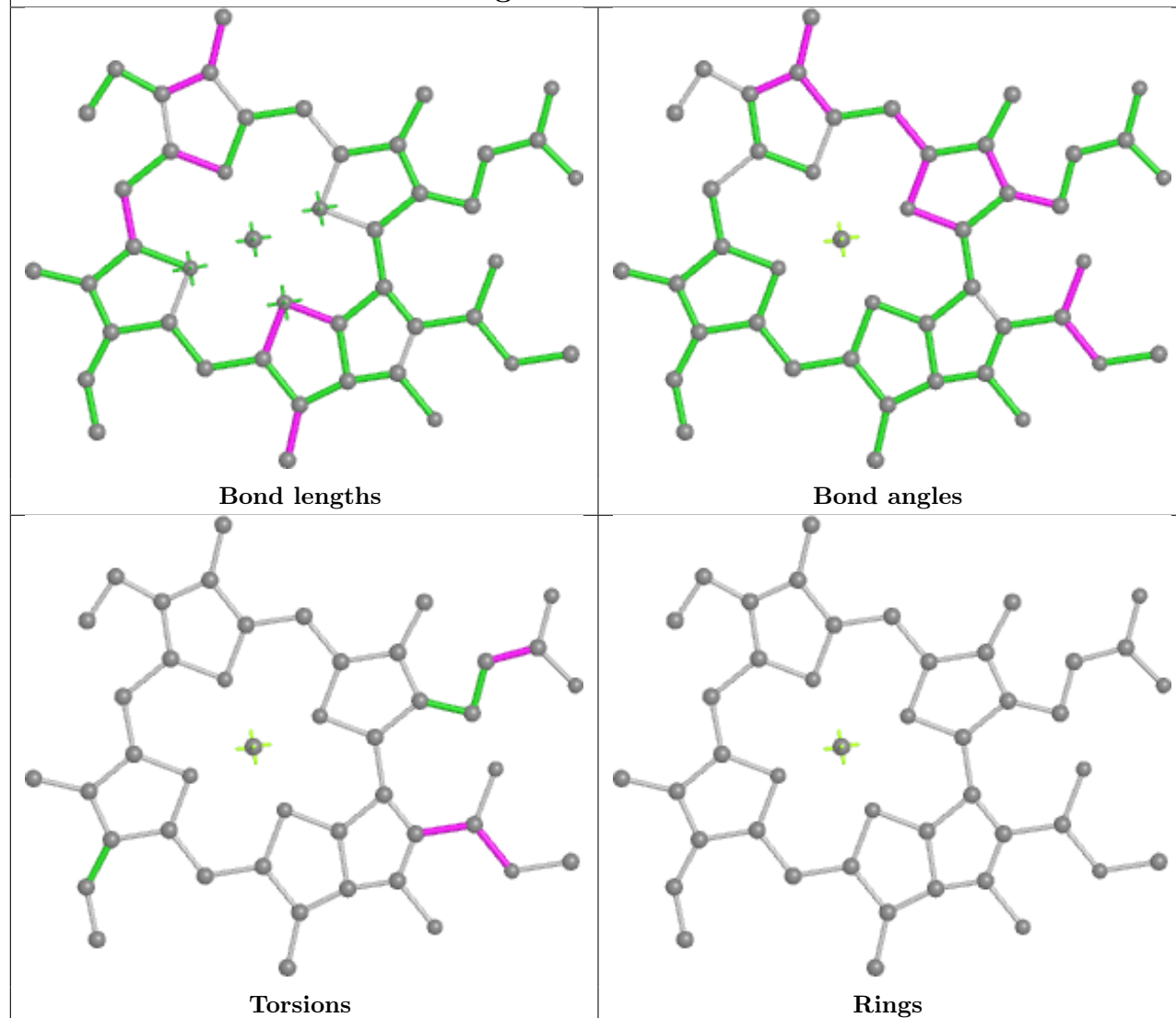




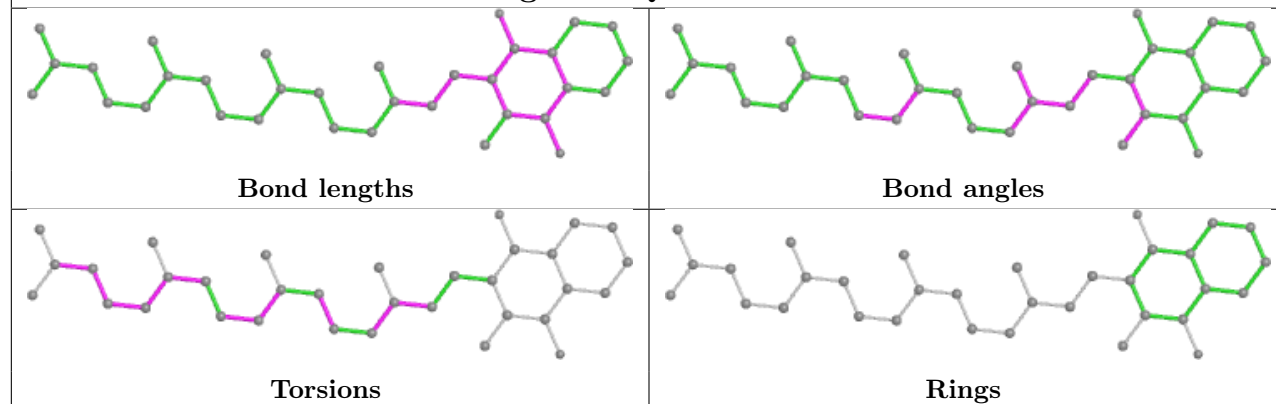
Ligand CLA u 519

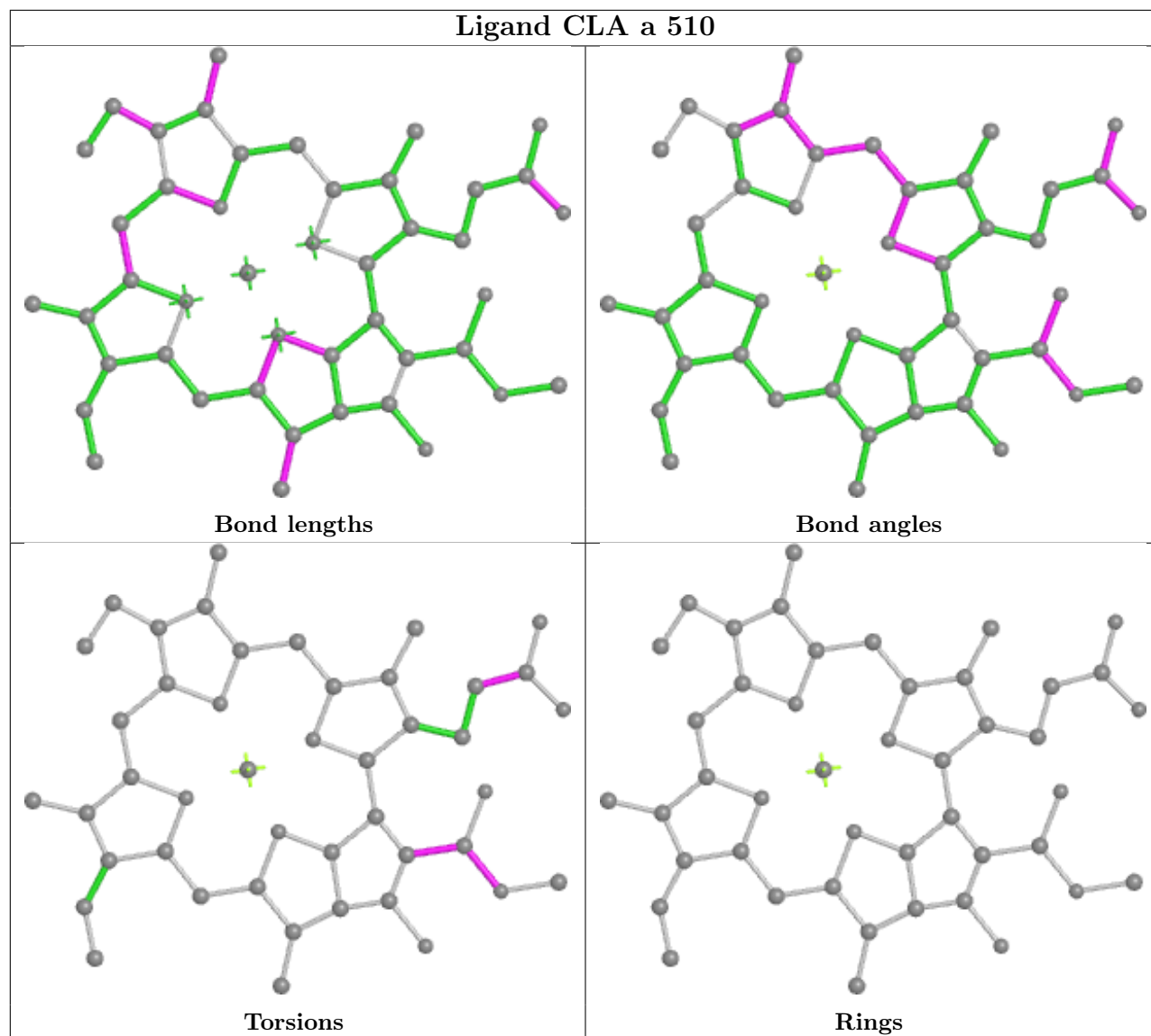
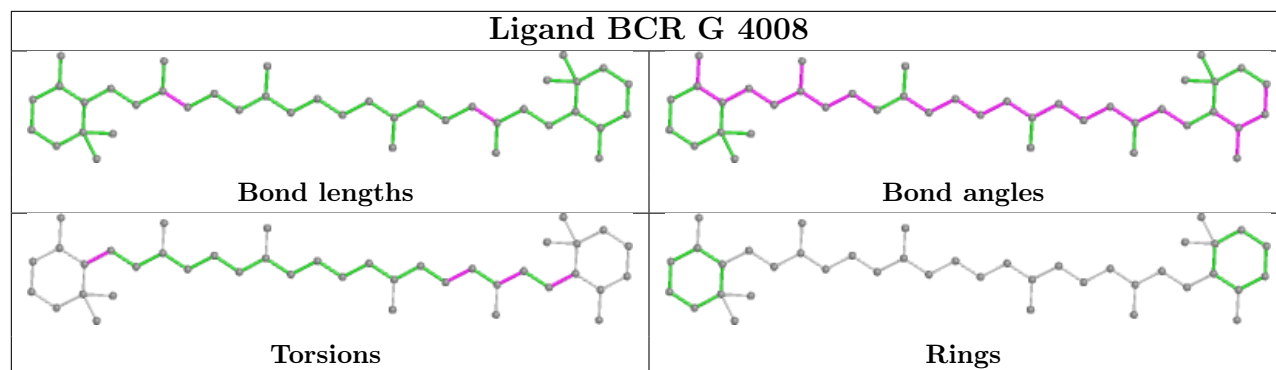


Ligand CLA c 512

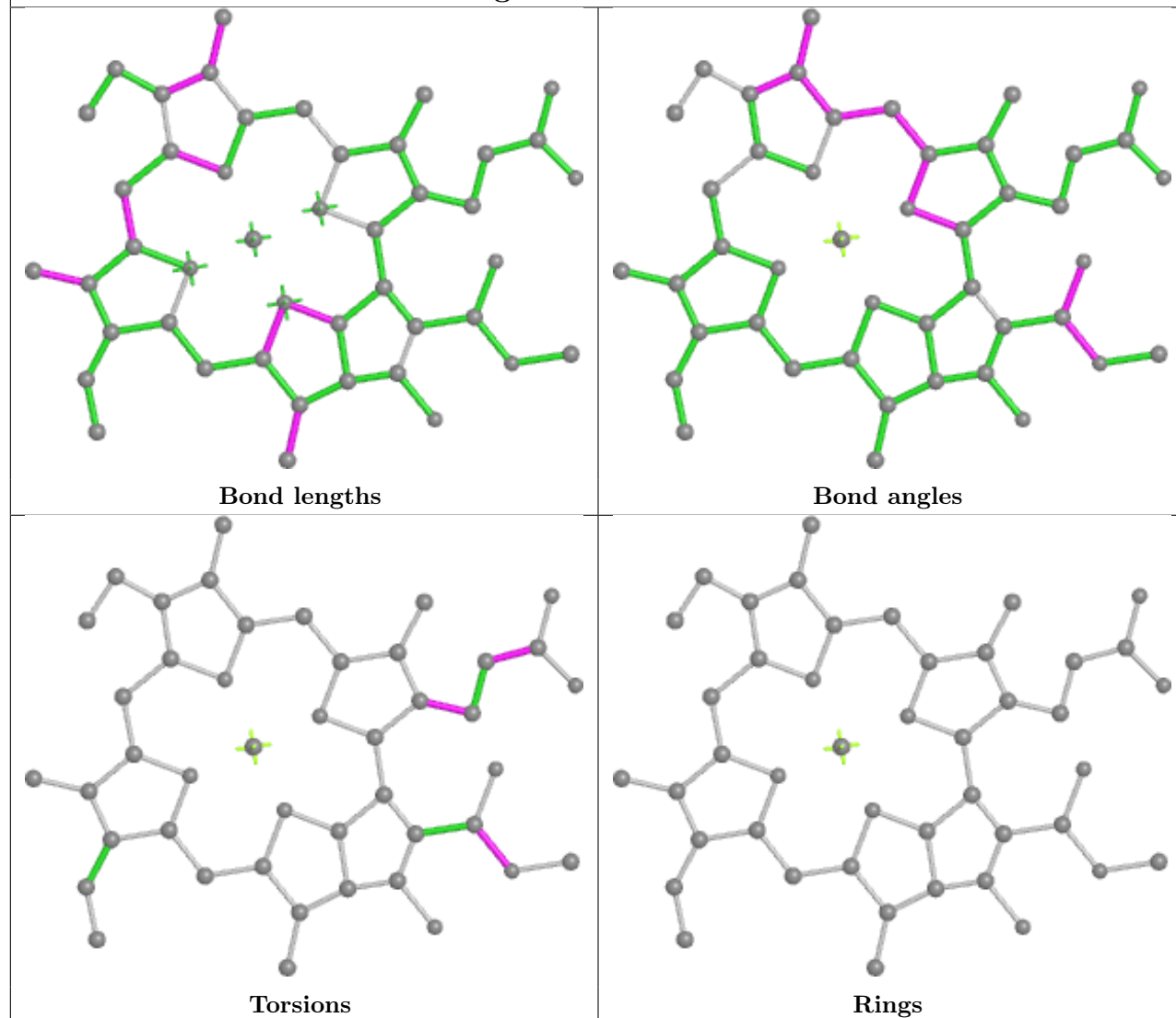


Ligand PQN G 2001

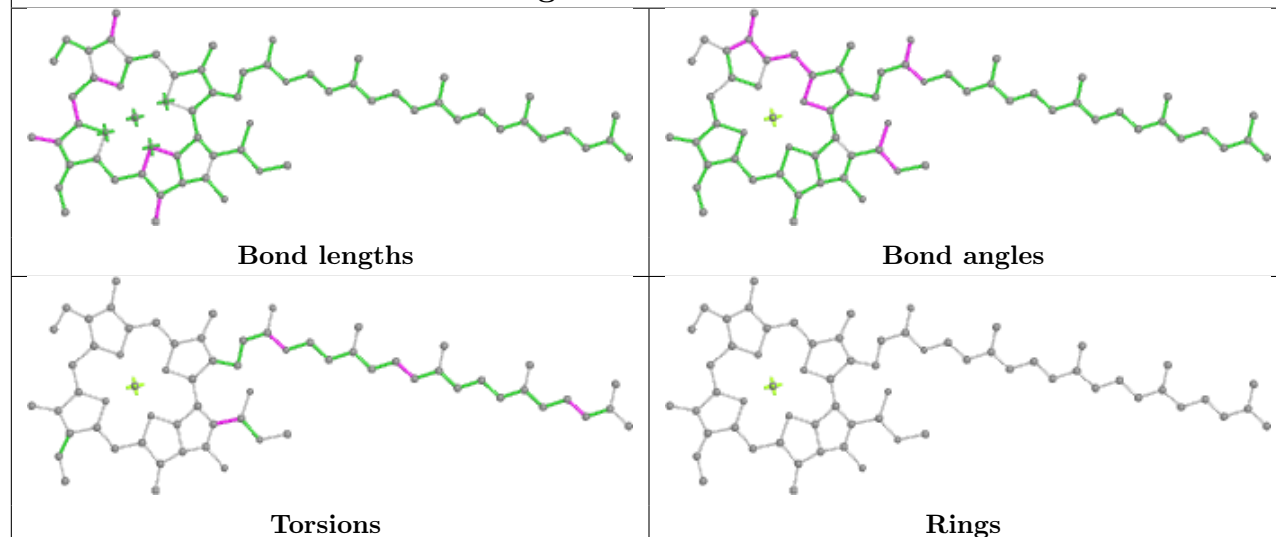




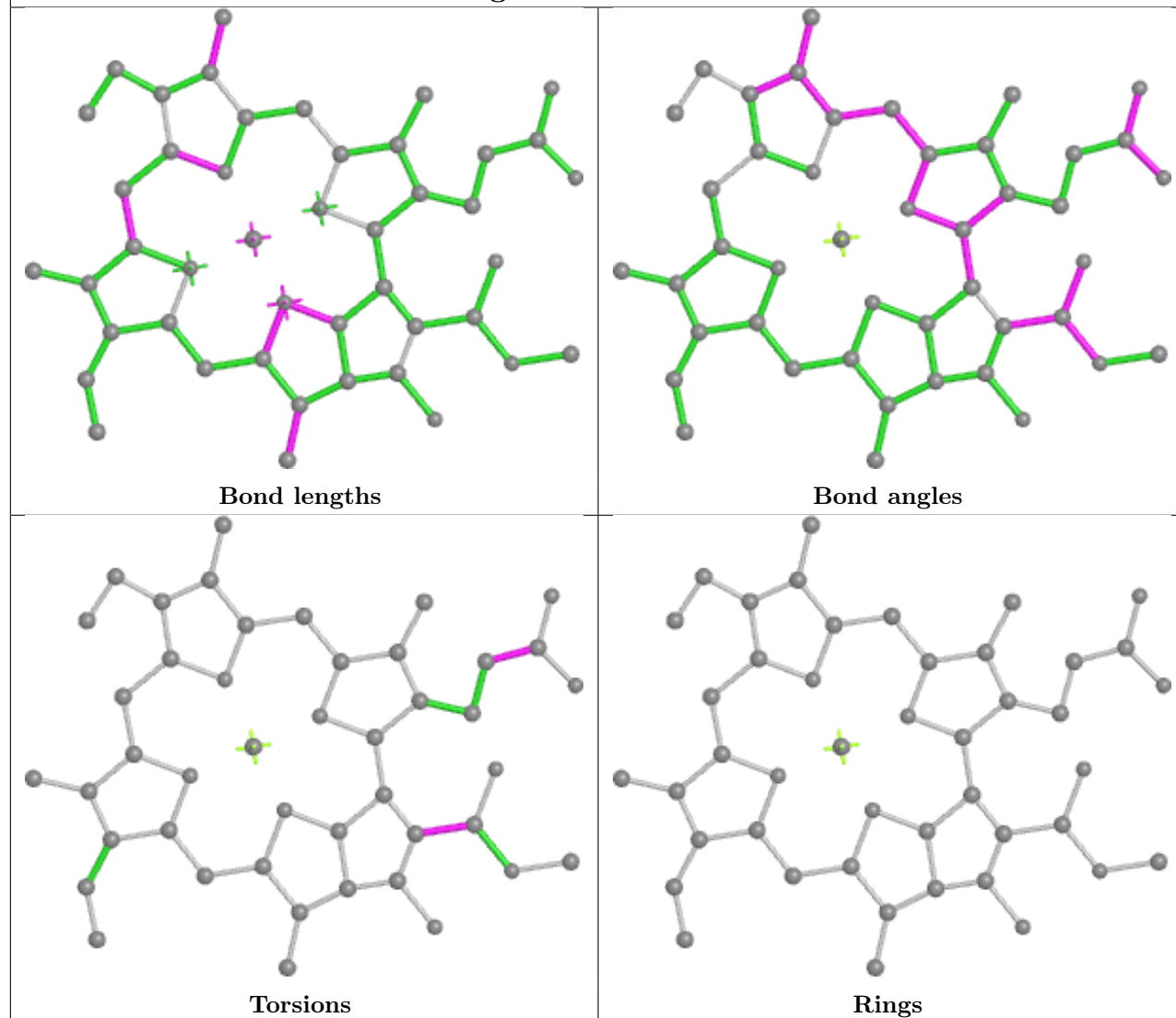
Ligand CLA 5 513



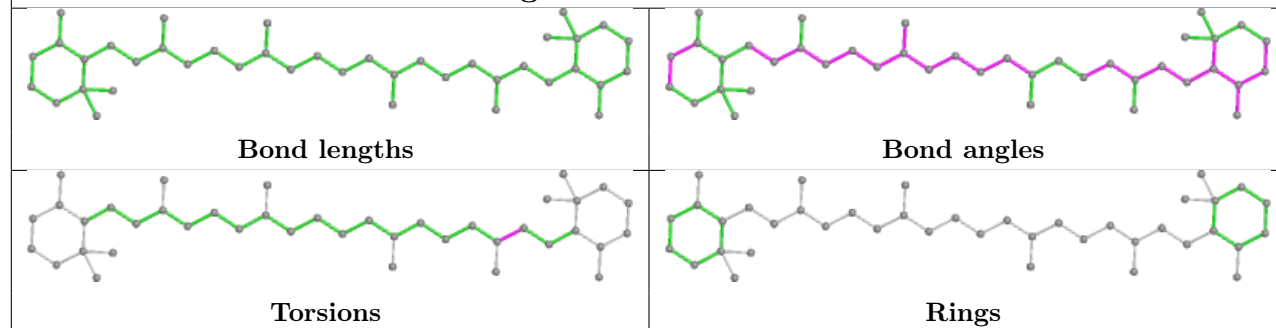
Ligand CLA r 509

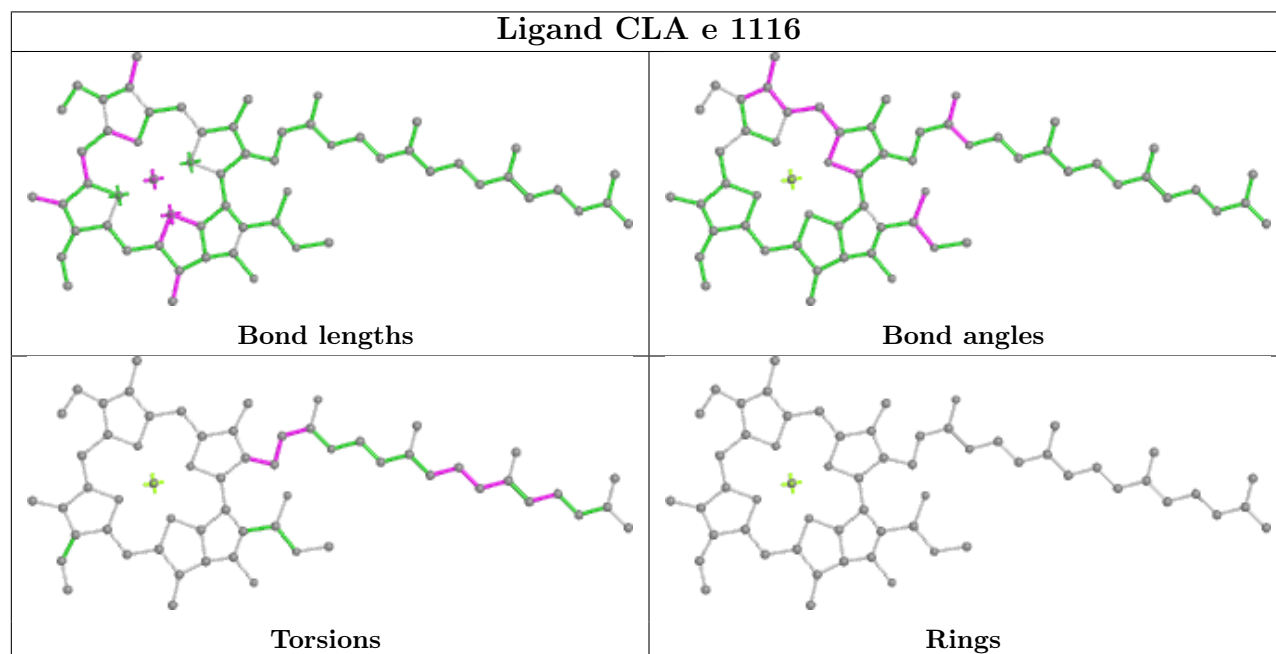
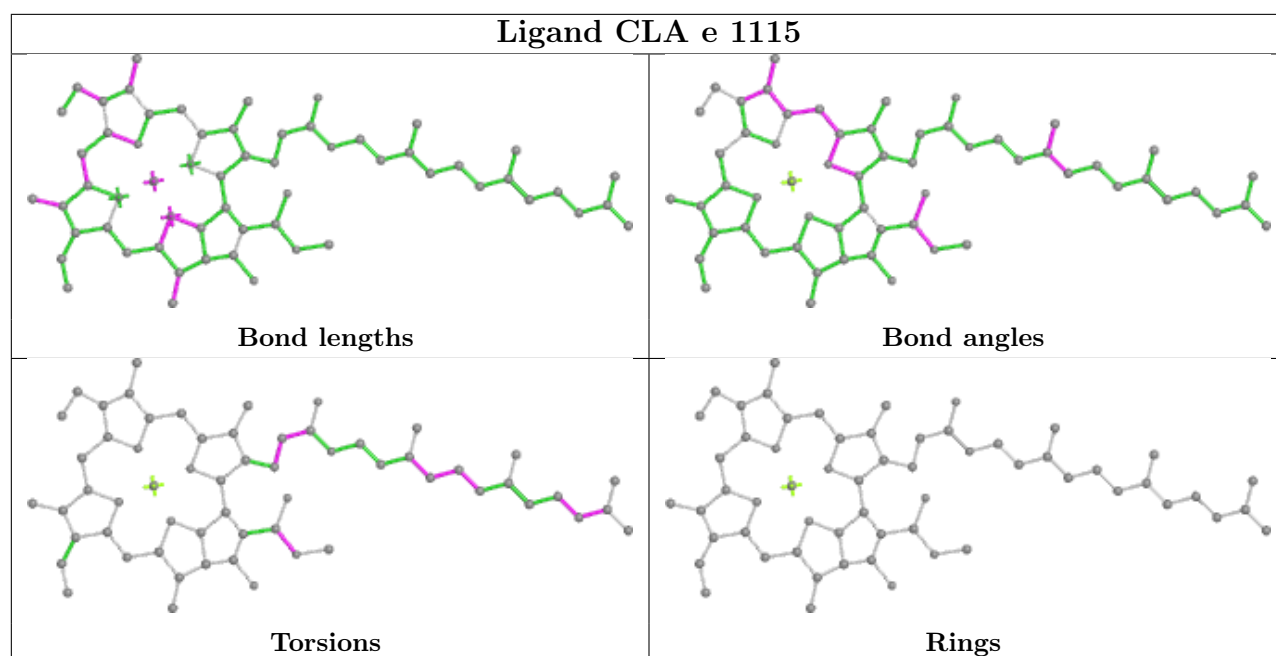


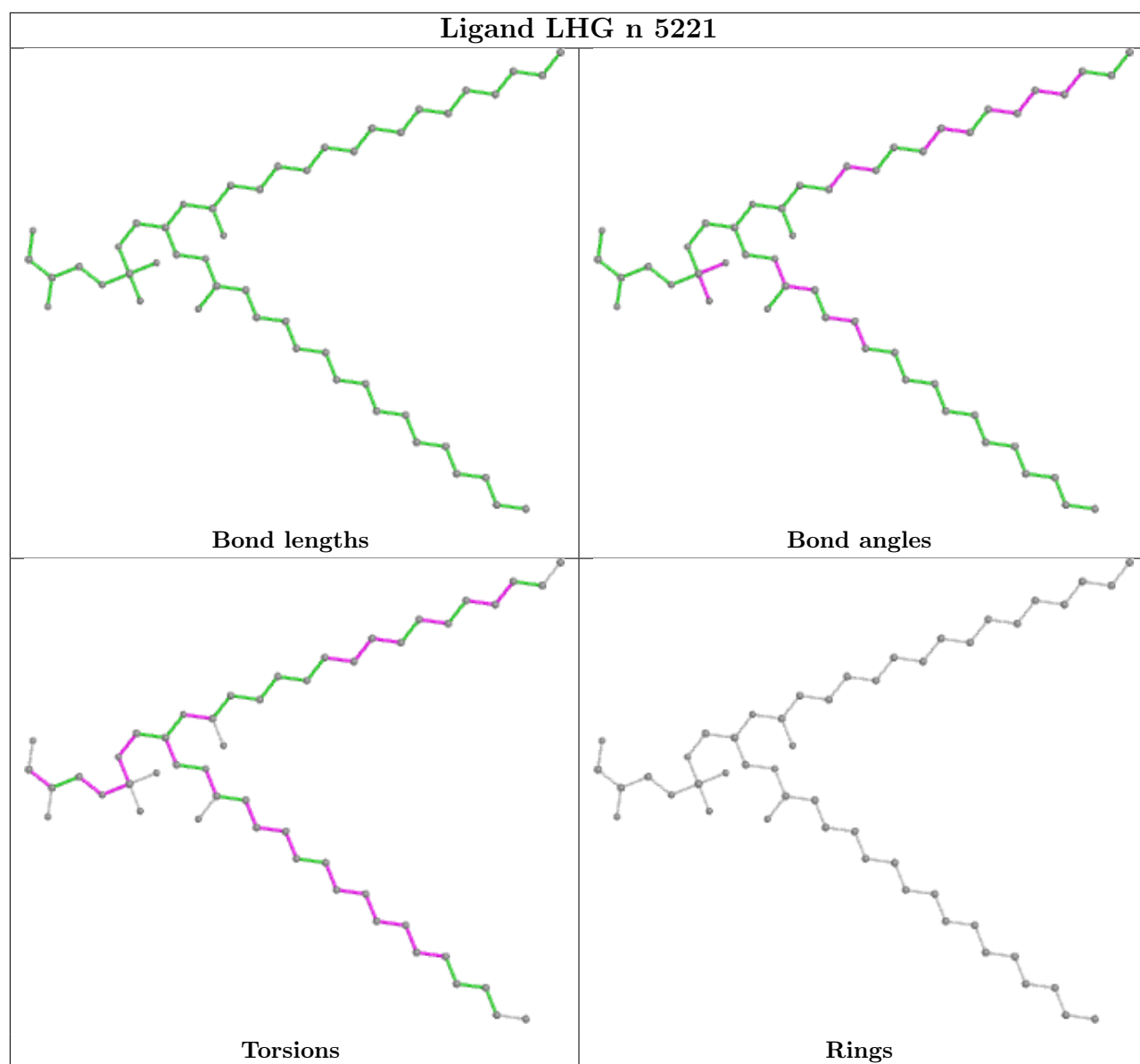
Ligand CLA Y 509

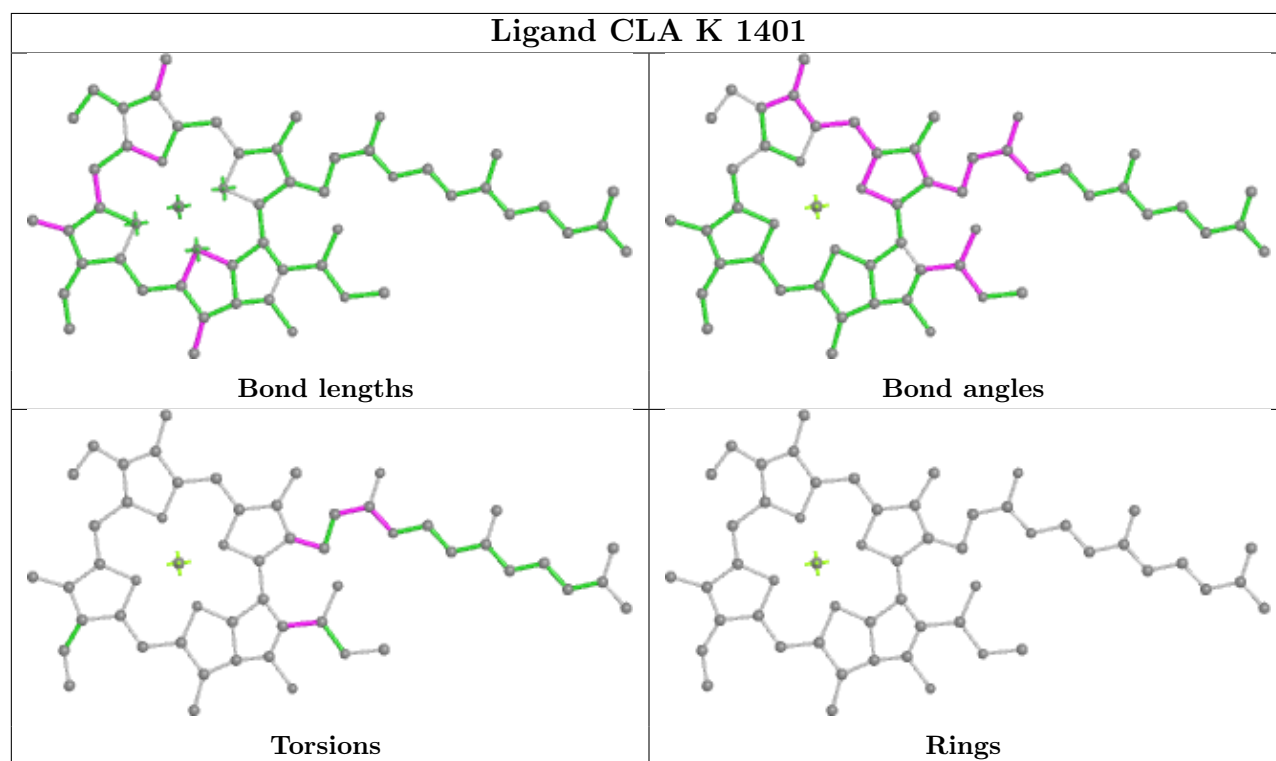
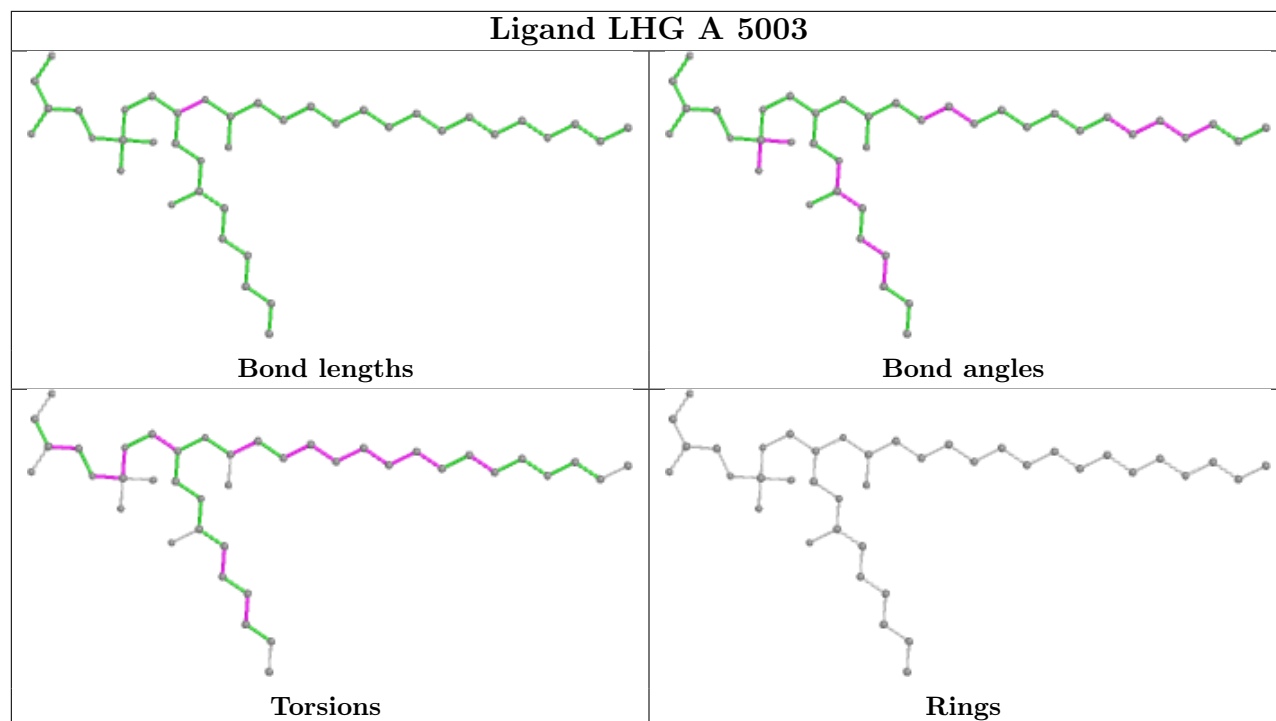


Ligand BCR K 4104

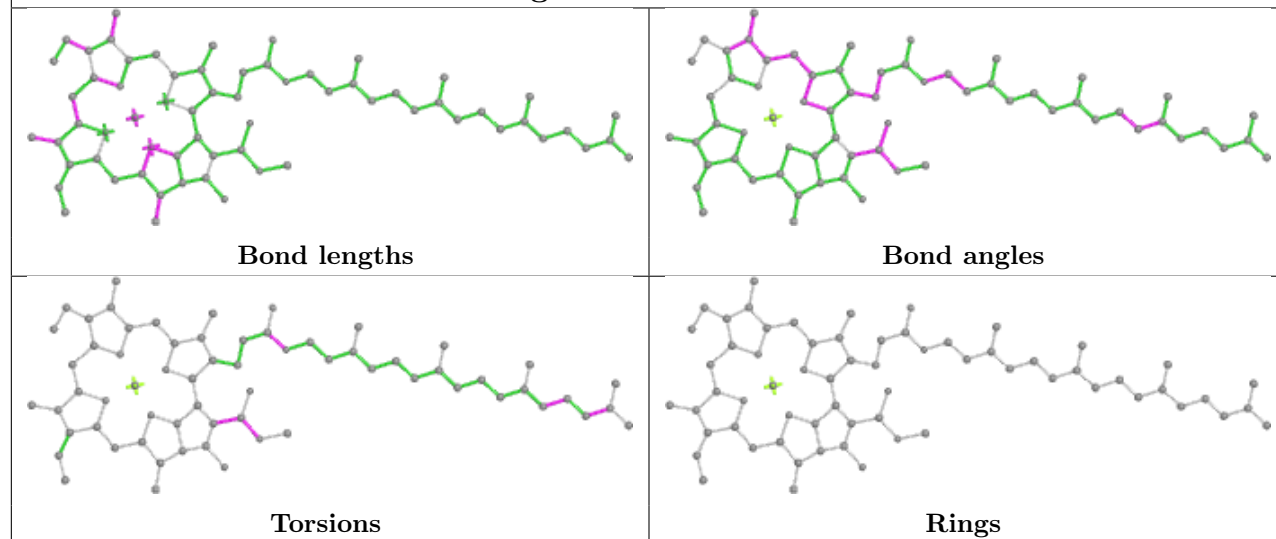




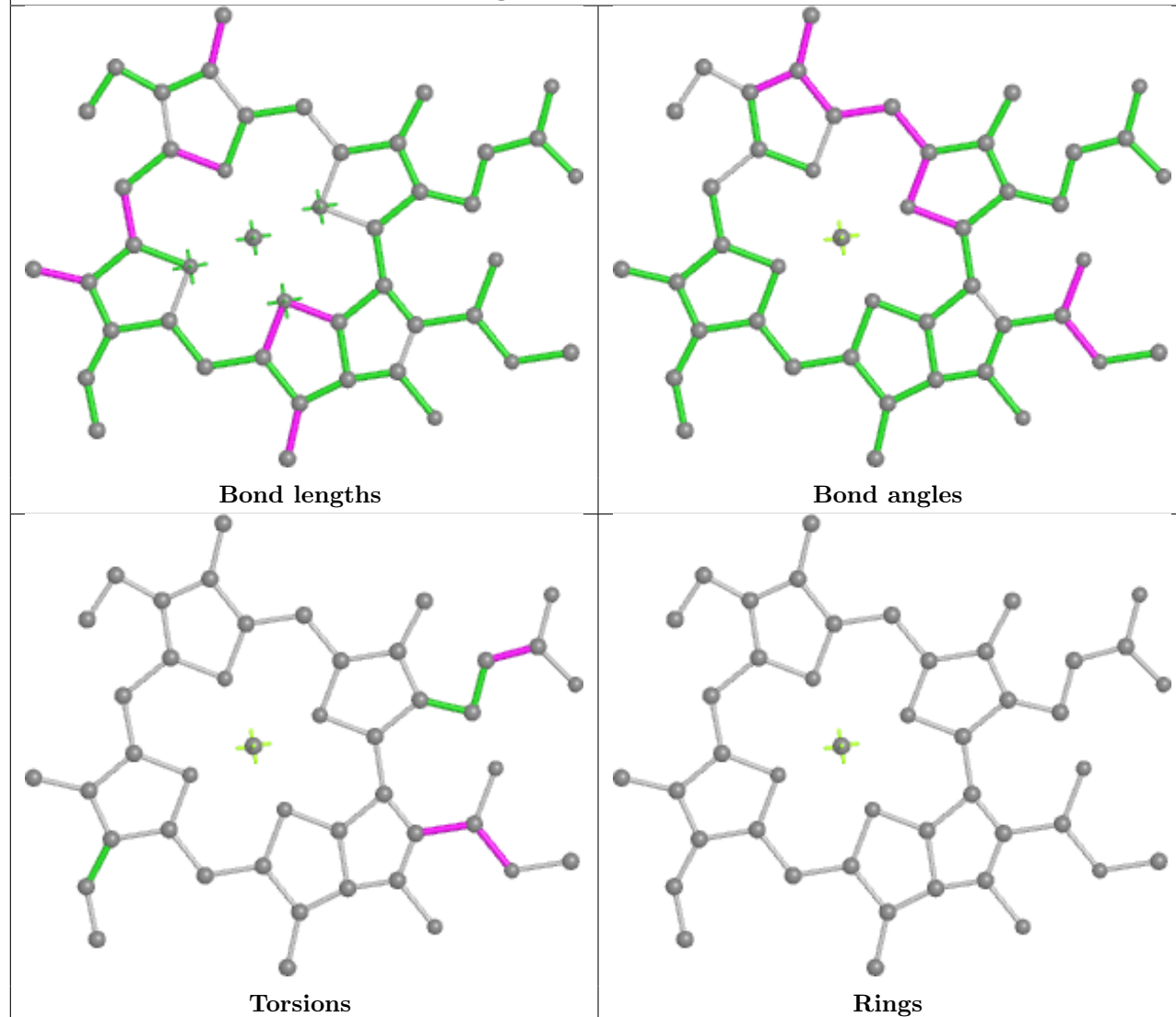


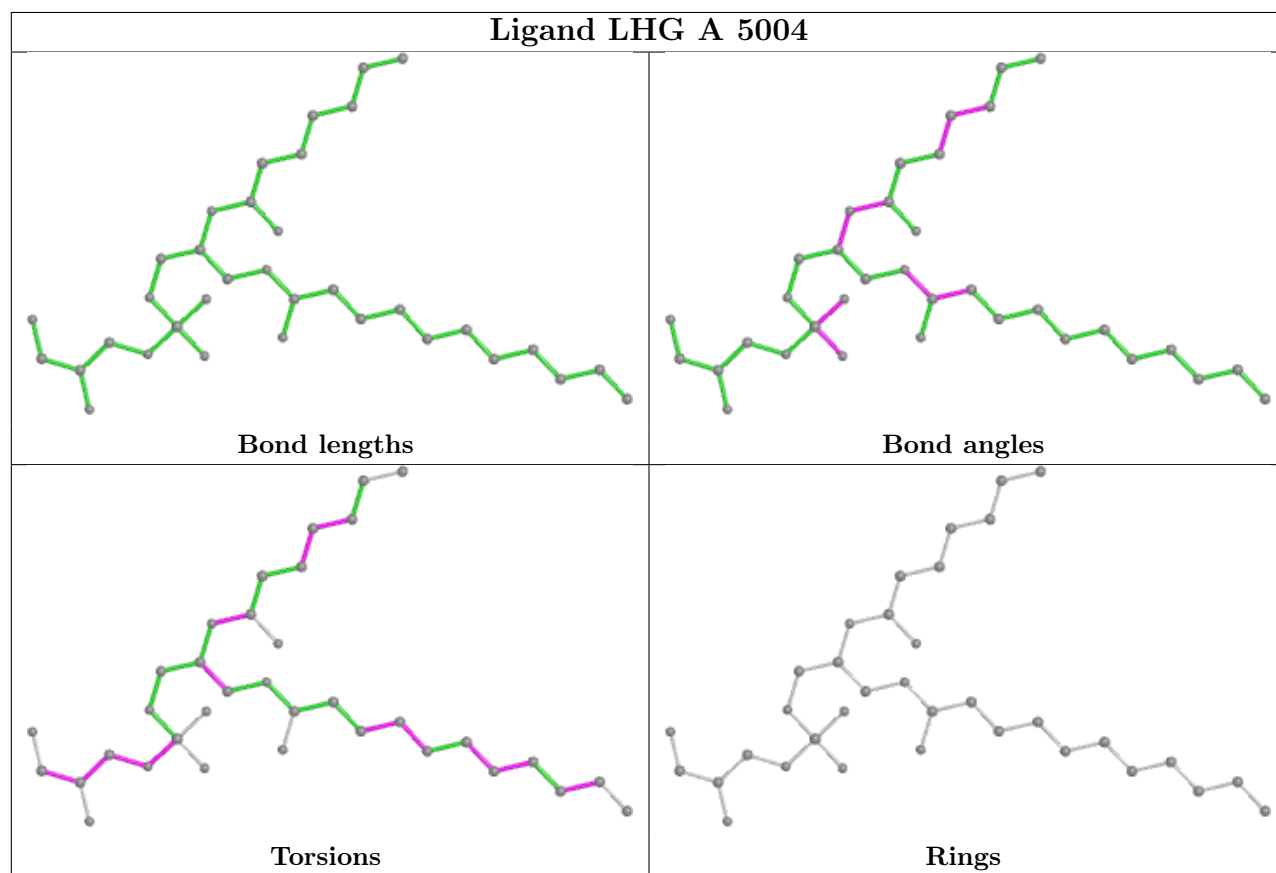
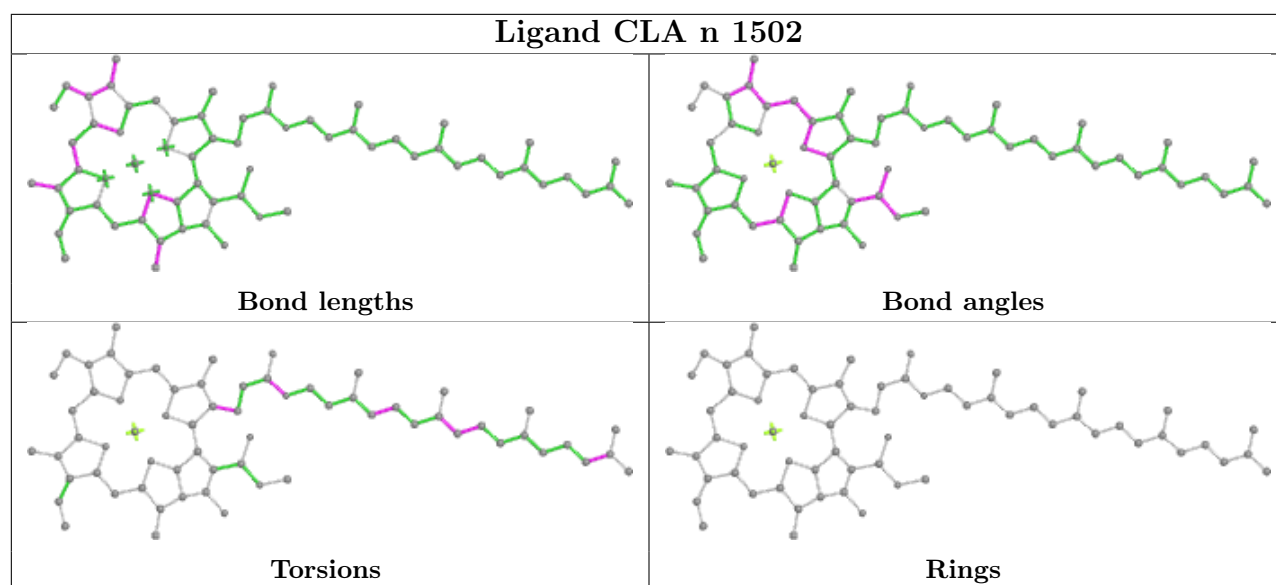


Ligand CLA f 1021

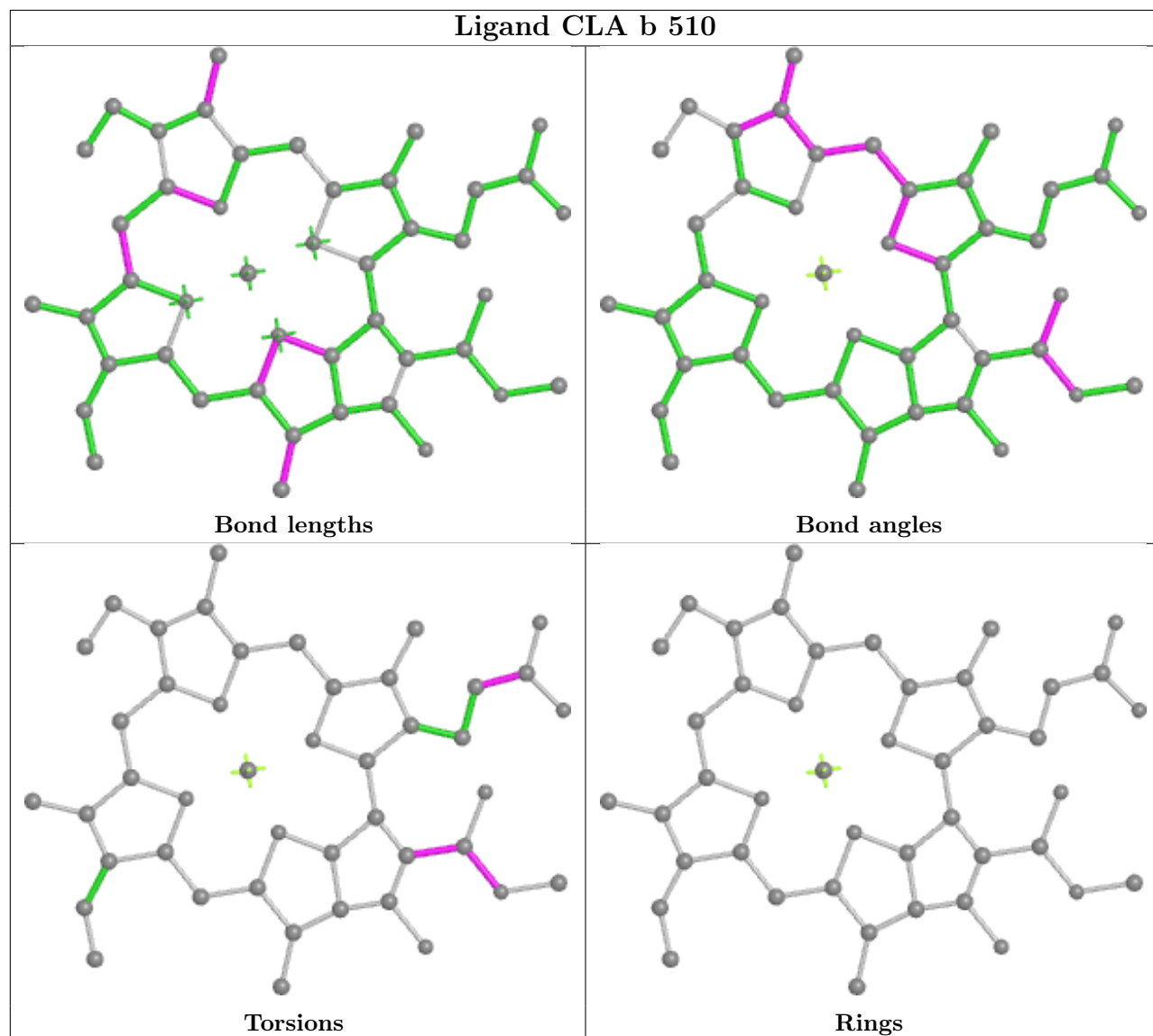


Ligand CLA d 510

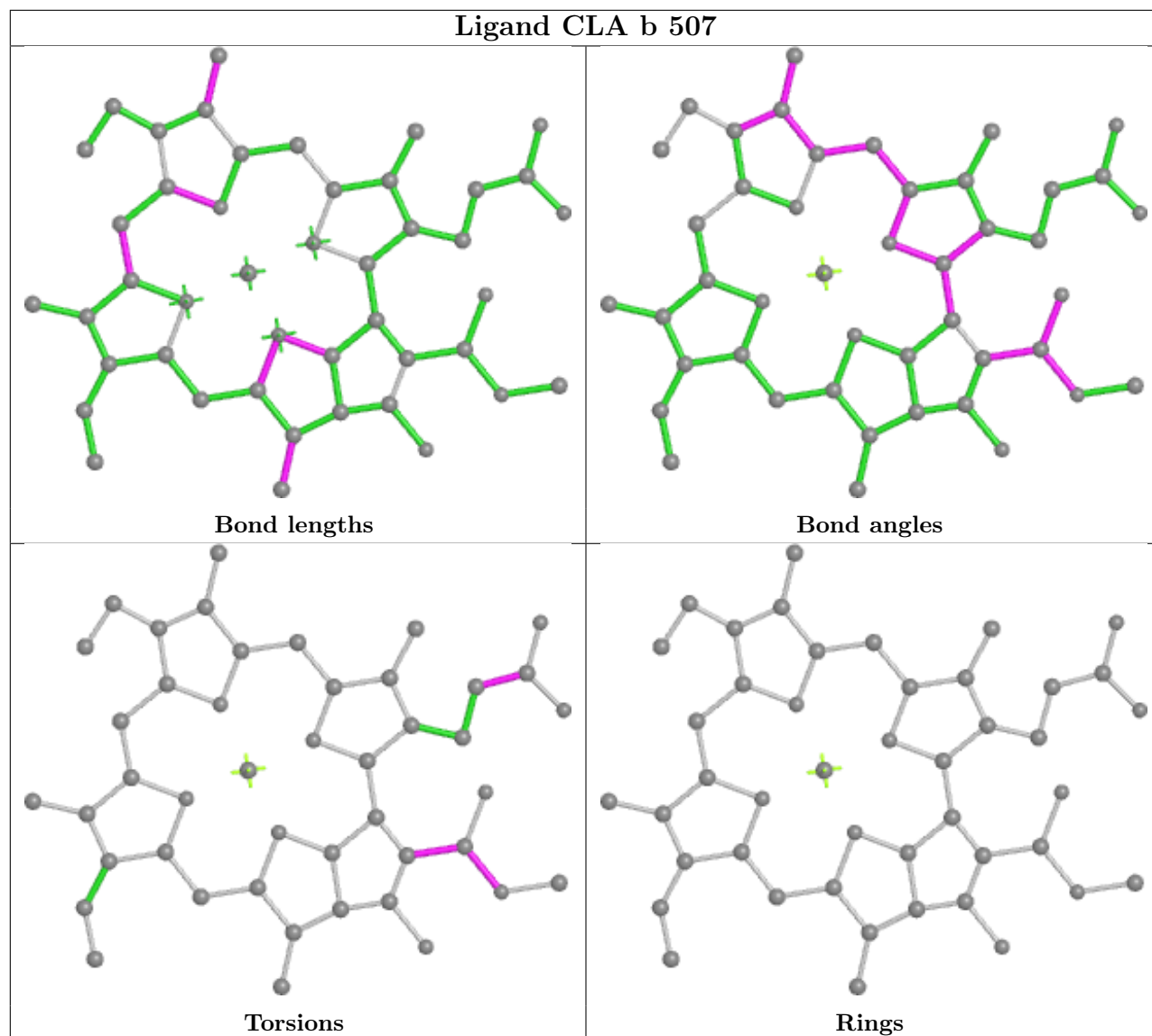




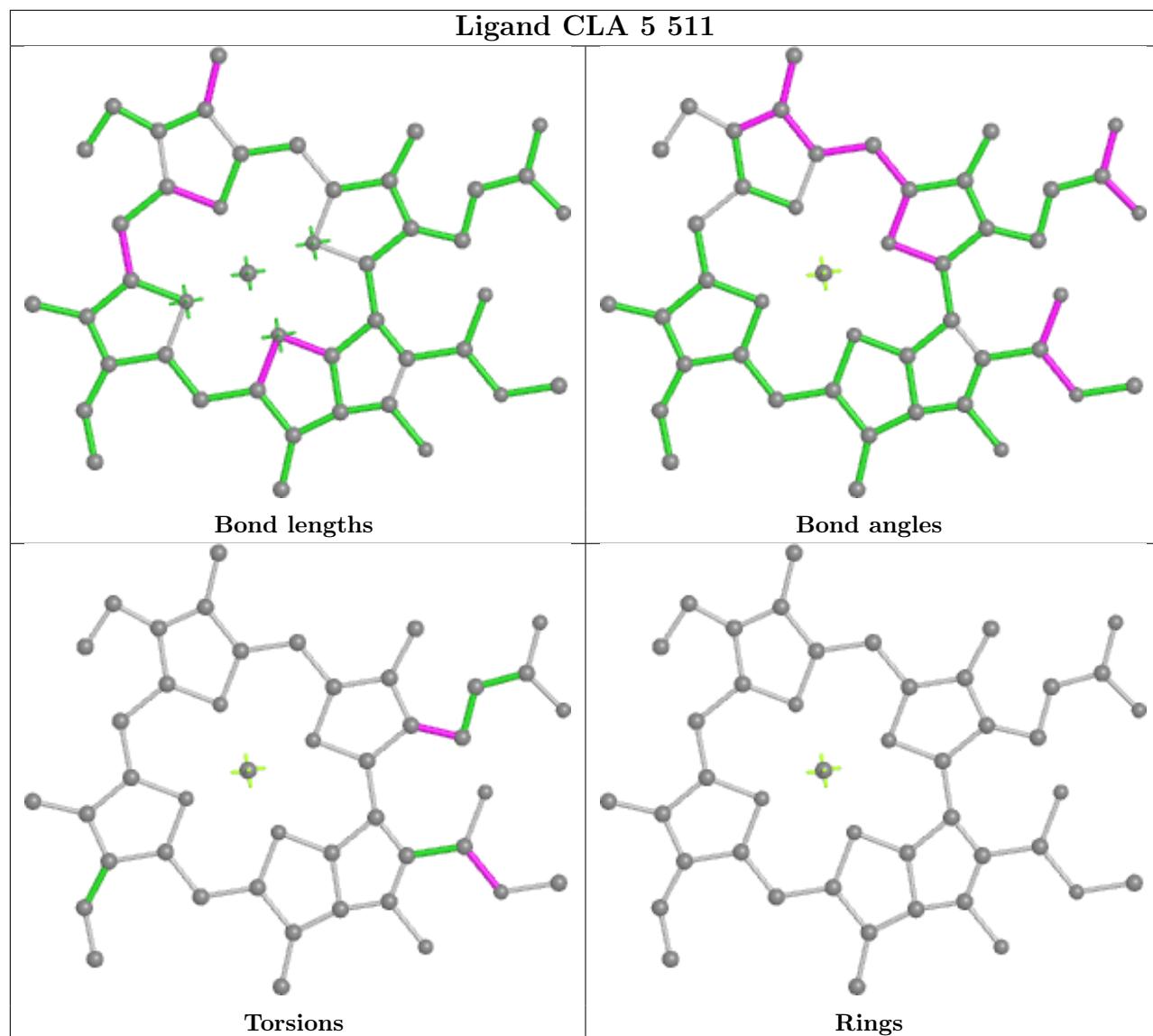
Ligand CLA b 510



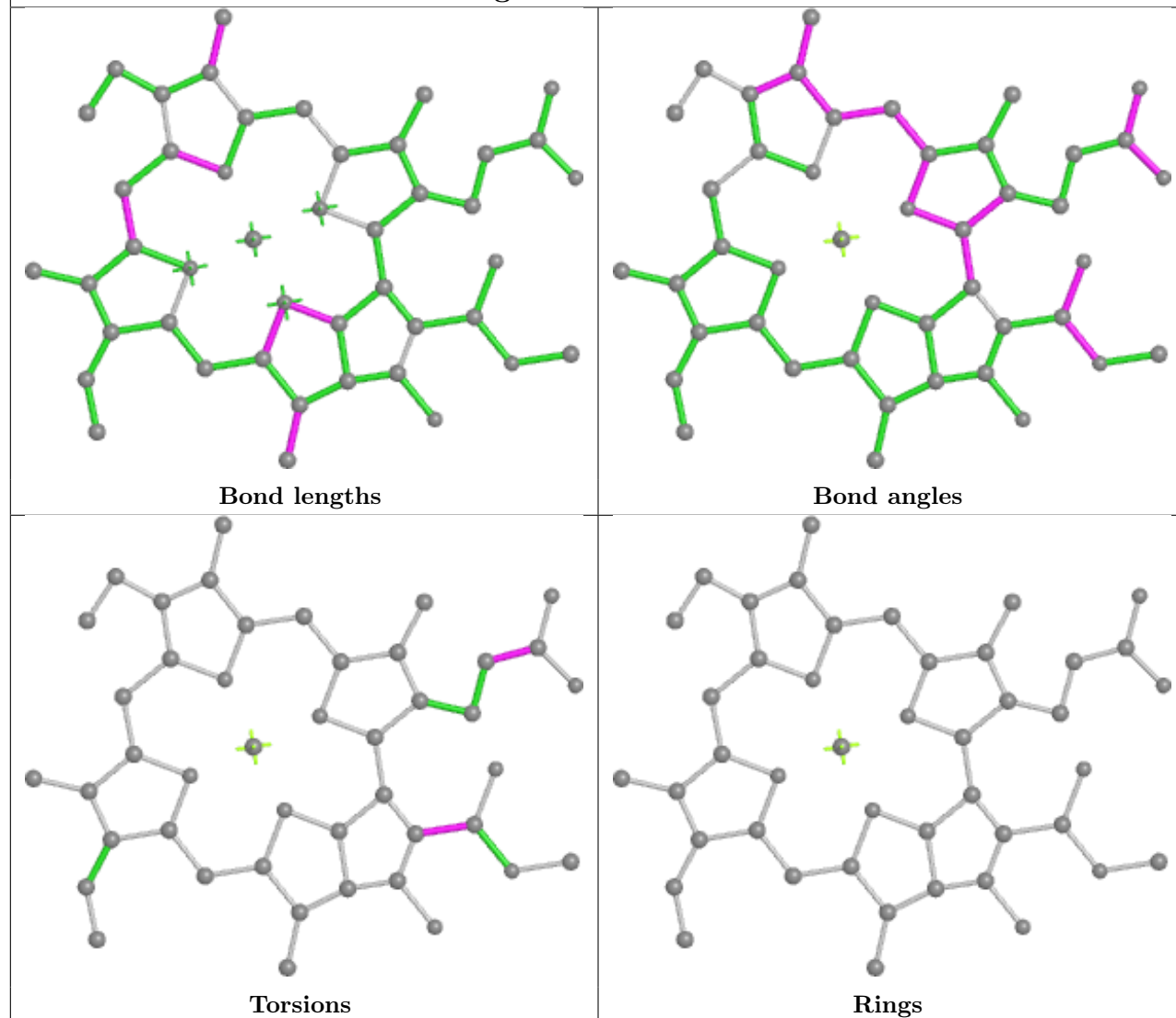
Ligand CLA b 507



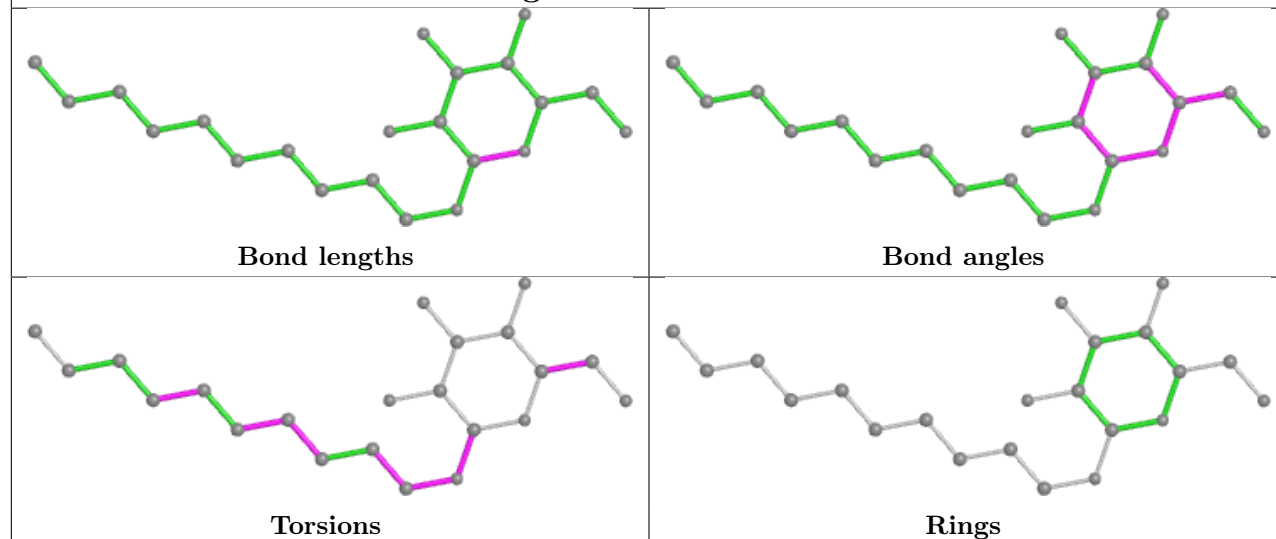
Ligand CLA 5 511

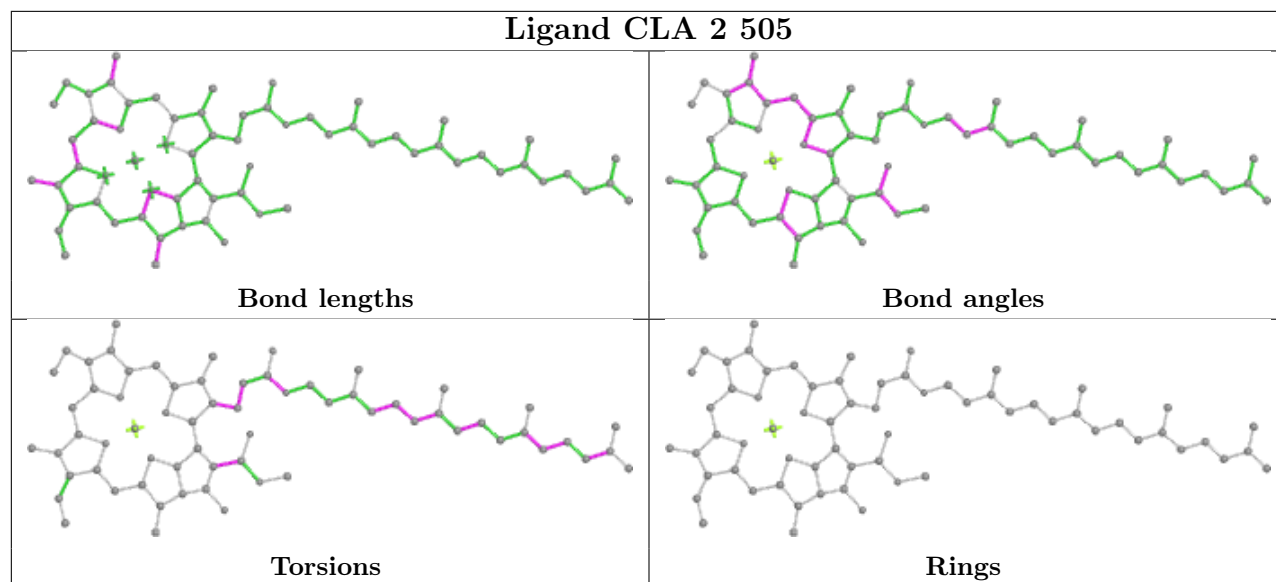
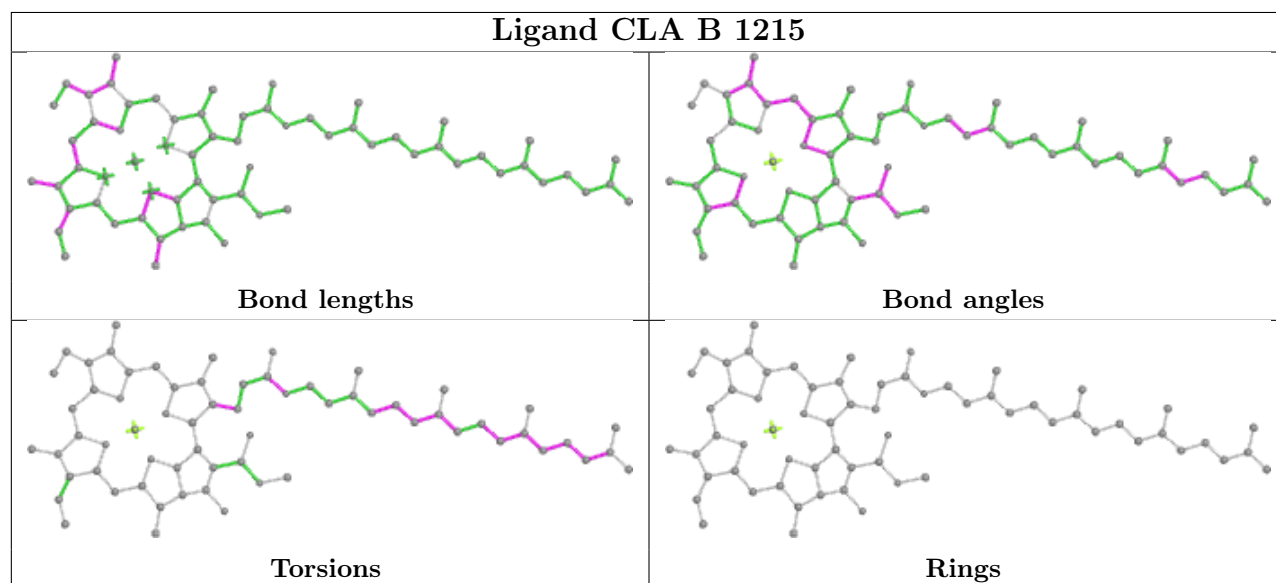


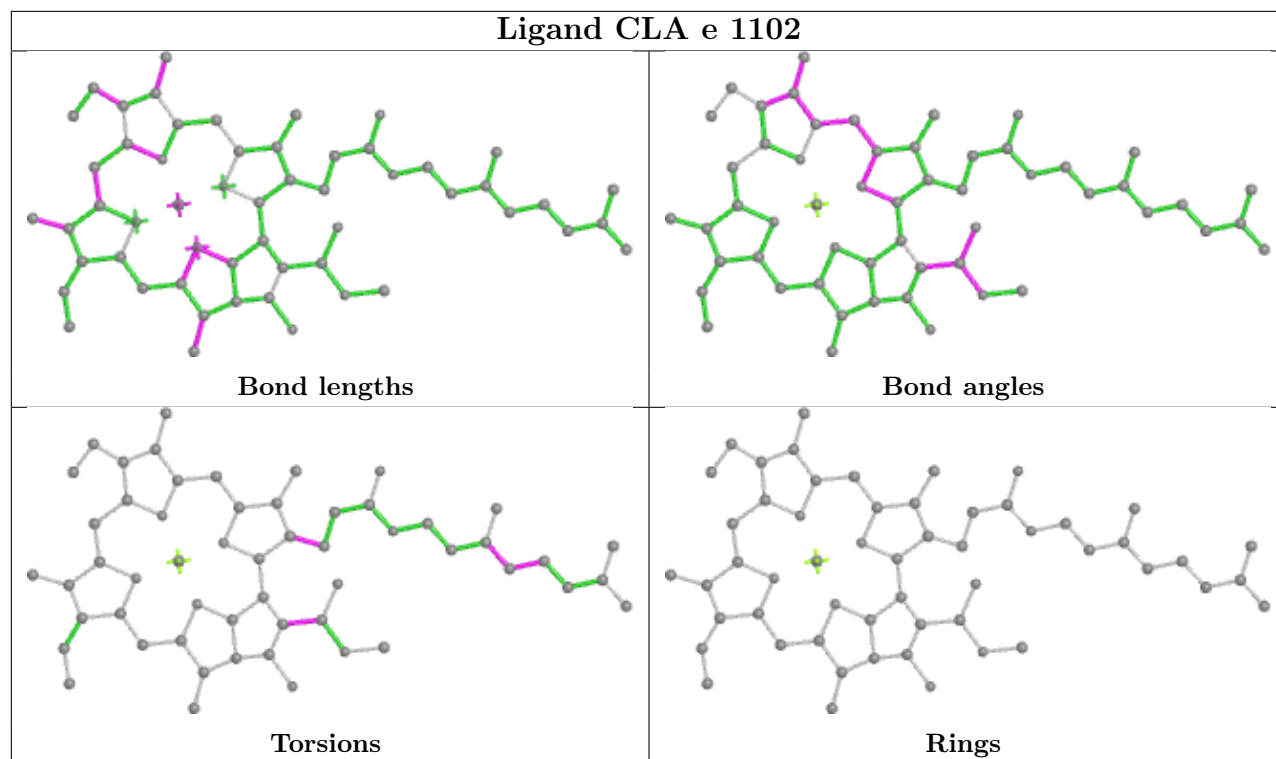
Ligand CLA a 507



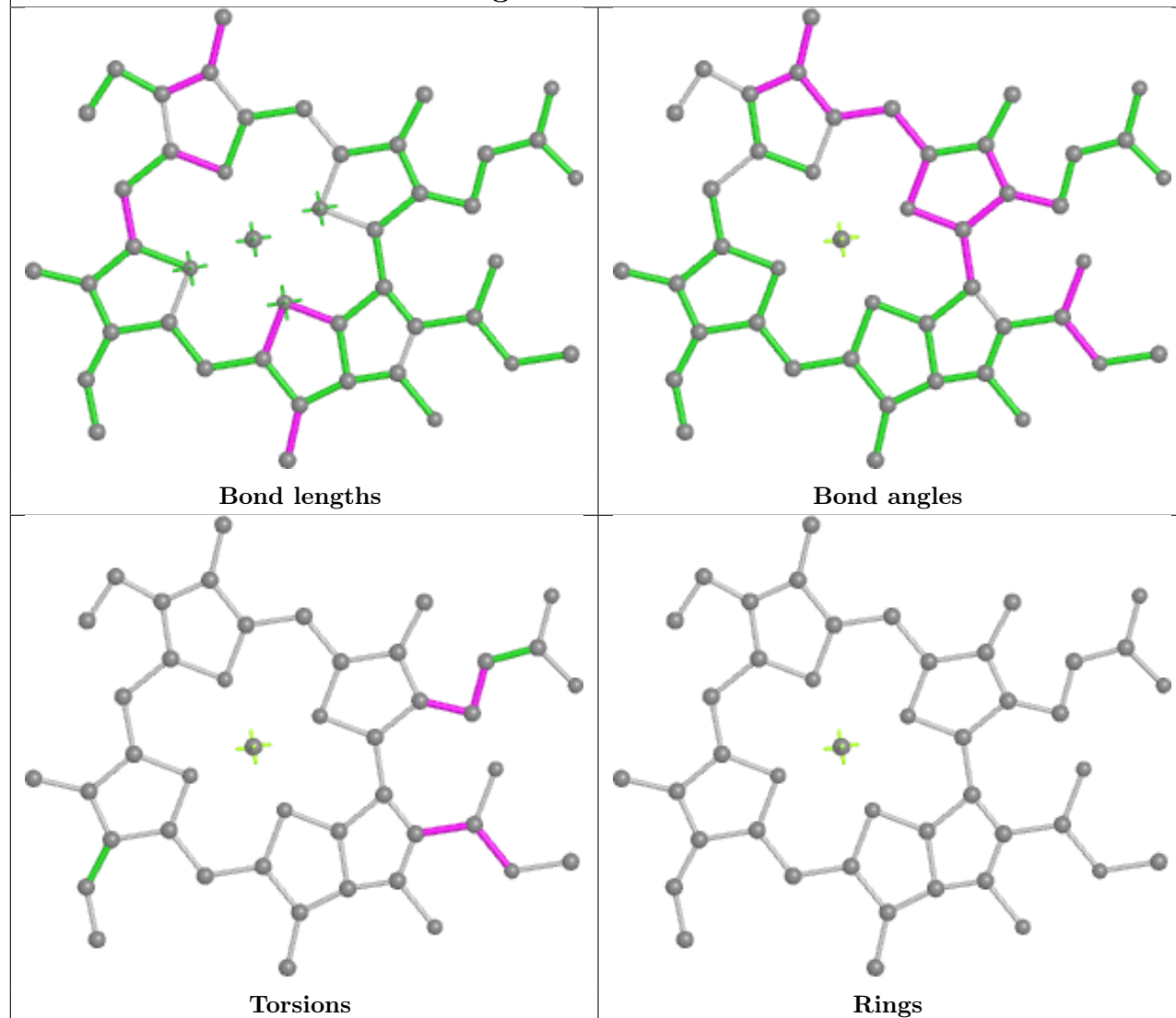
Ligand LMU J 5105



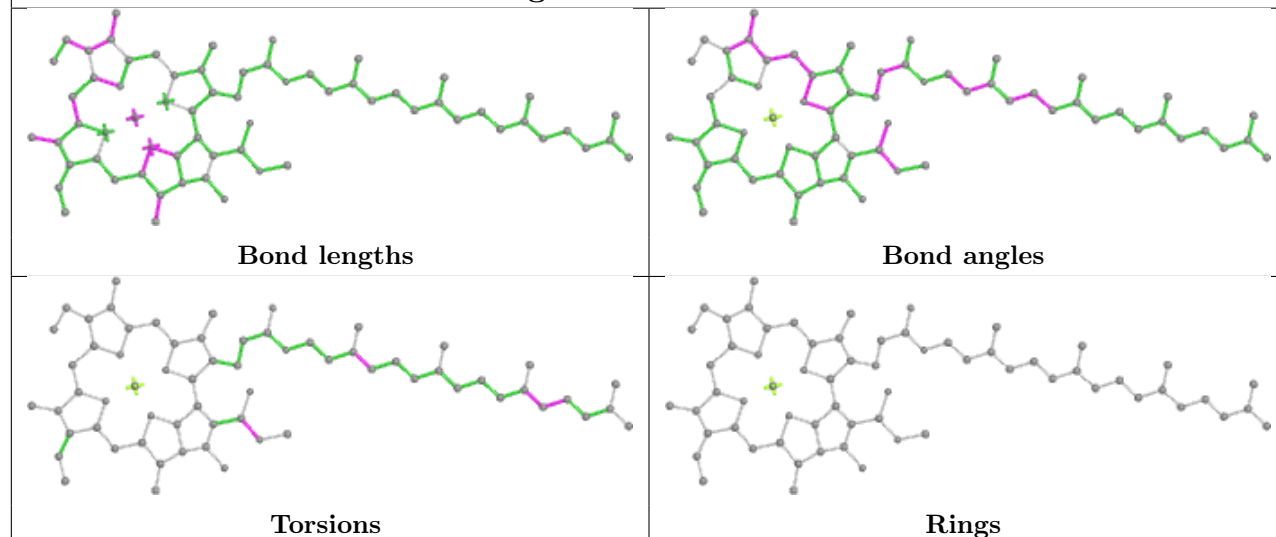
Ligand CLA 2 505**Ligand CLA B 1215**

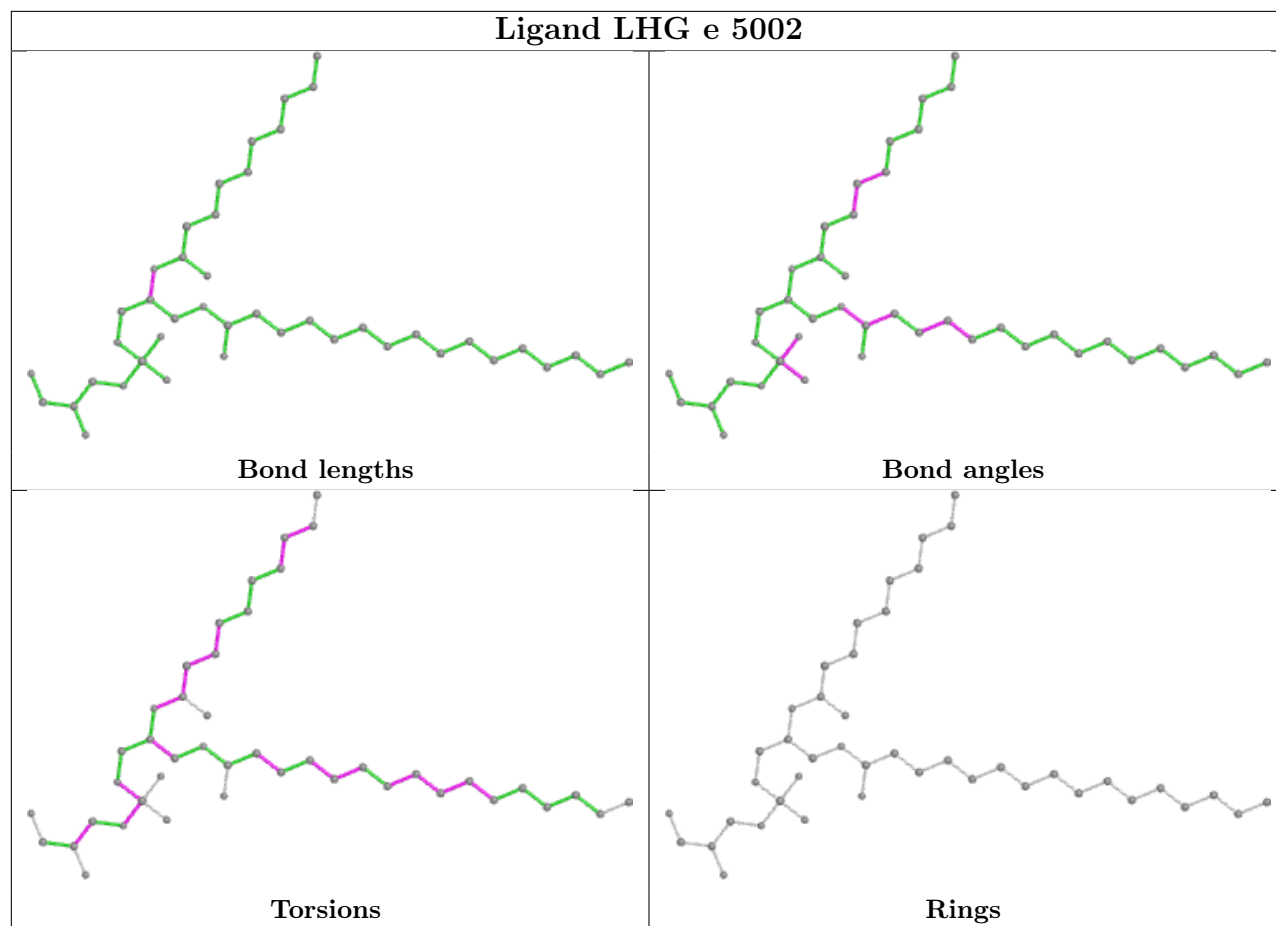


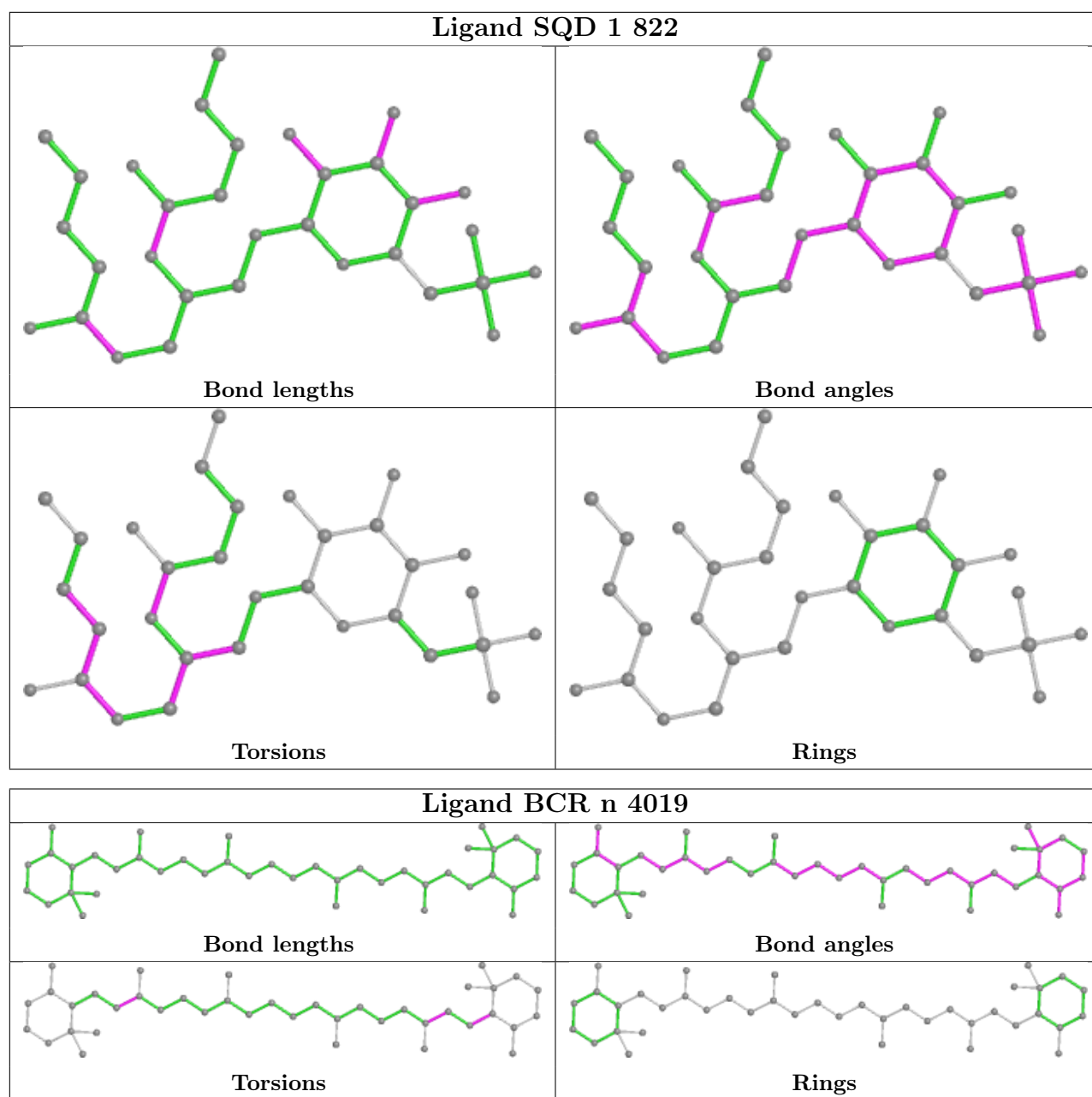
Ligand CLA Z 504

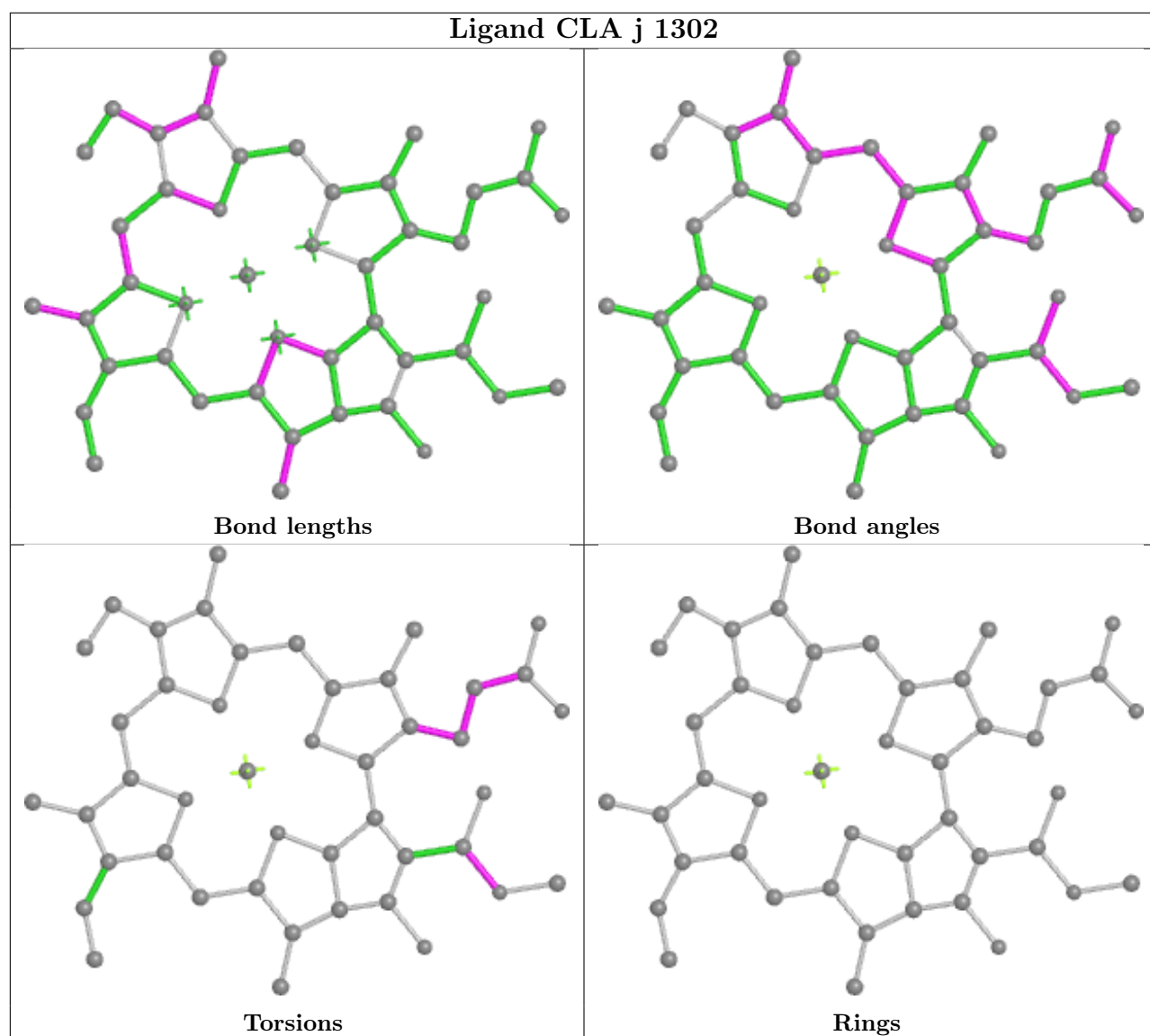


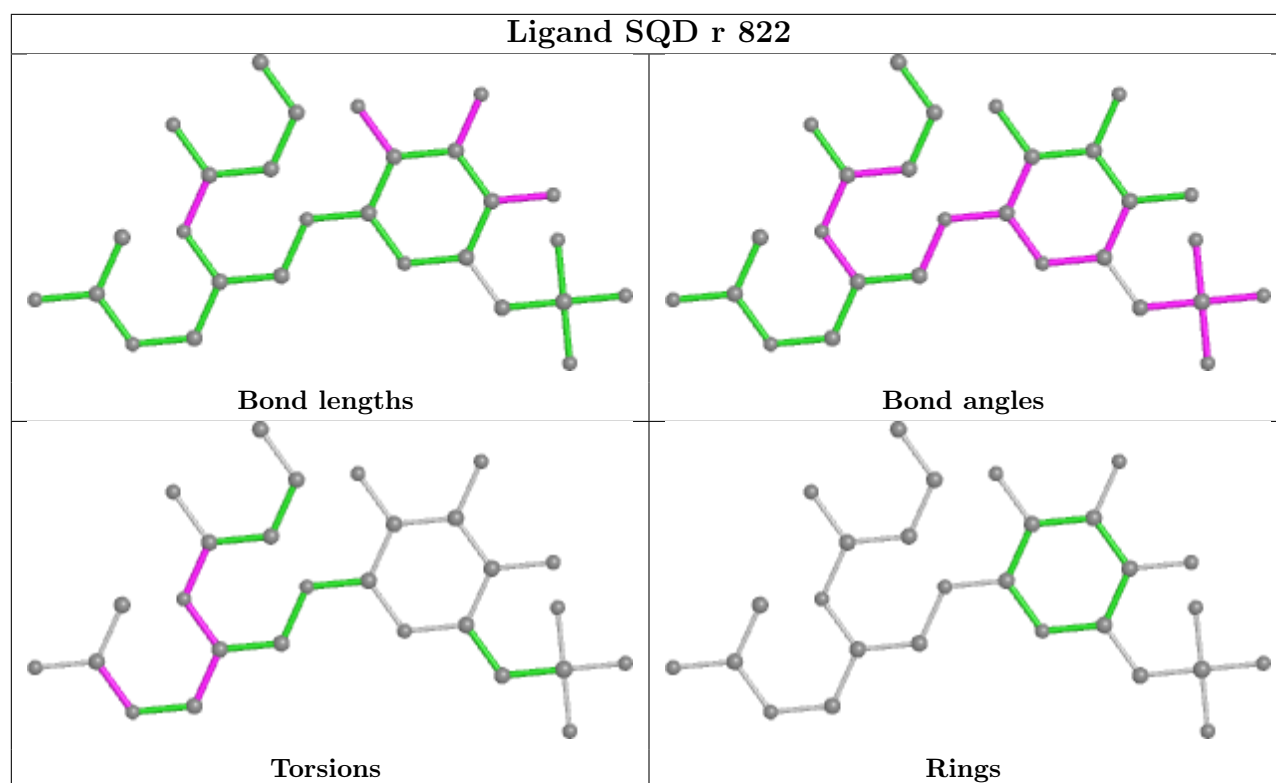
Ligand CLA e 1131



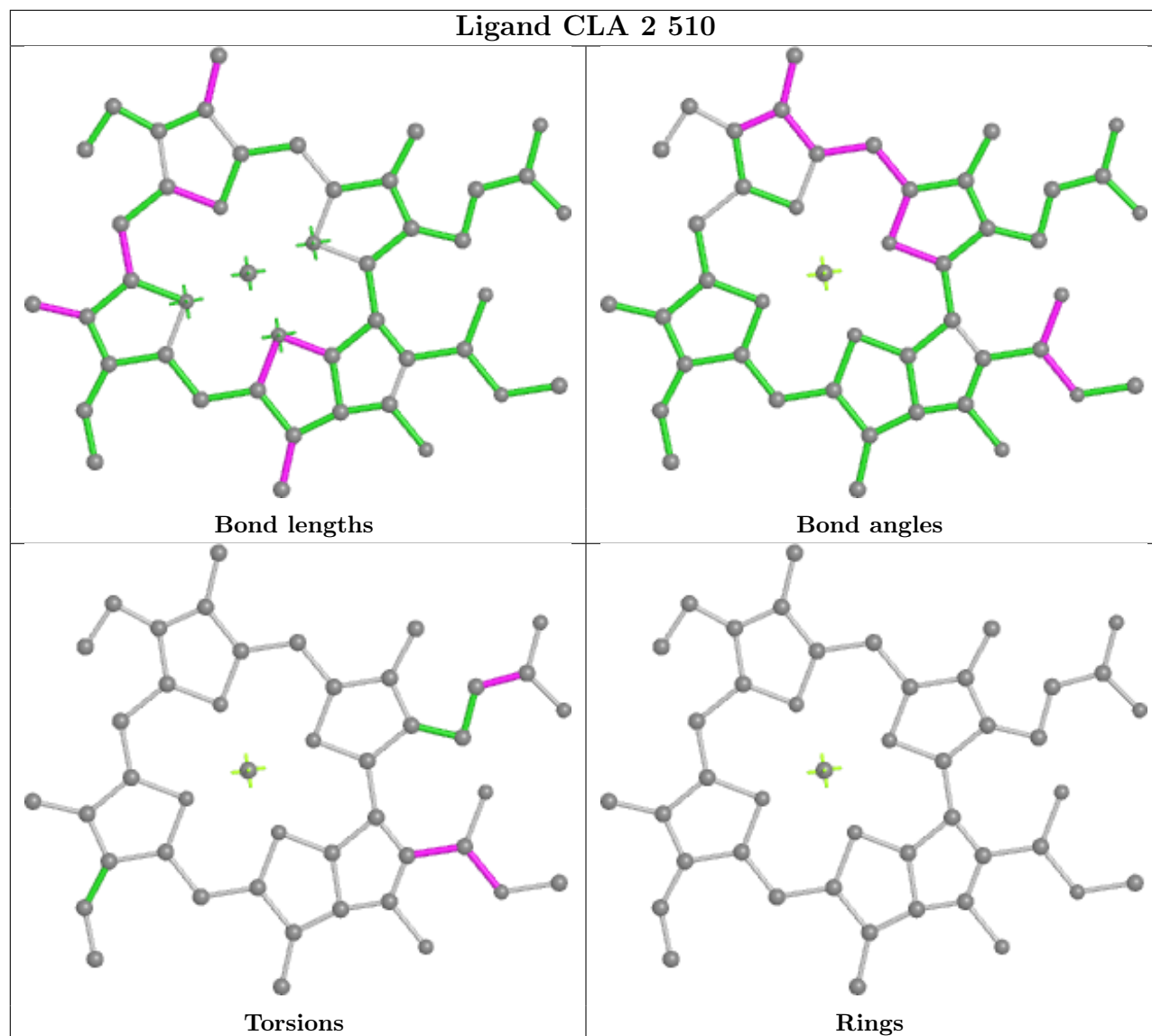




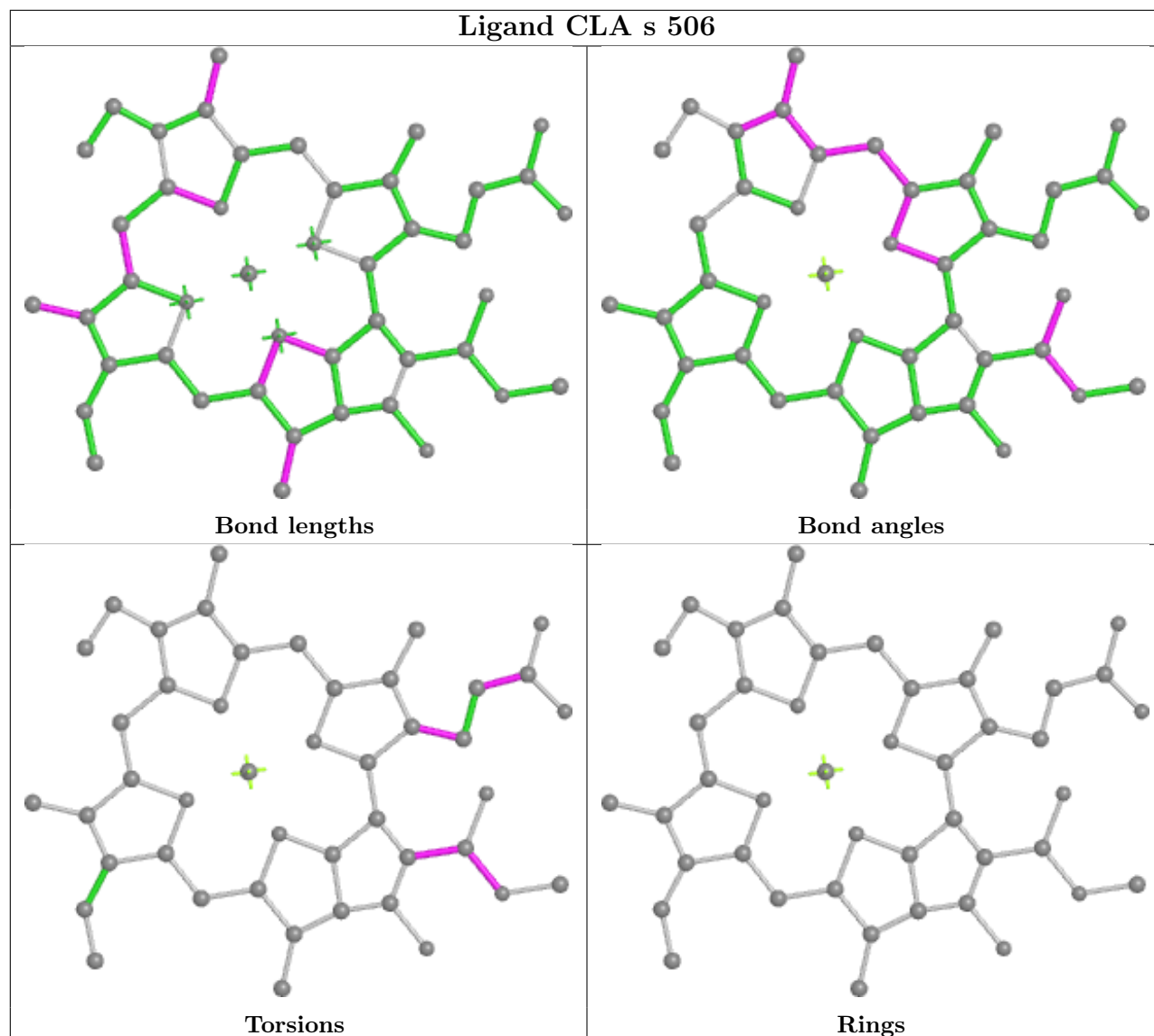




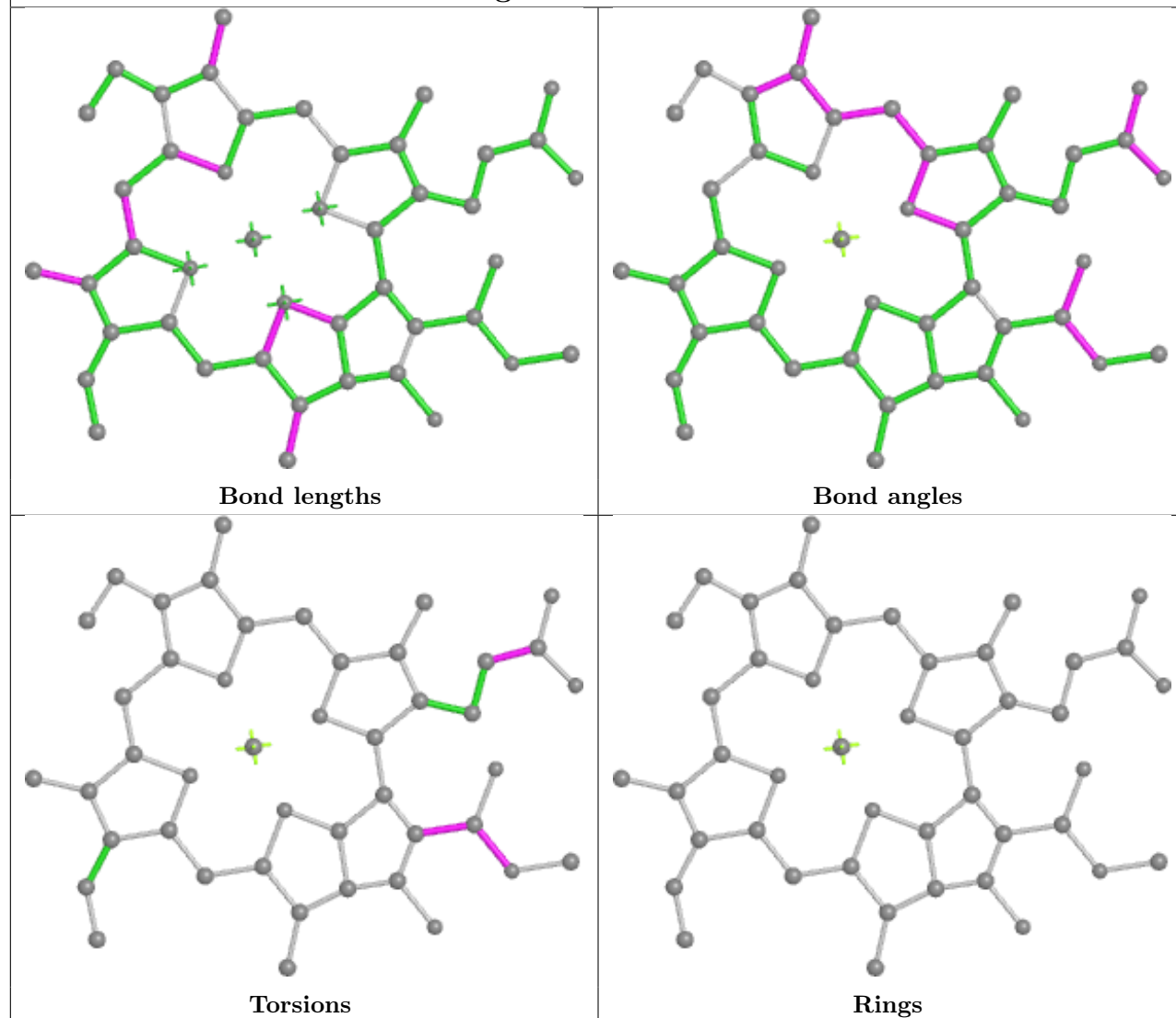
Ligand CLA 2 510



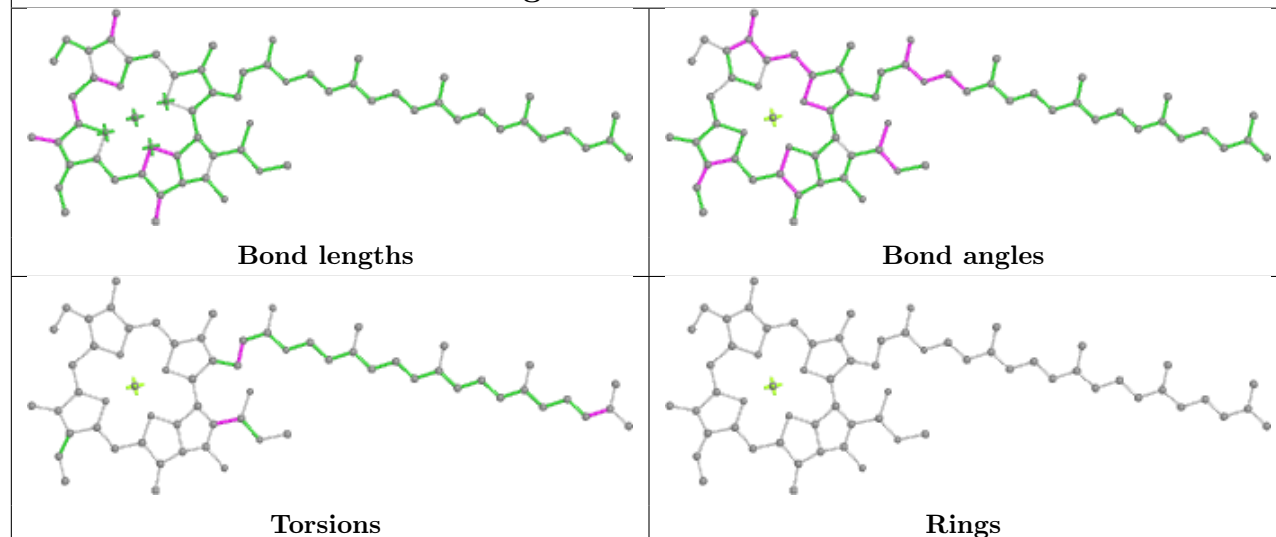
Ligand CLA s 506



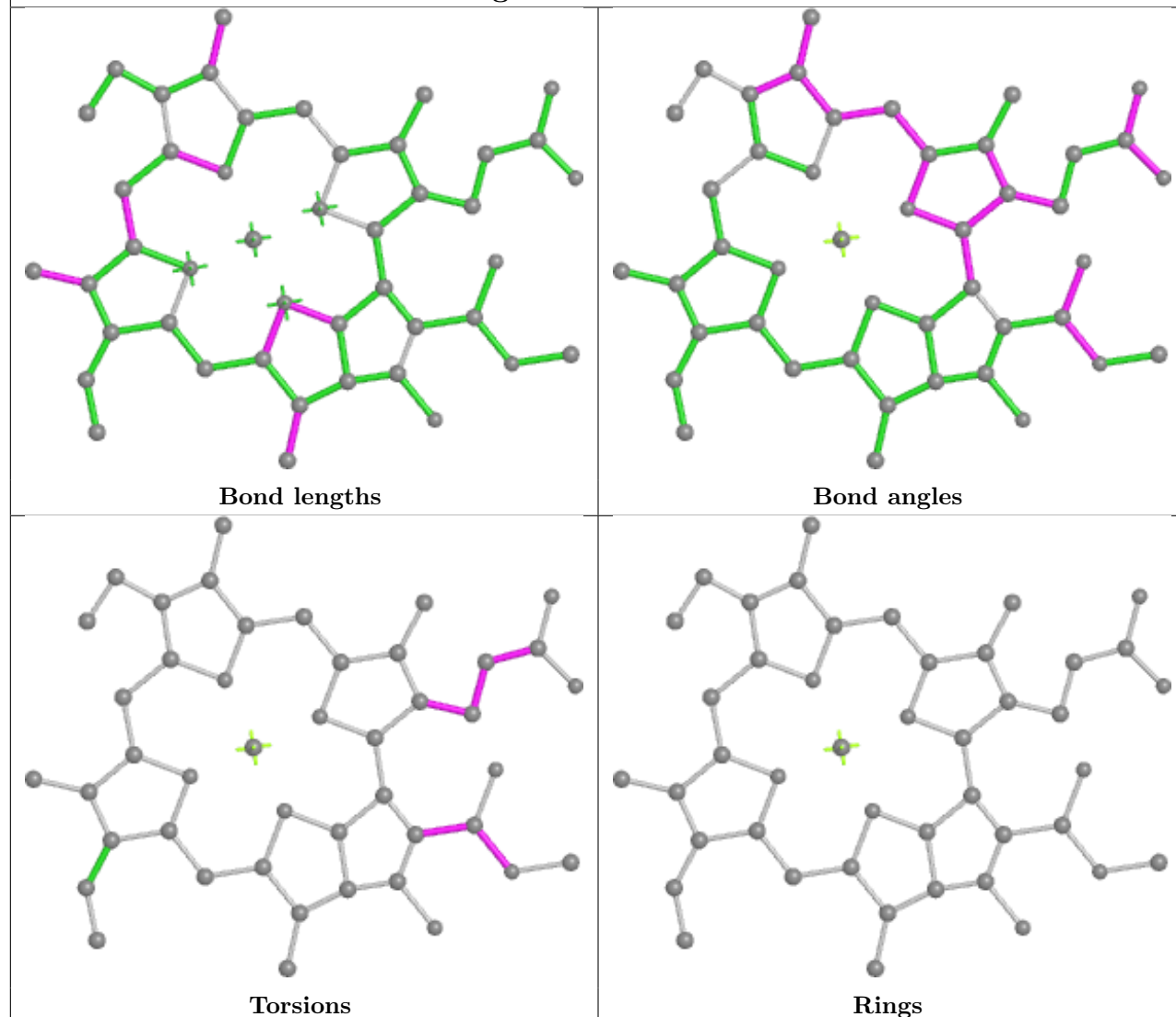
Ligand CLA c 510



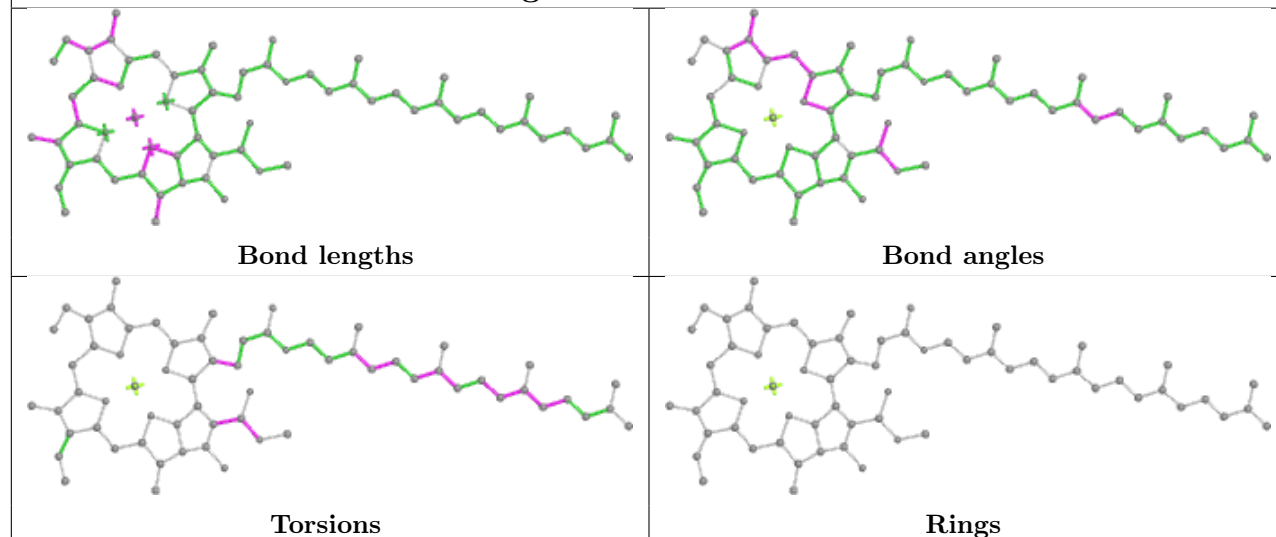
Ligand CLA B 1238



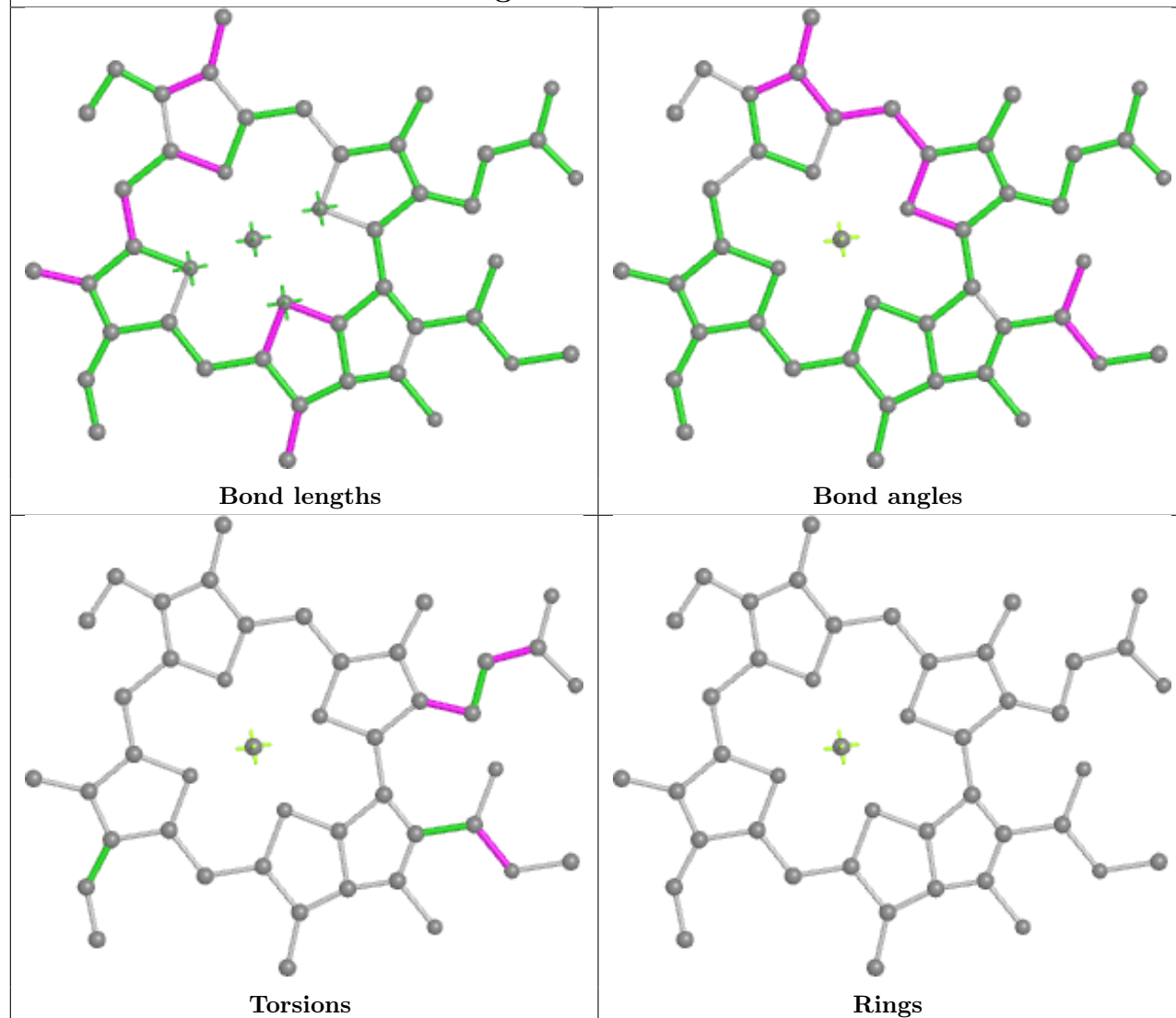
Ligand CLA Z 507



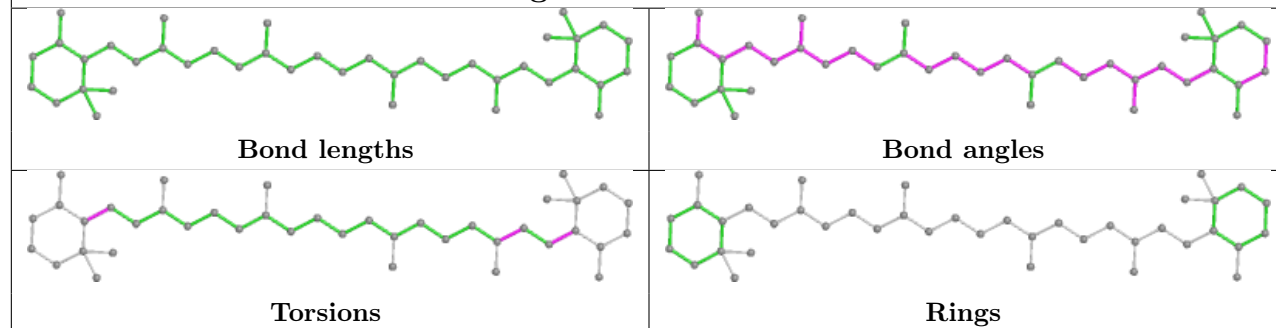
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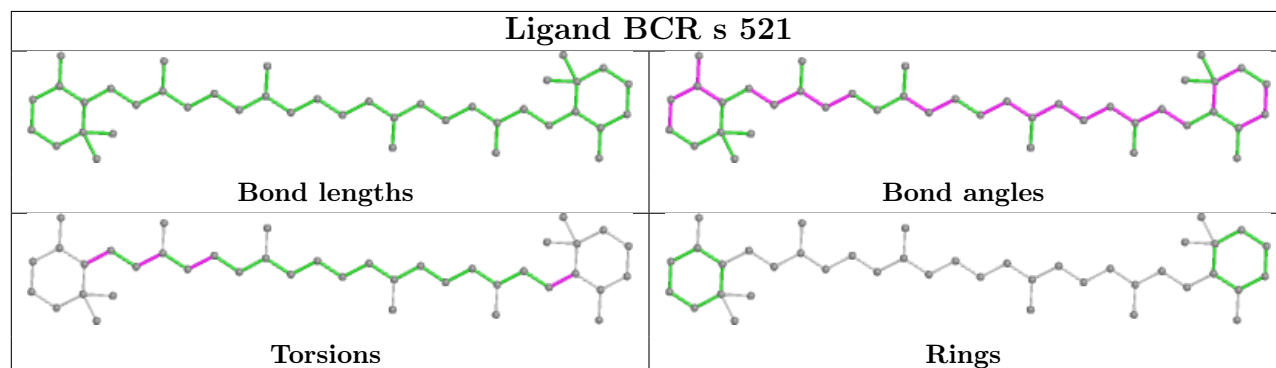
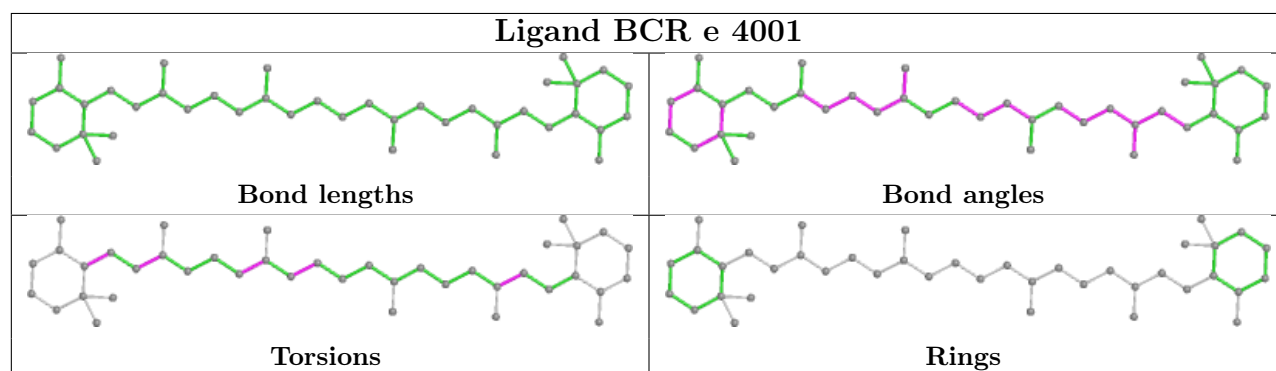
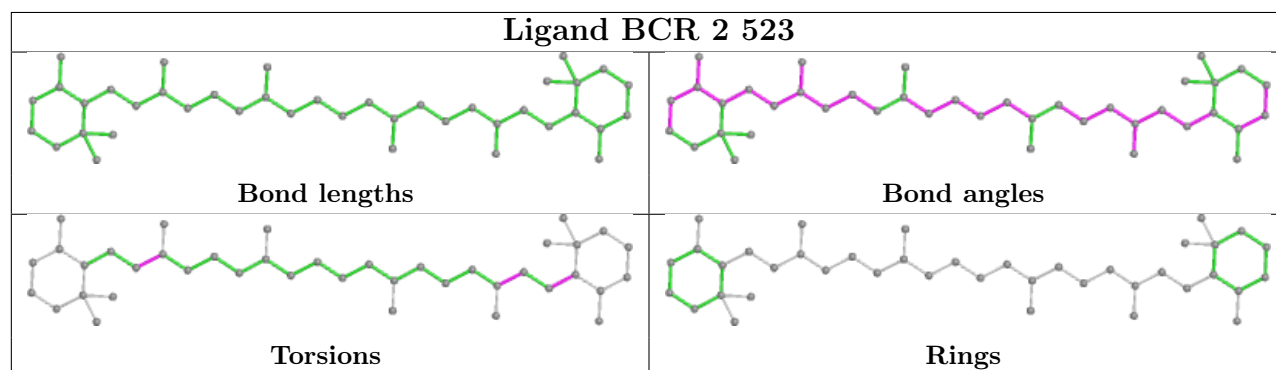
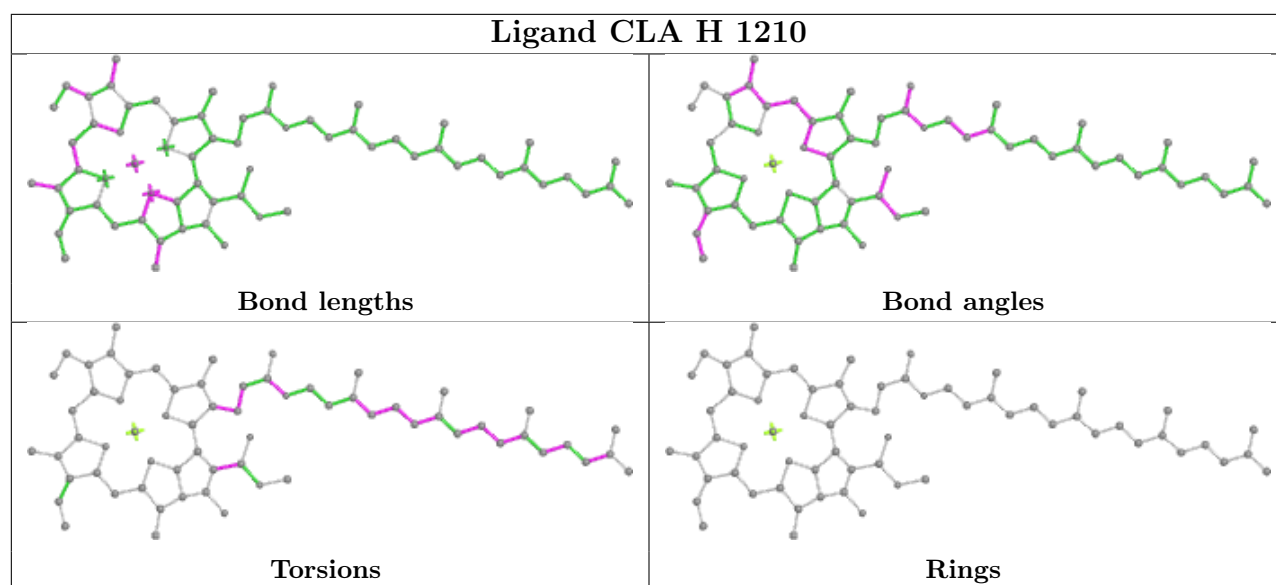


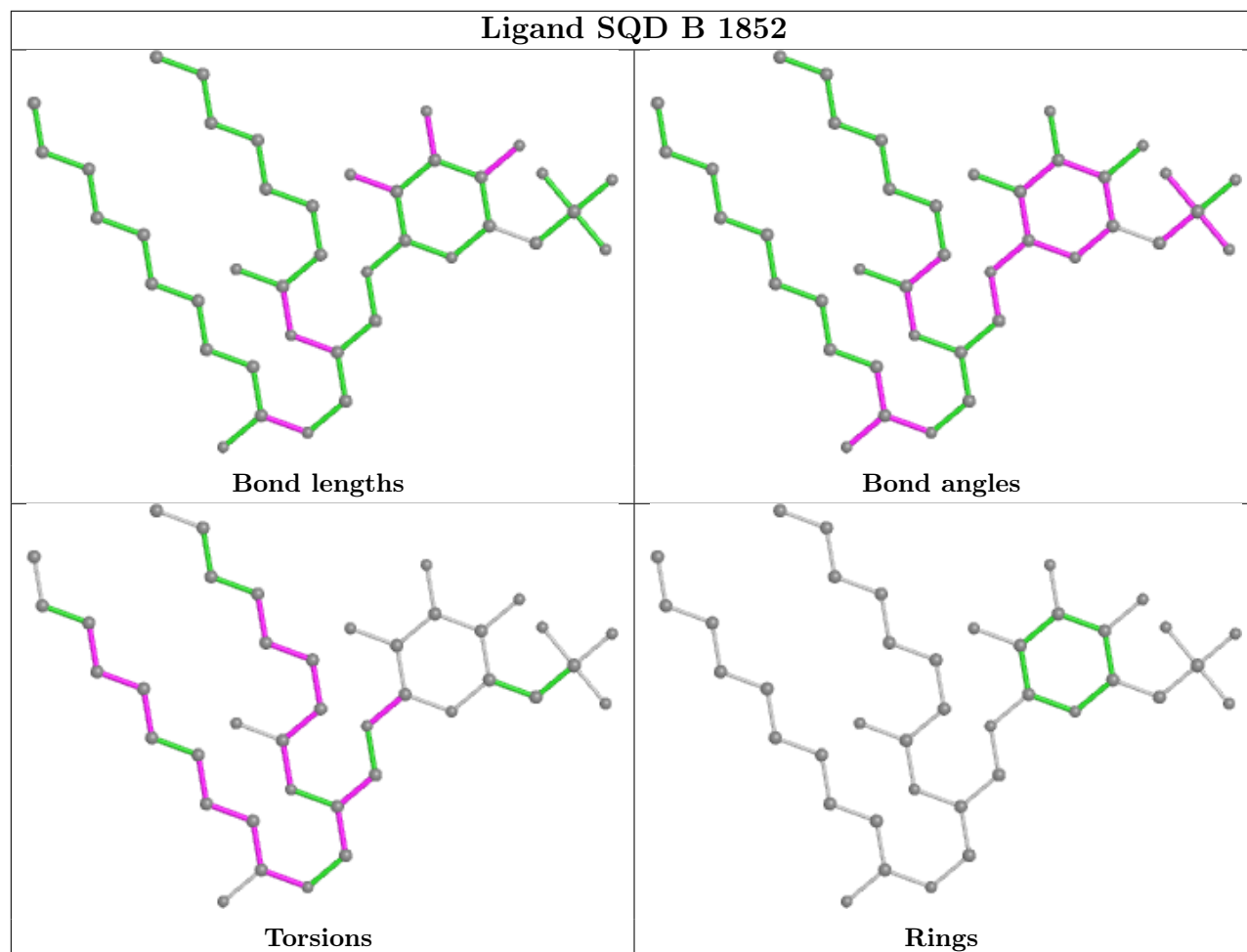
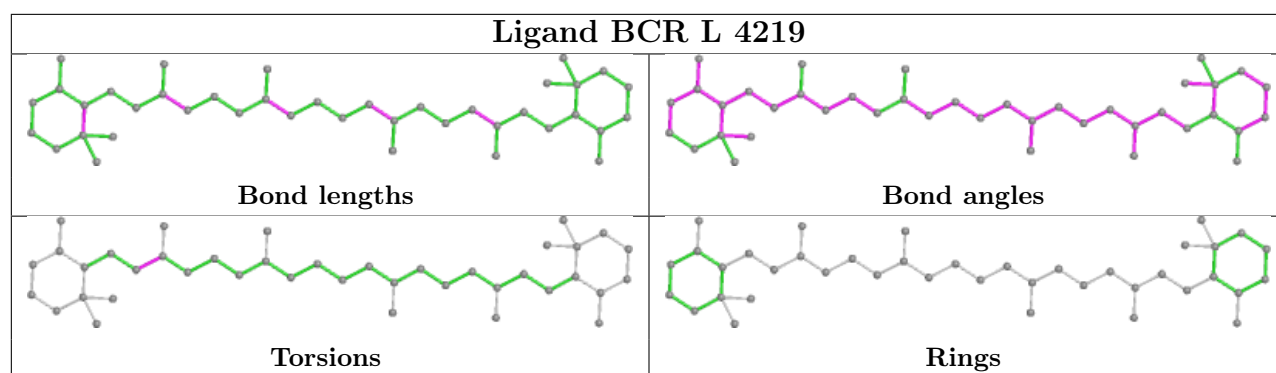
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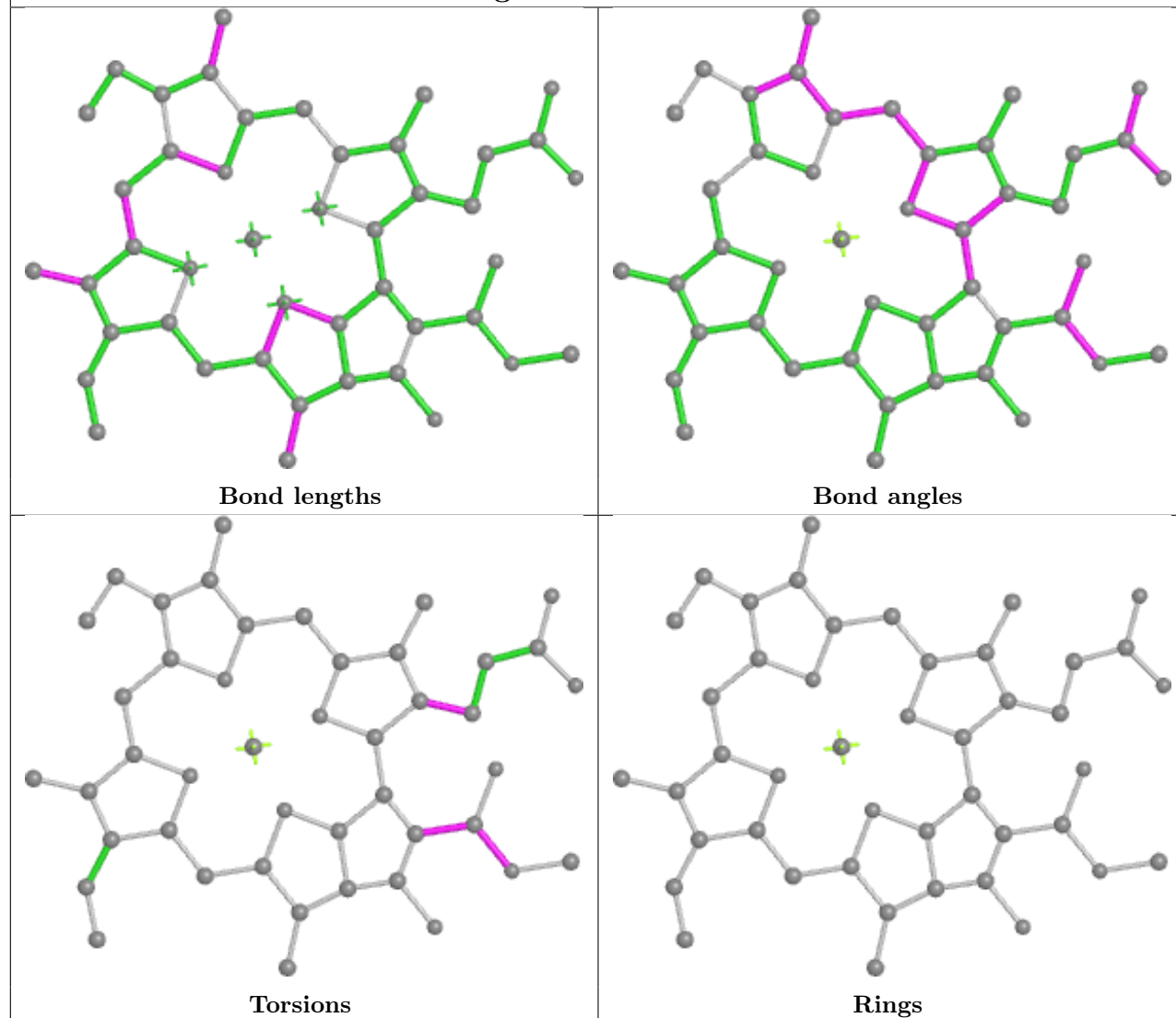
Ligand BCR Y 523



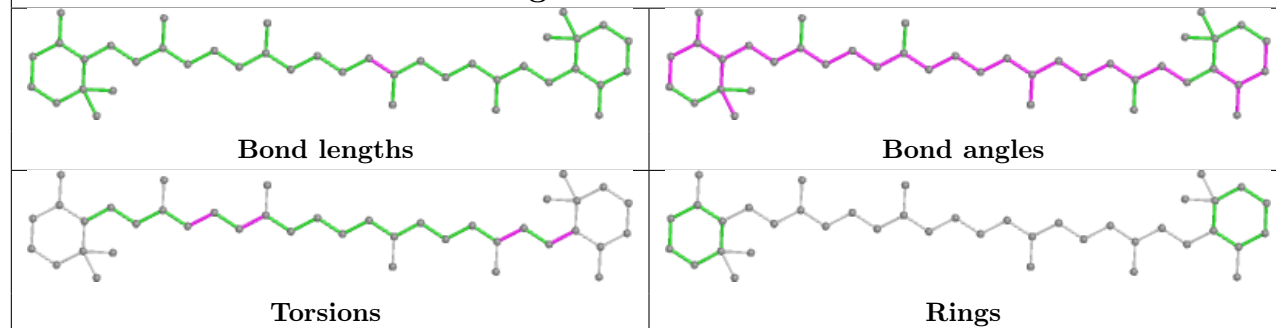


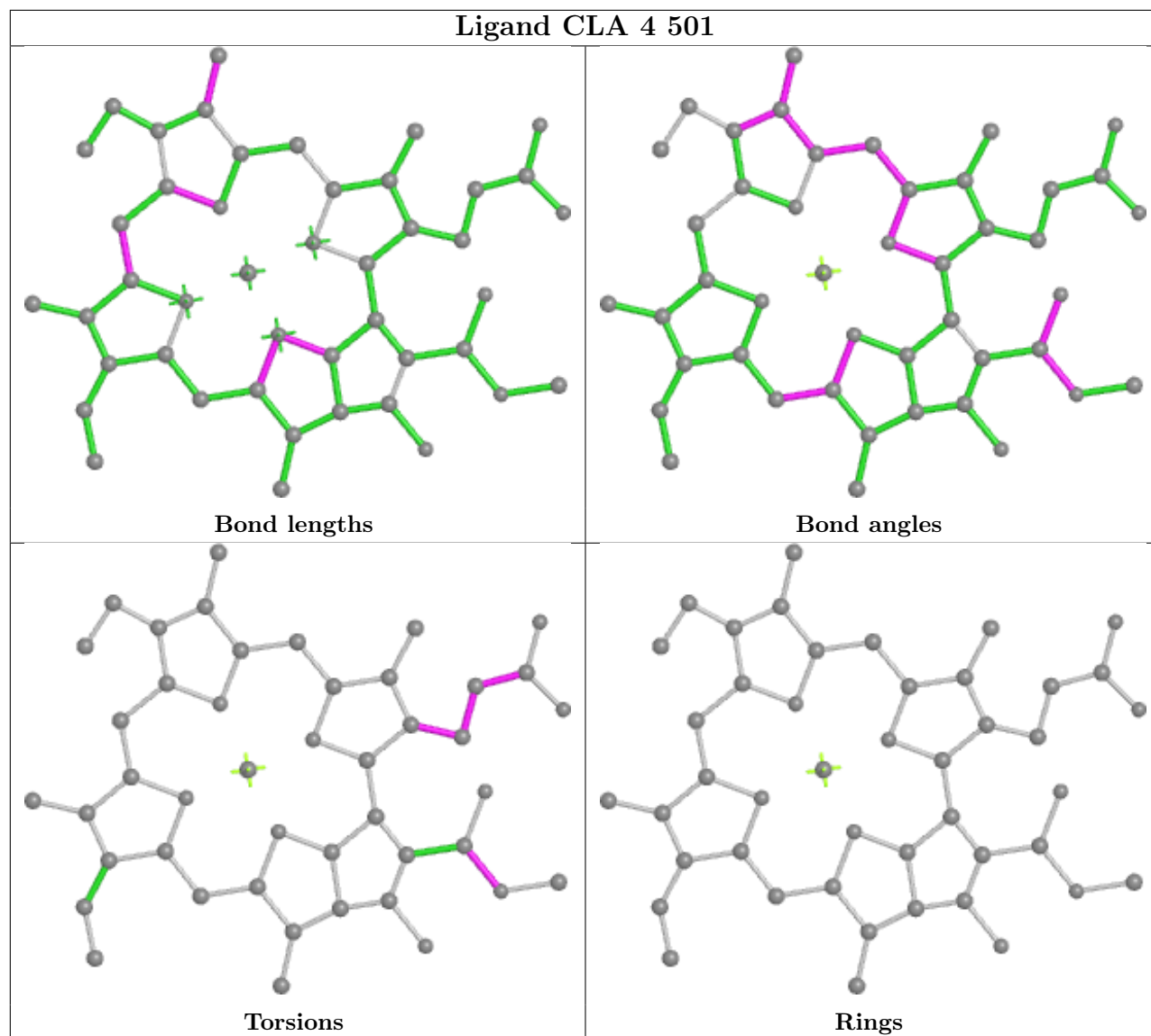
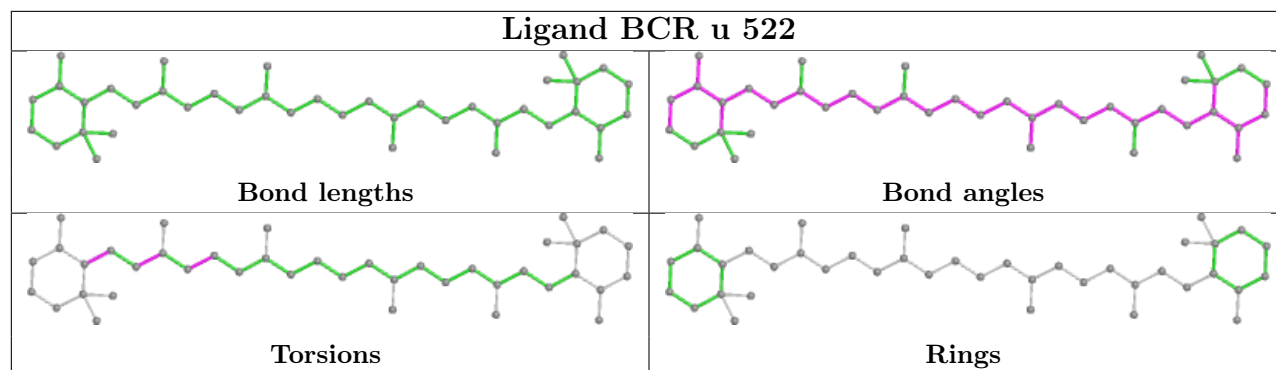


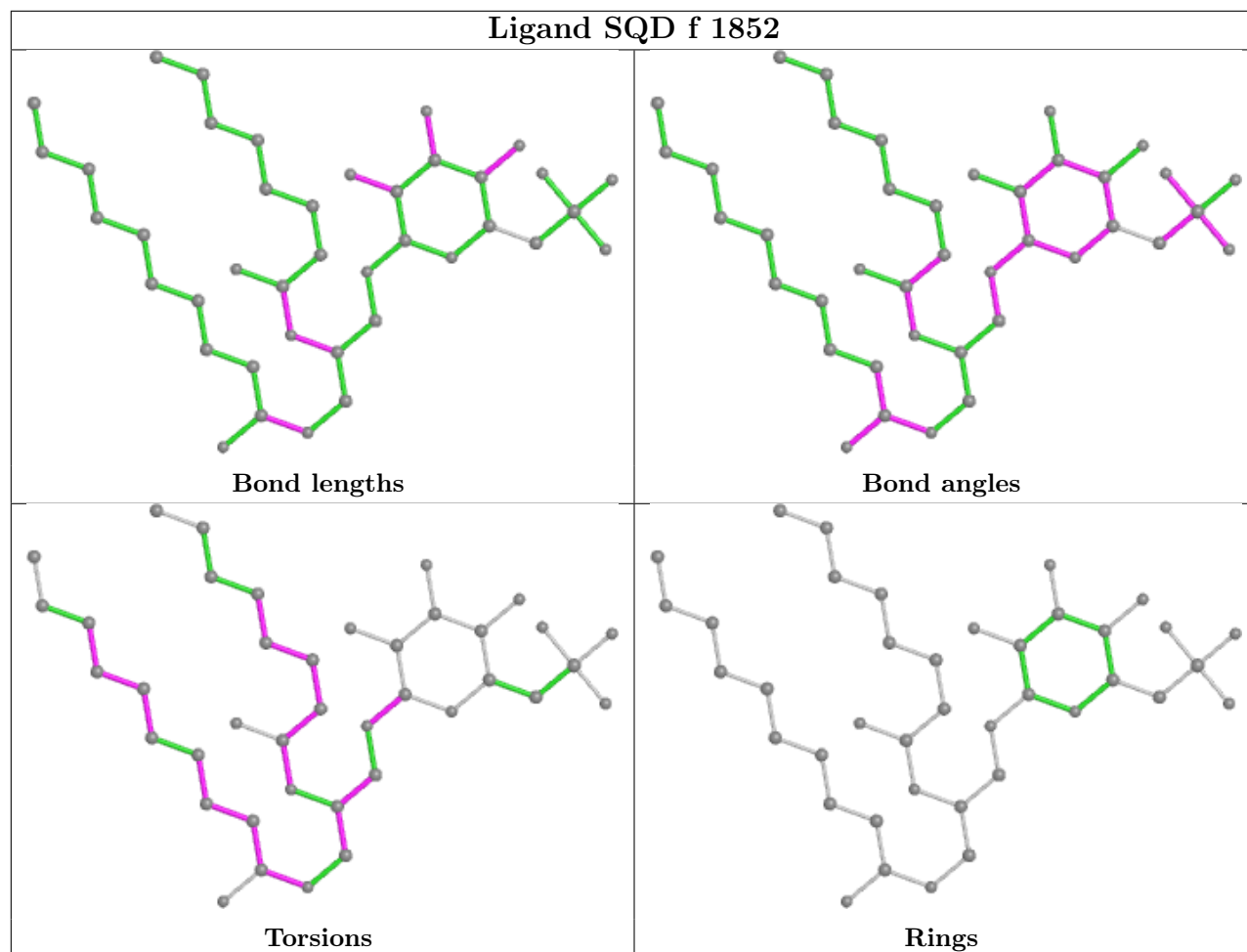
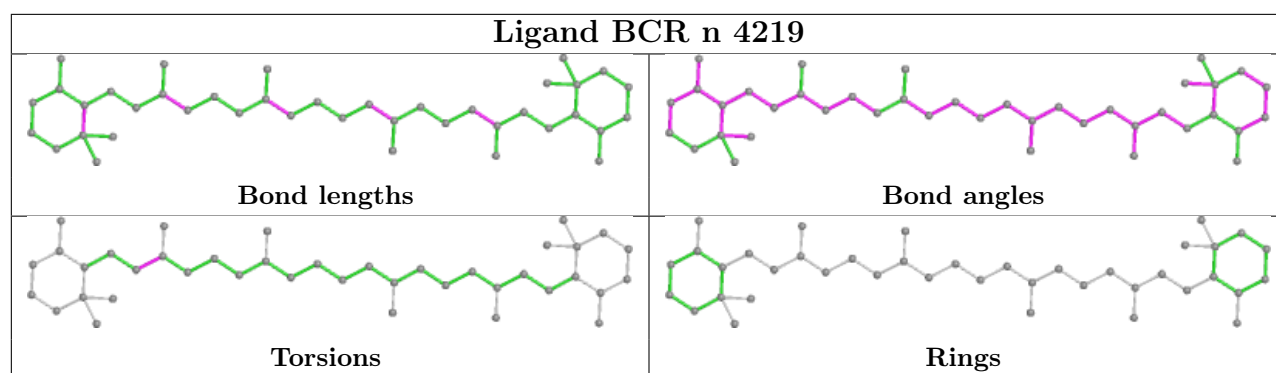
Ligand CLA 4 517



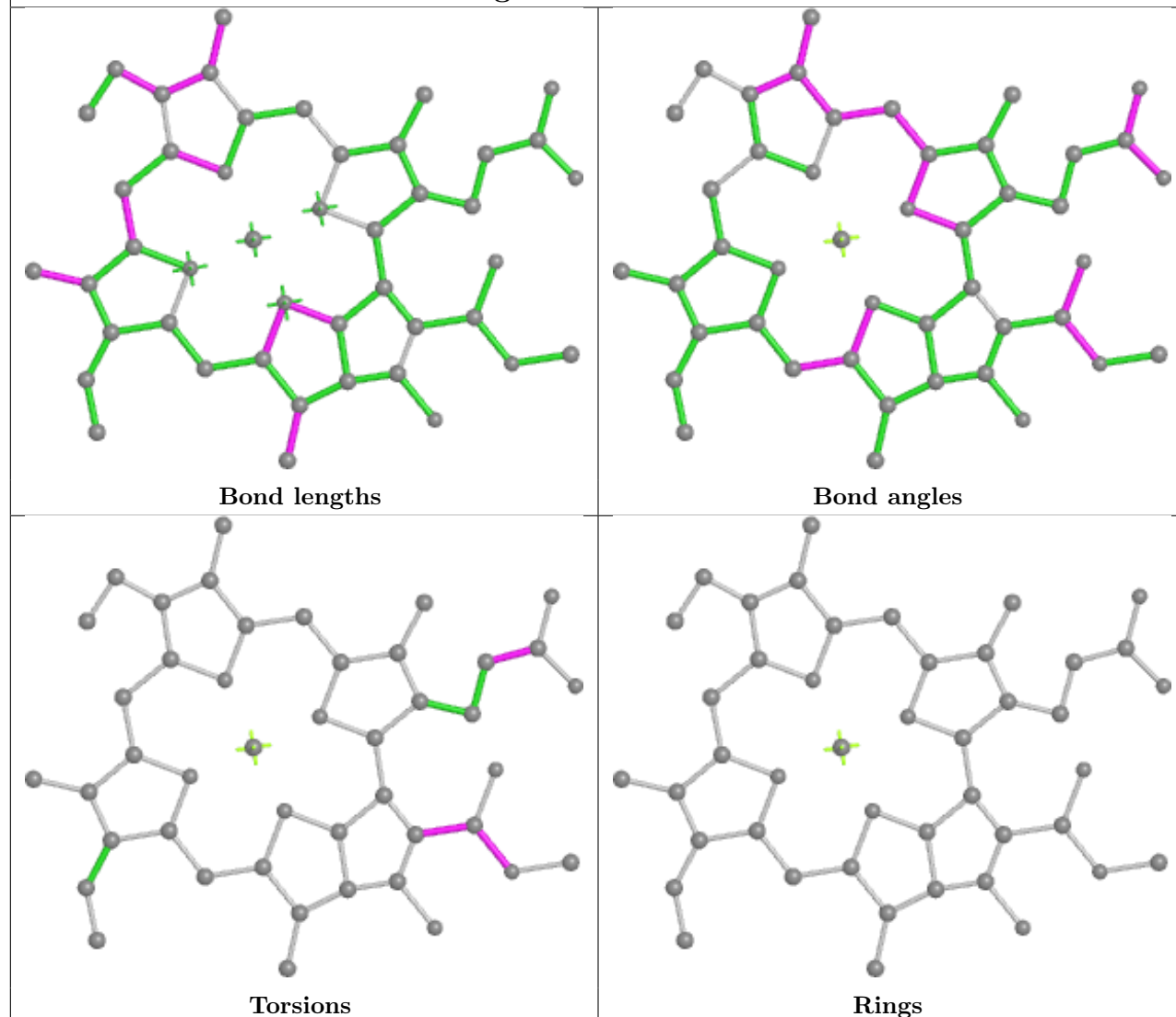
Ligand BCR f 4010



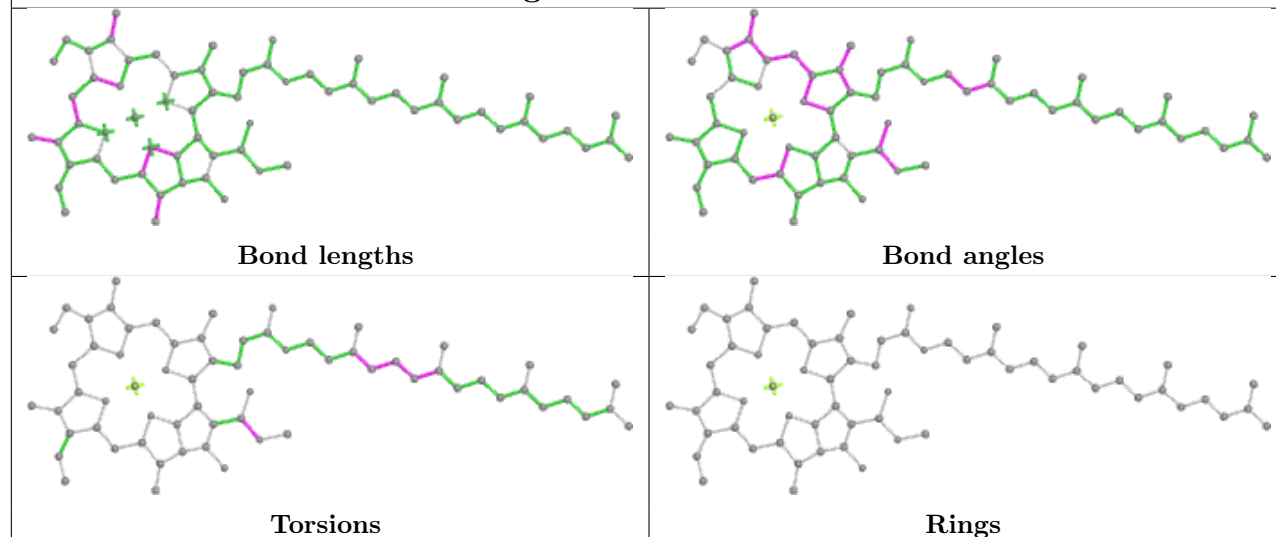




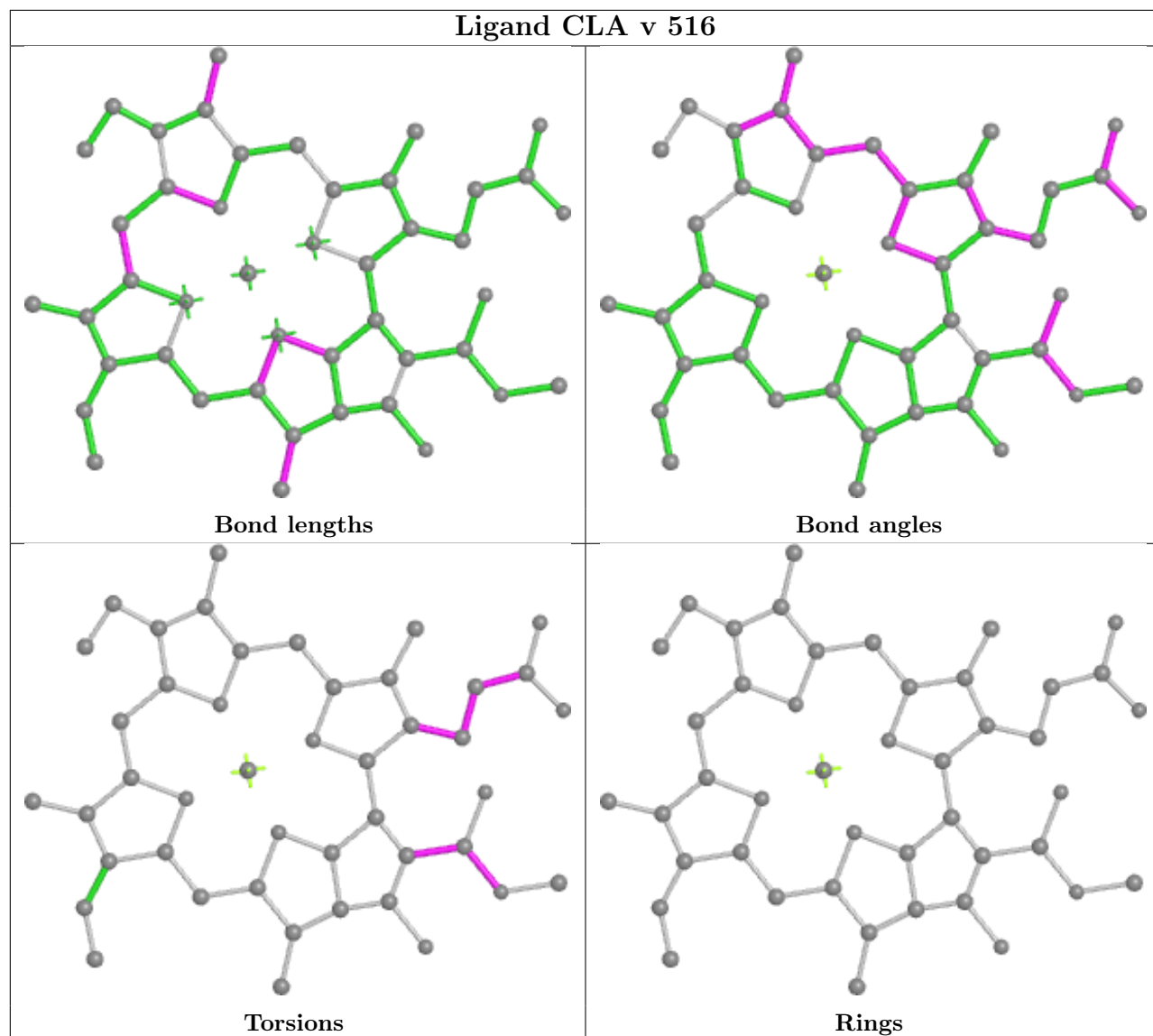
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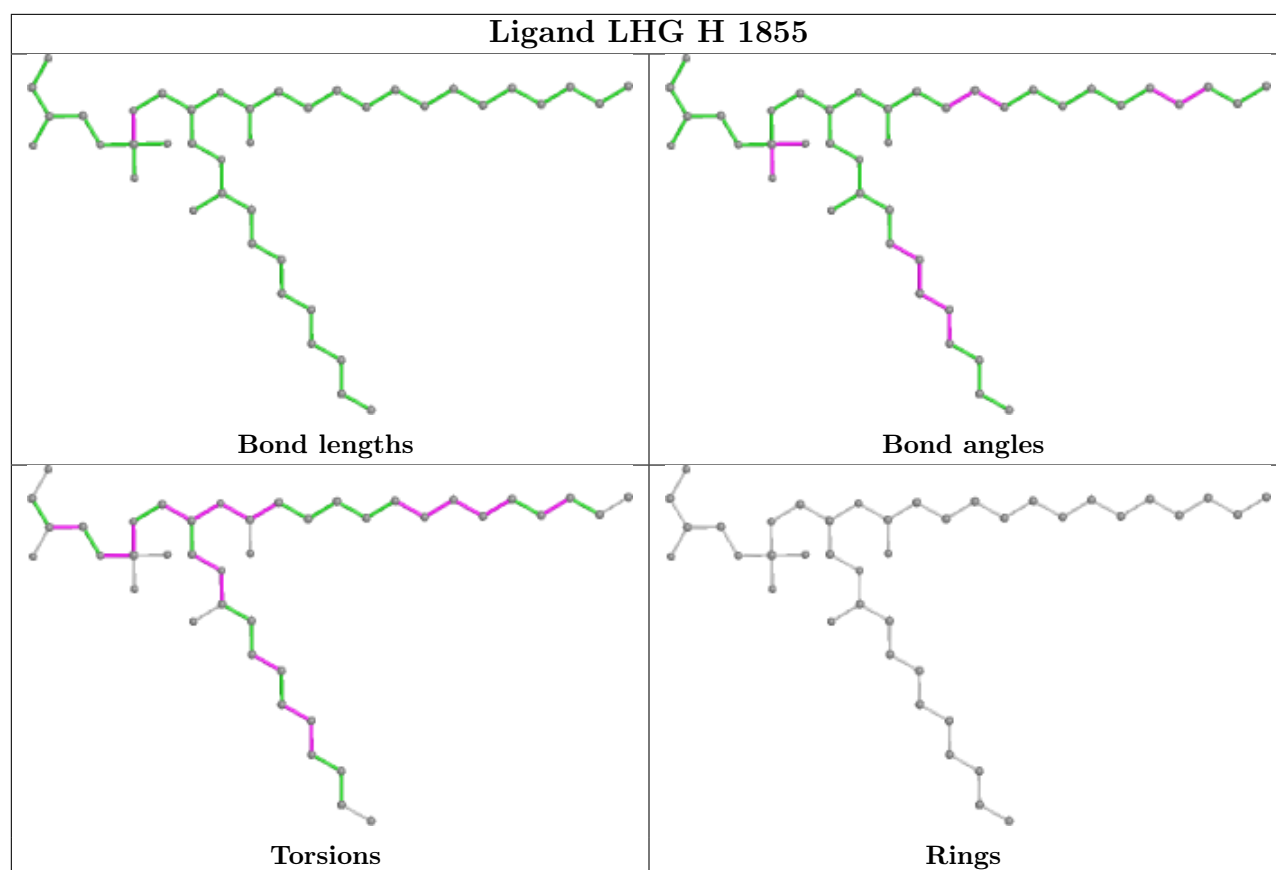


Ligand CLA B 1231

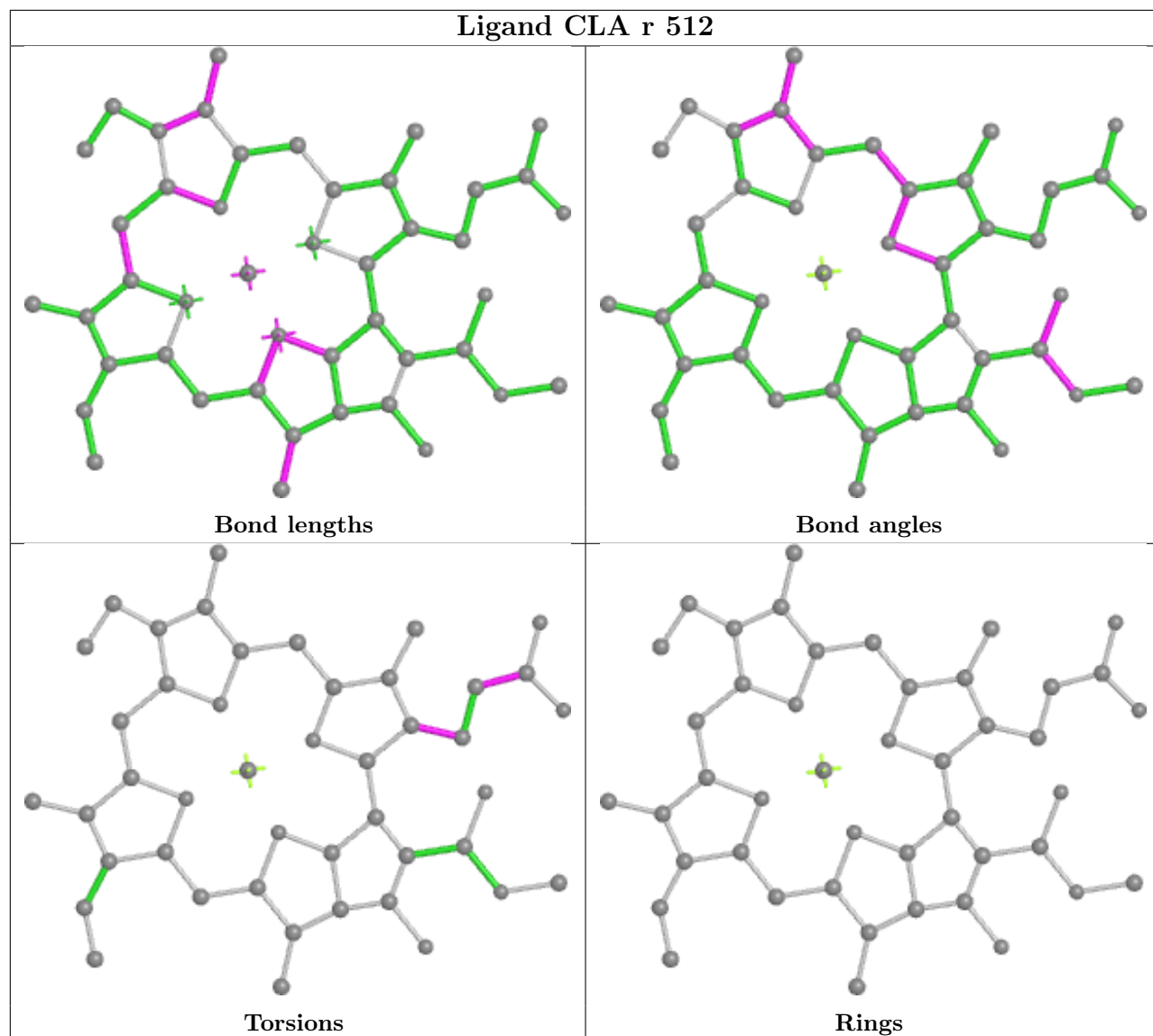


Ligand CLA v 516

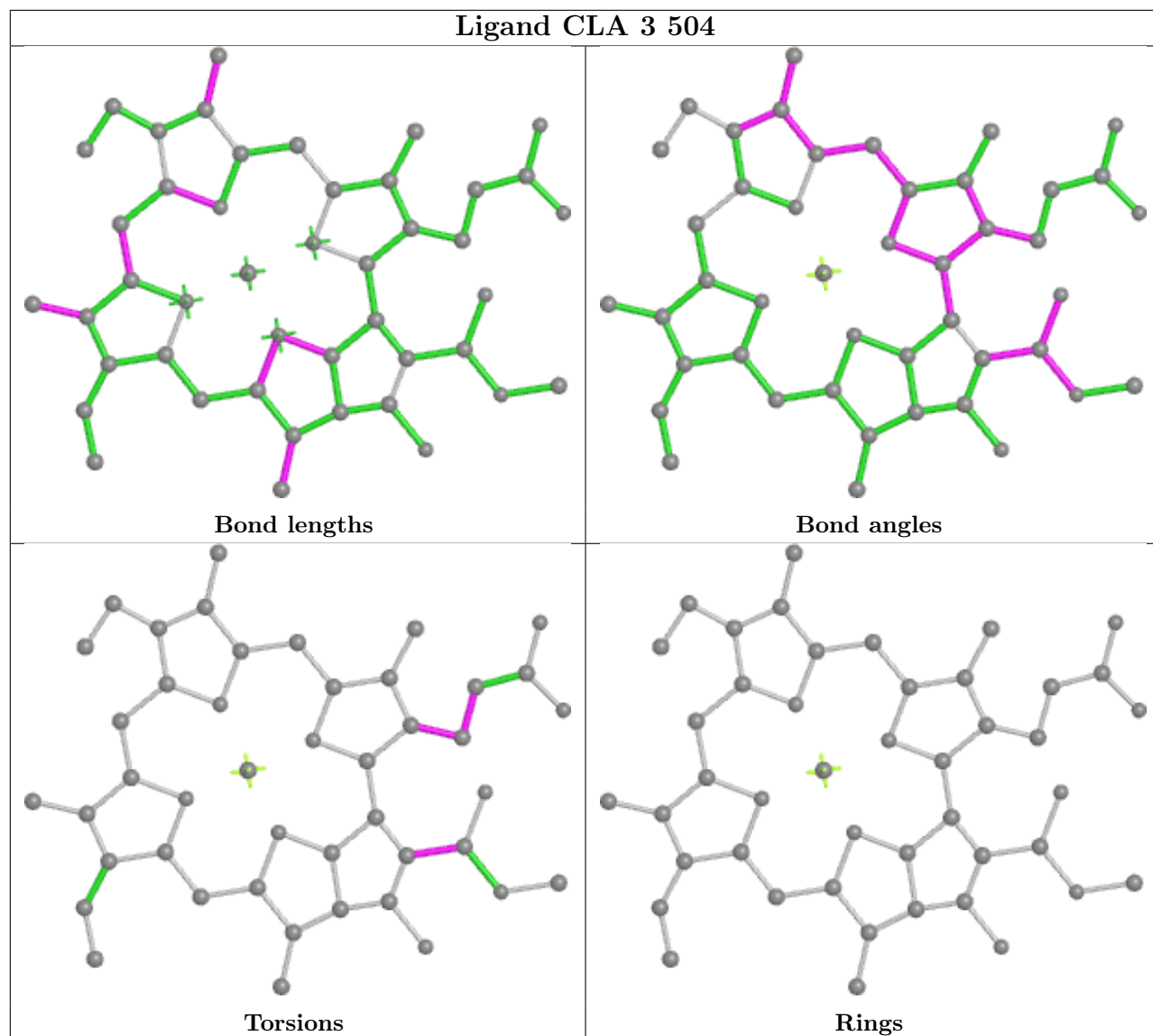


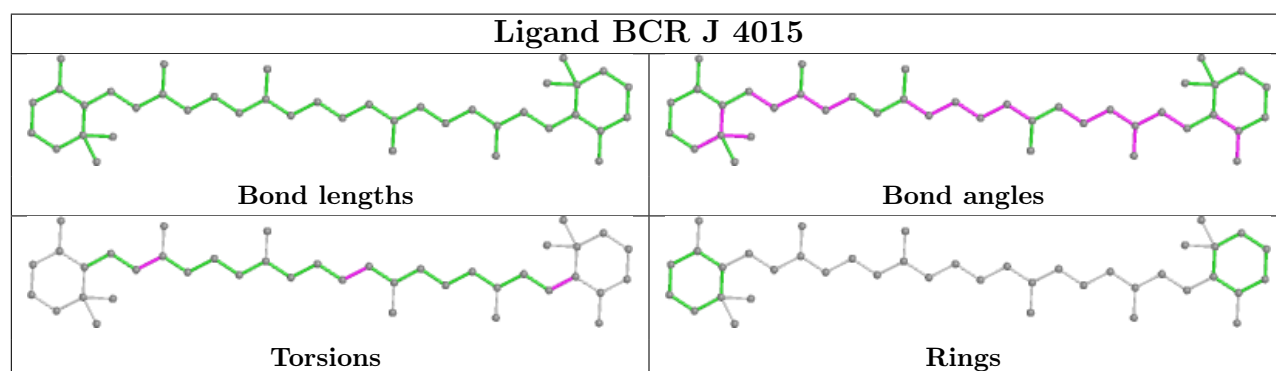
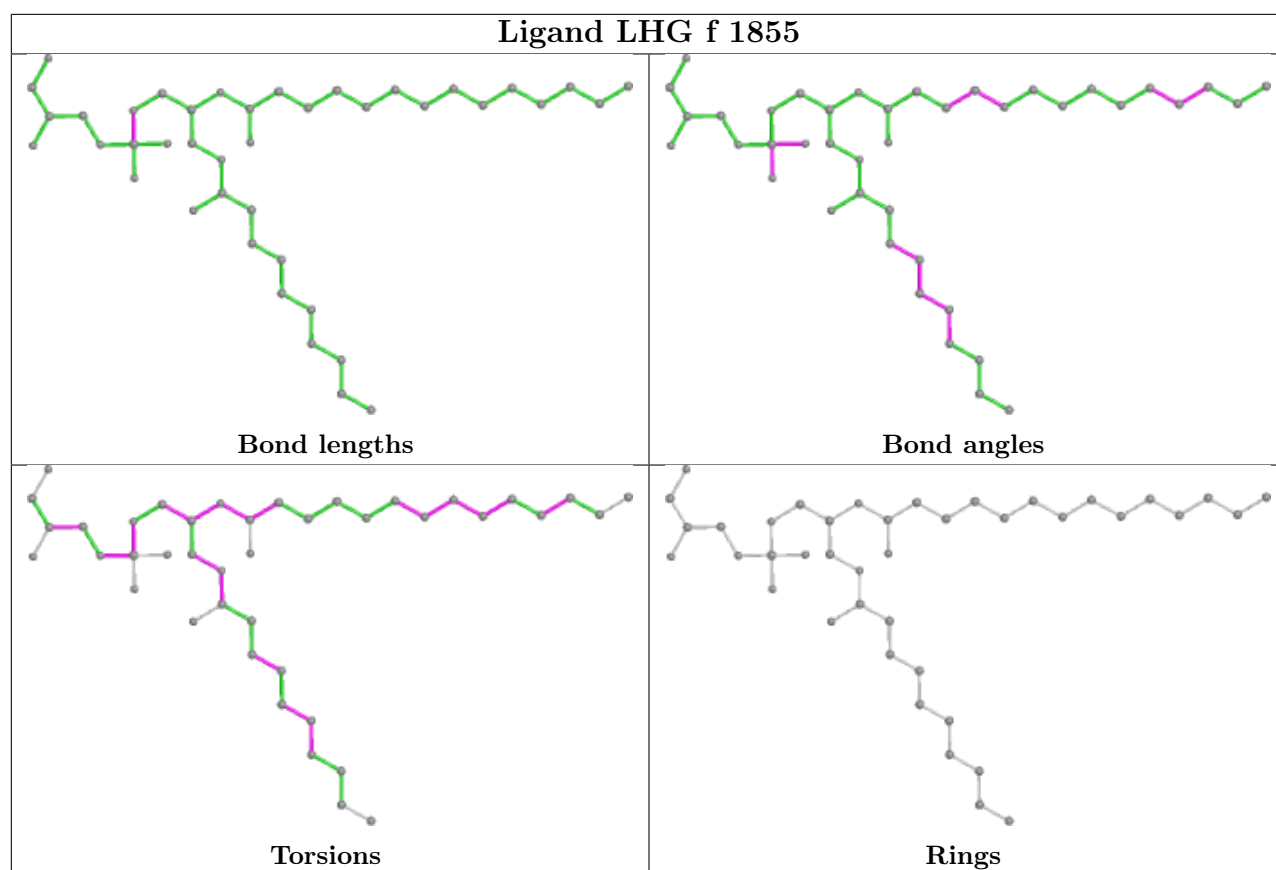


Ligand CLA r 512

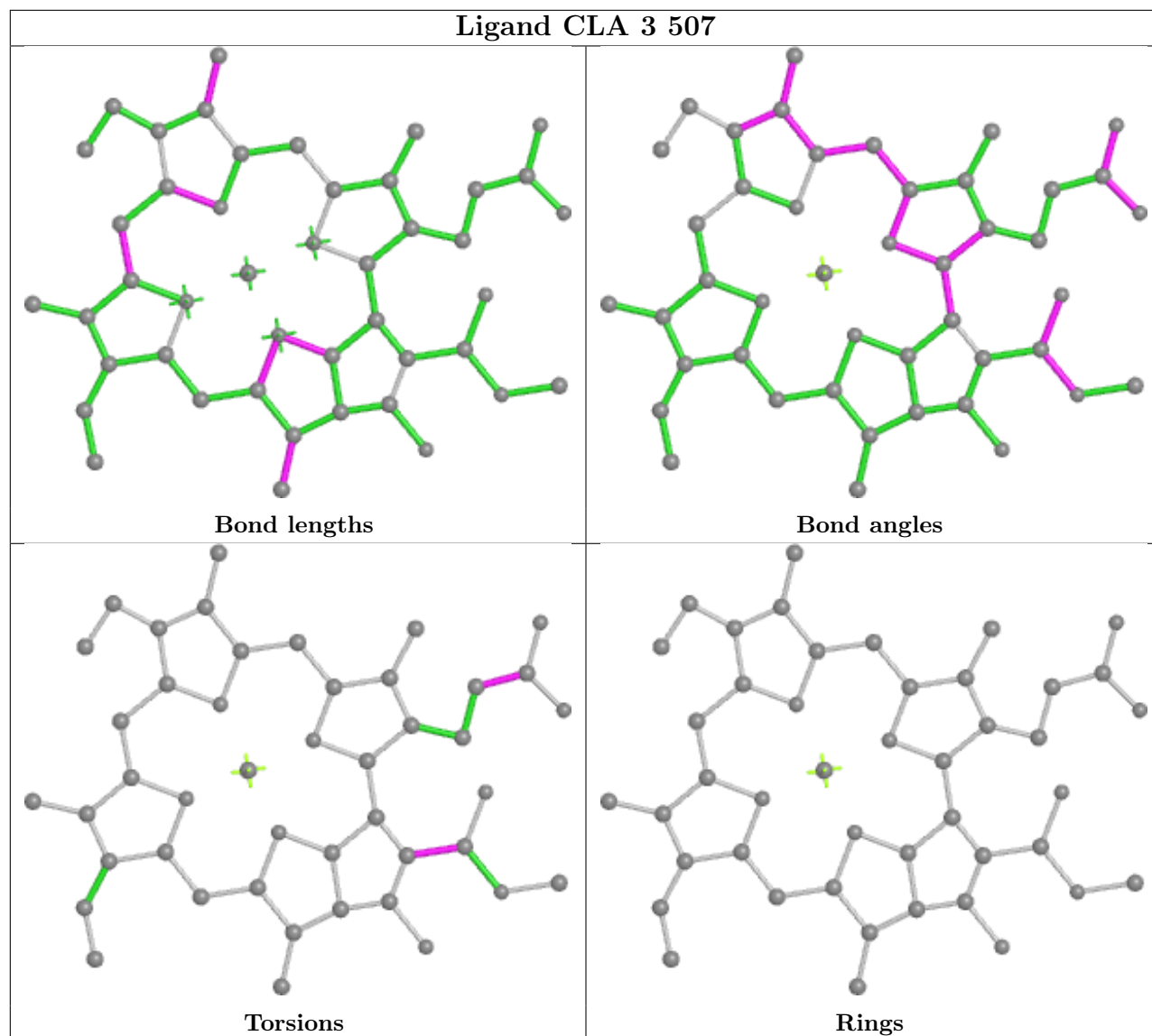


Ligand CLA 3 504

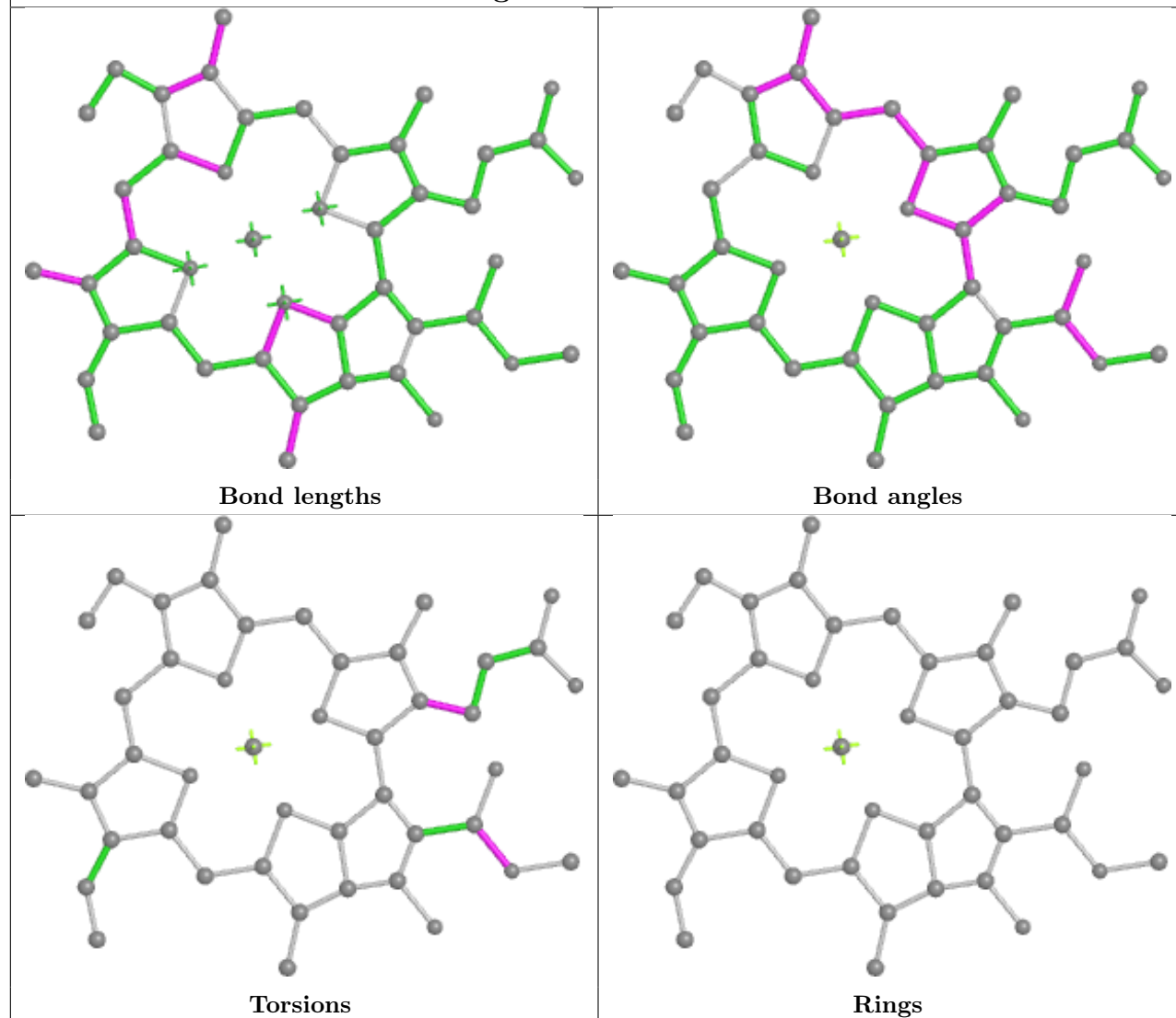




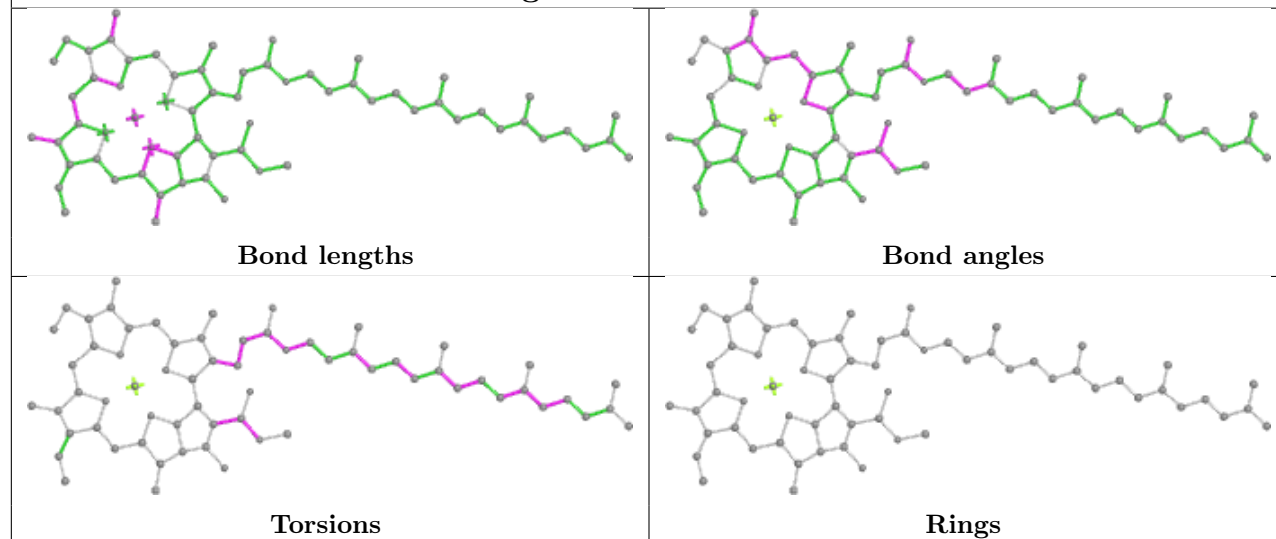
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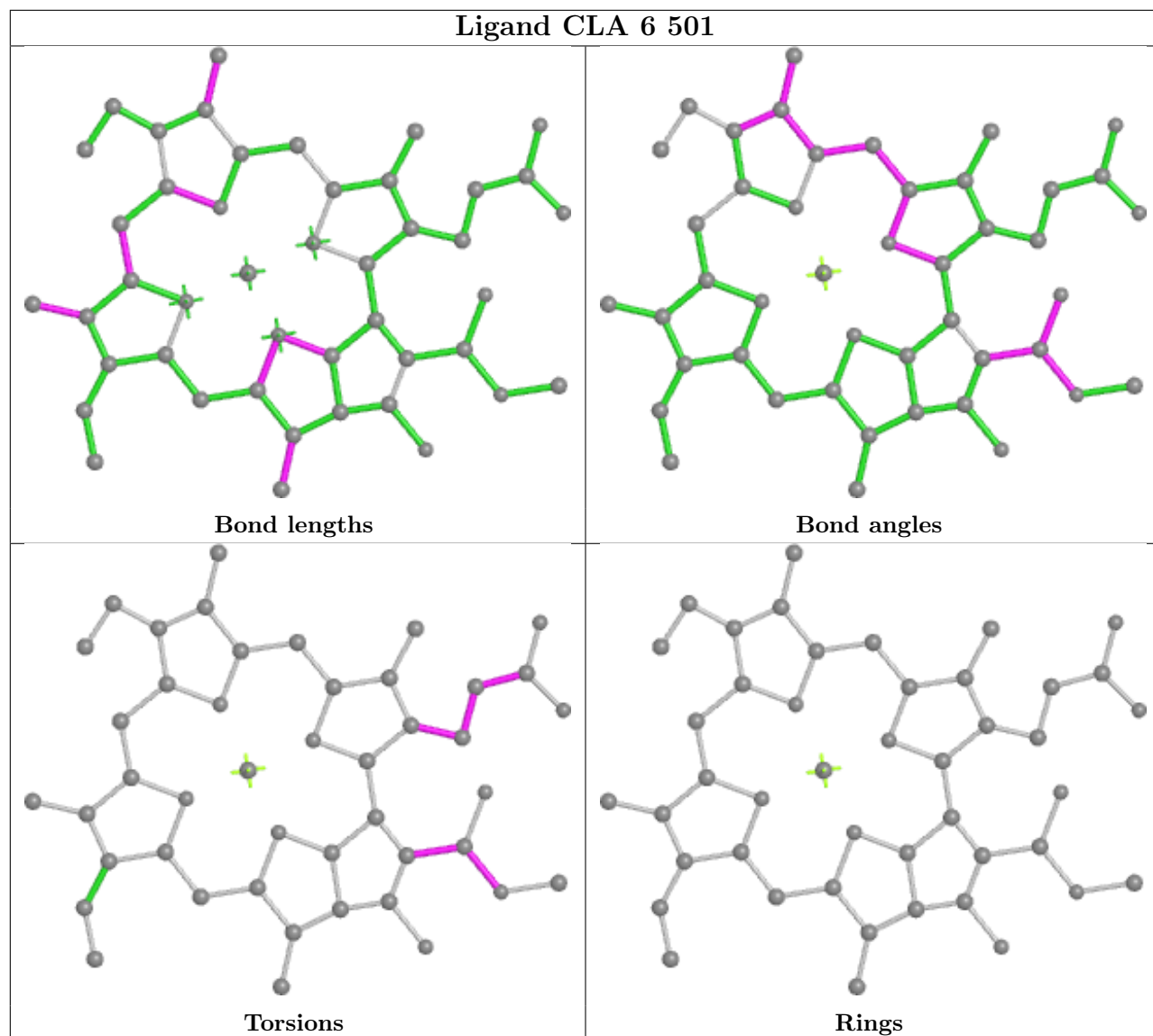
Ligand CLA u 504



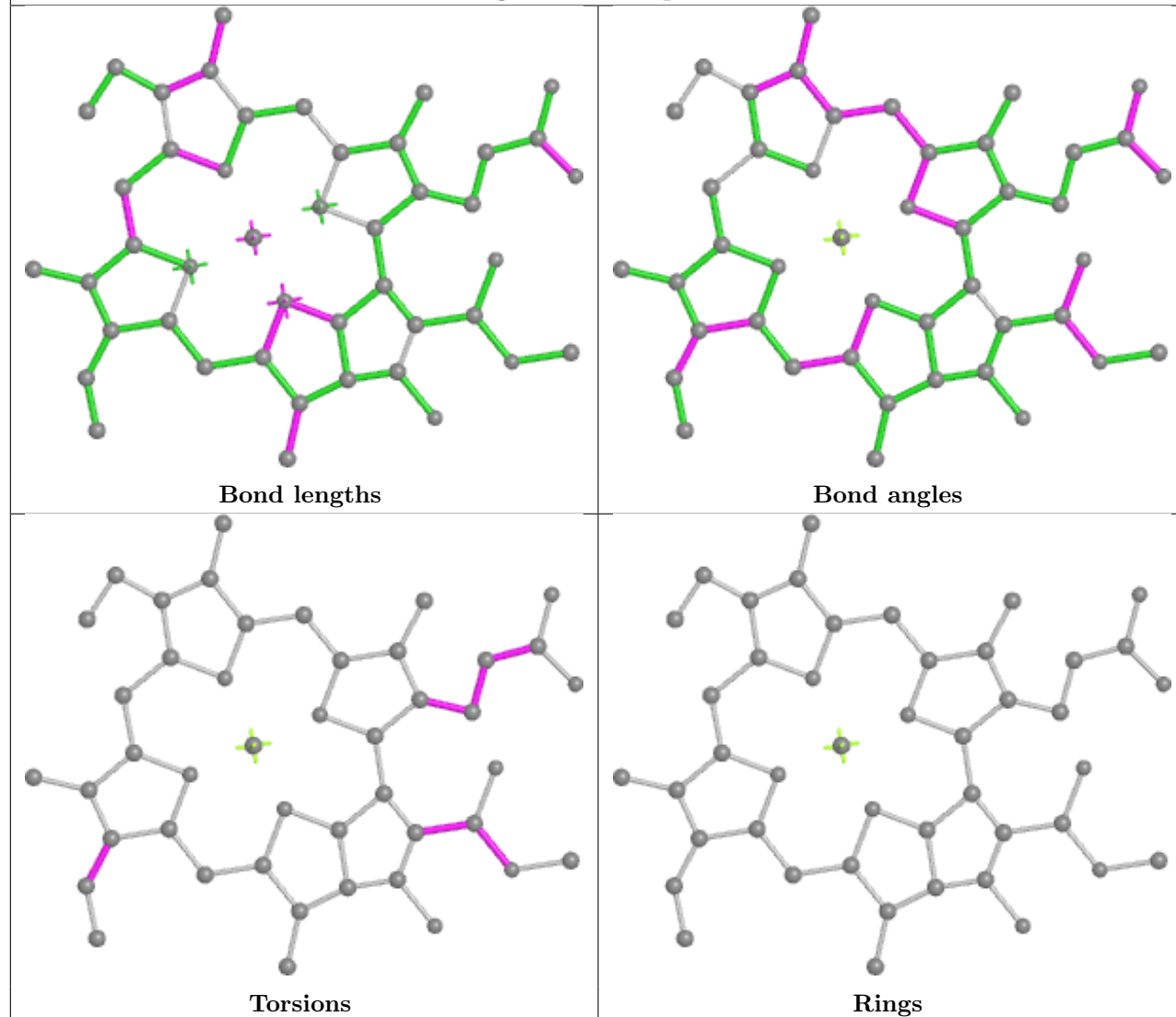
Ligand CLA G 1106



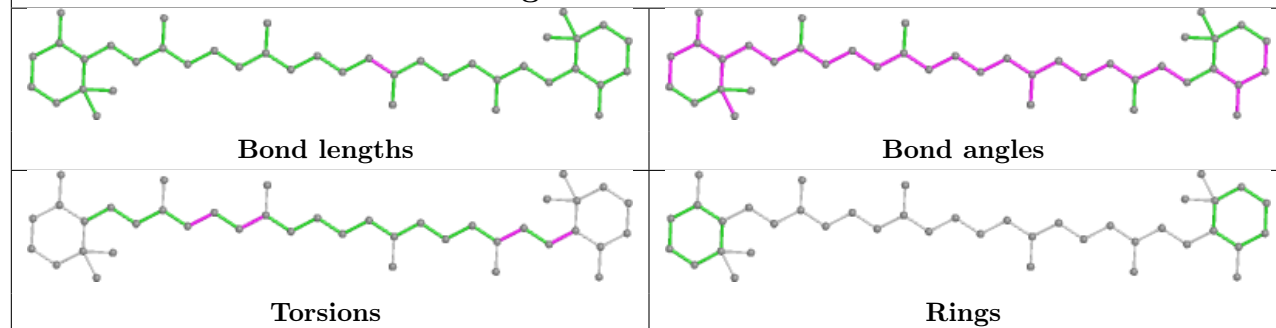
Ligand CLA 6 501

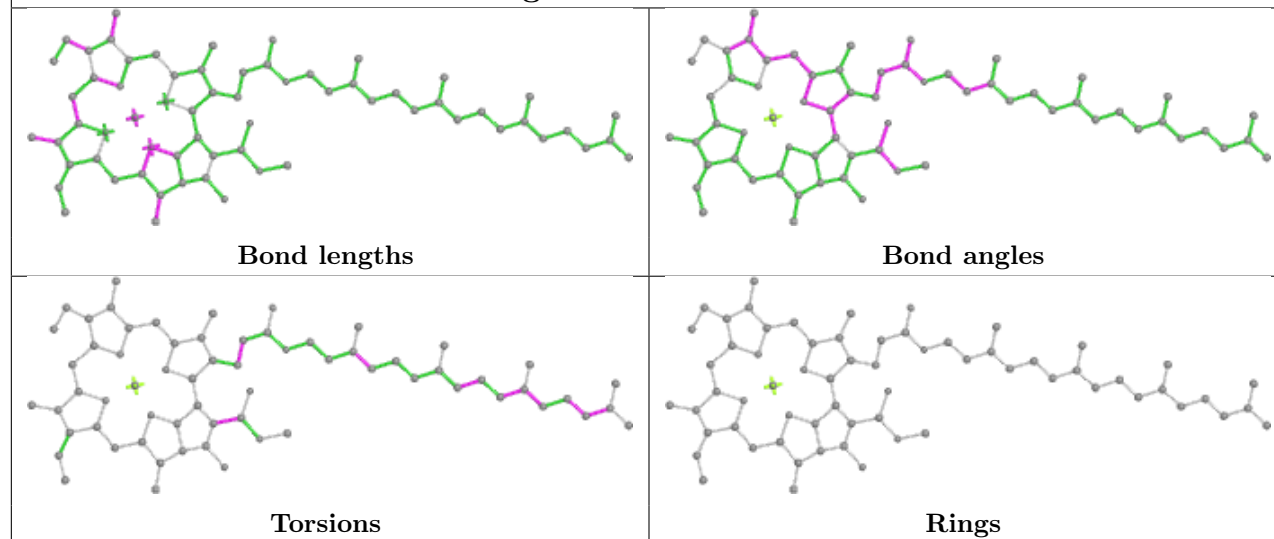
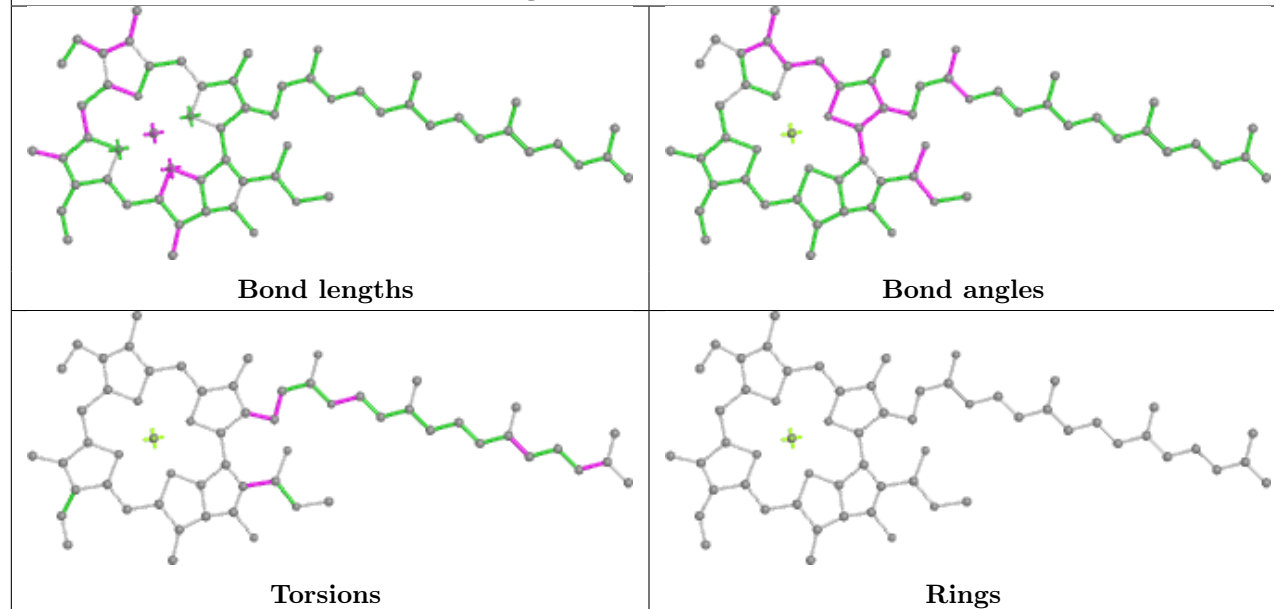


Ligand CLA q 516

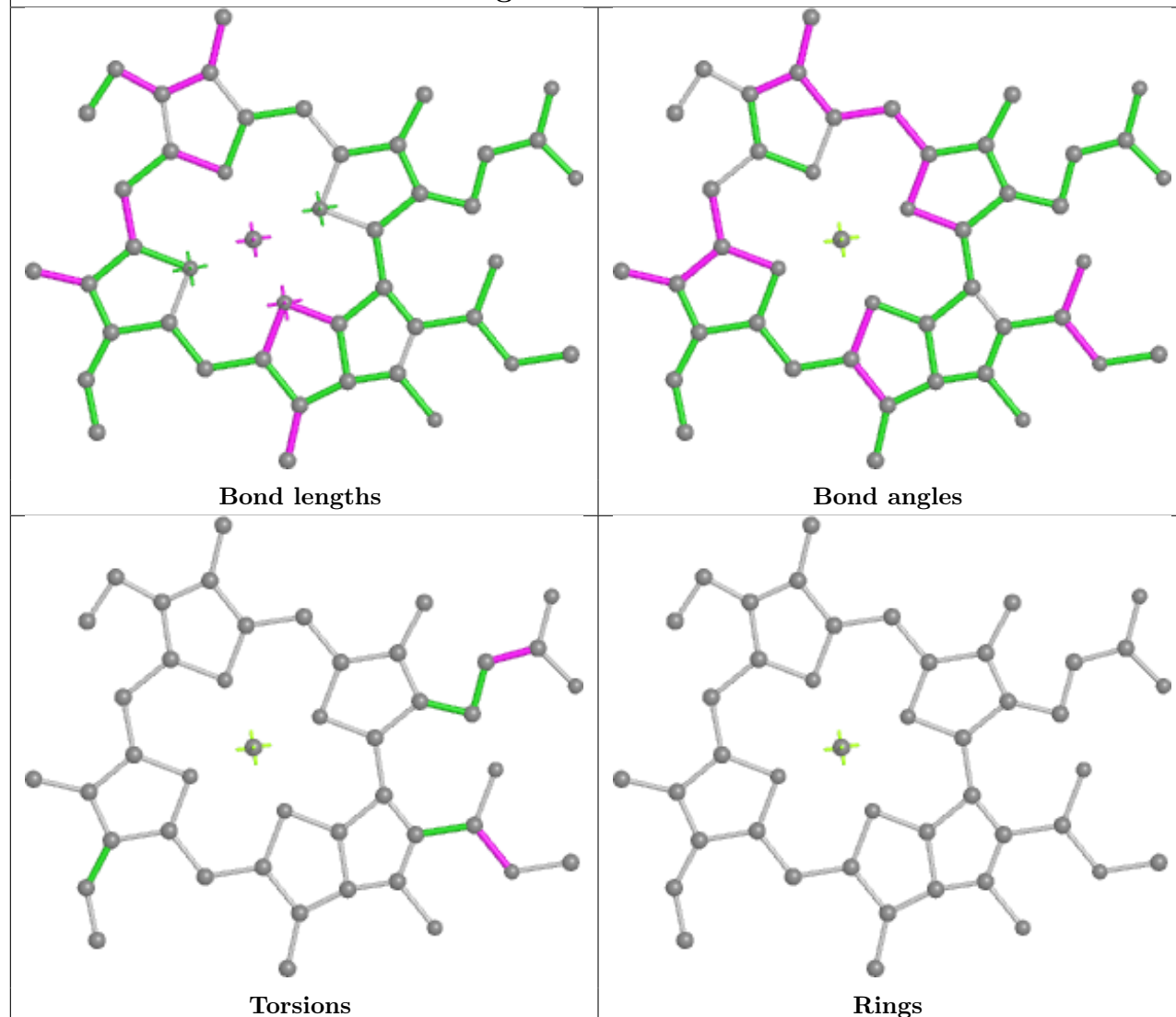


Ligand BCR B 4010

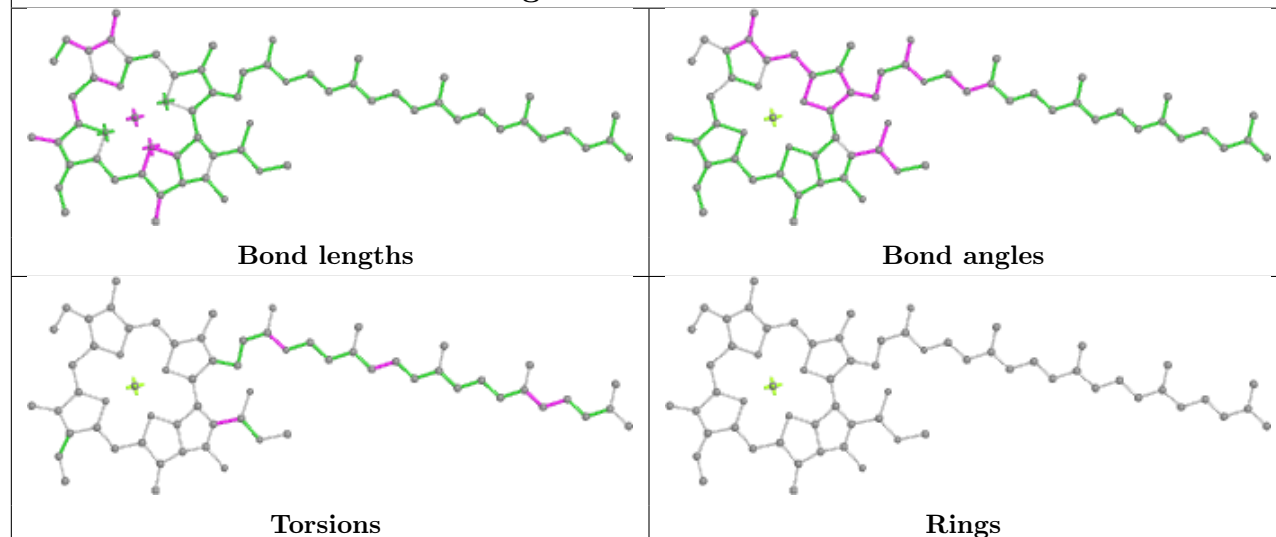


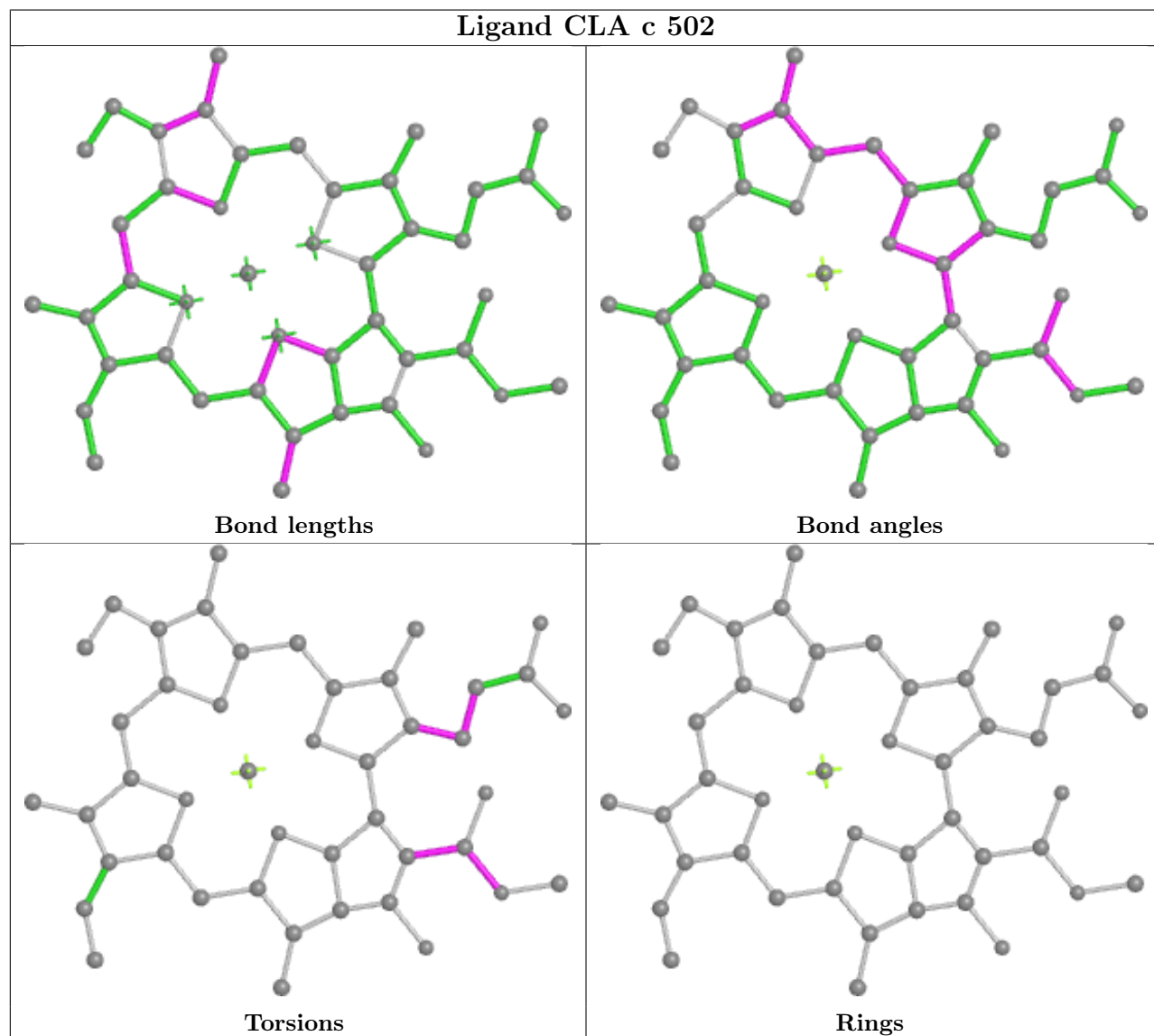
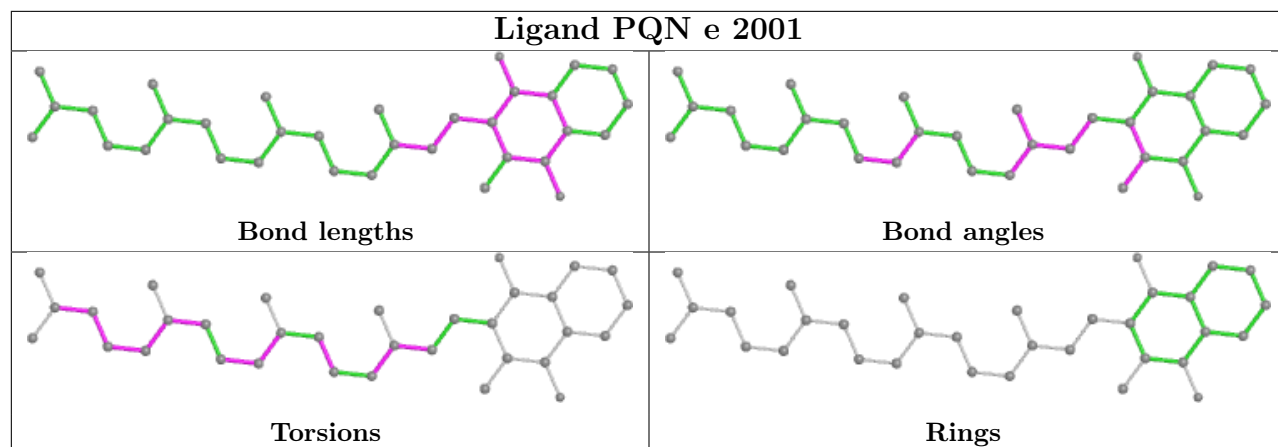
Ligand CLA A 1127**Ligand CLA V 1501**

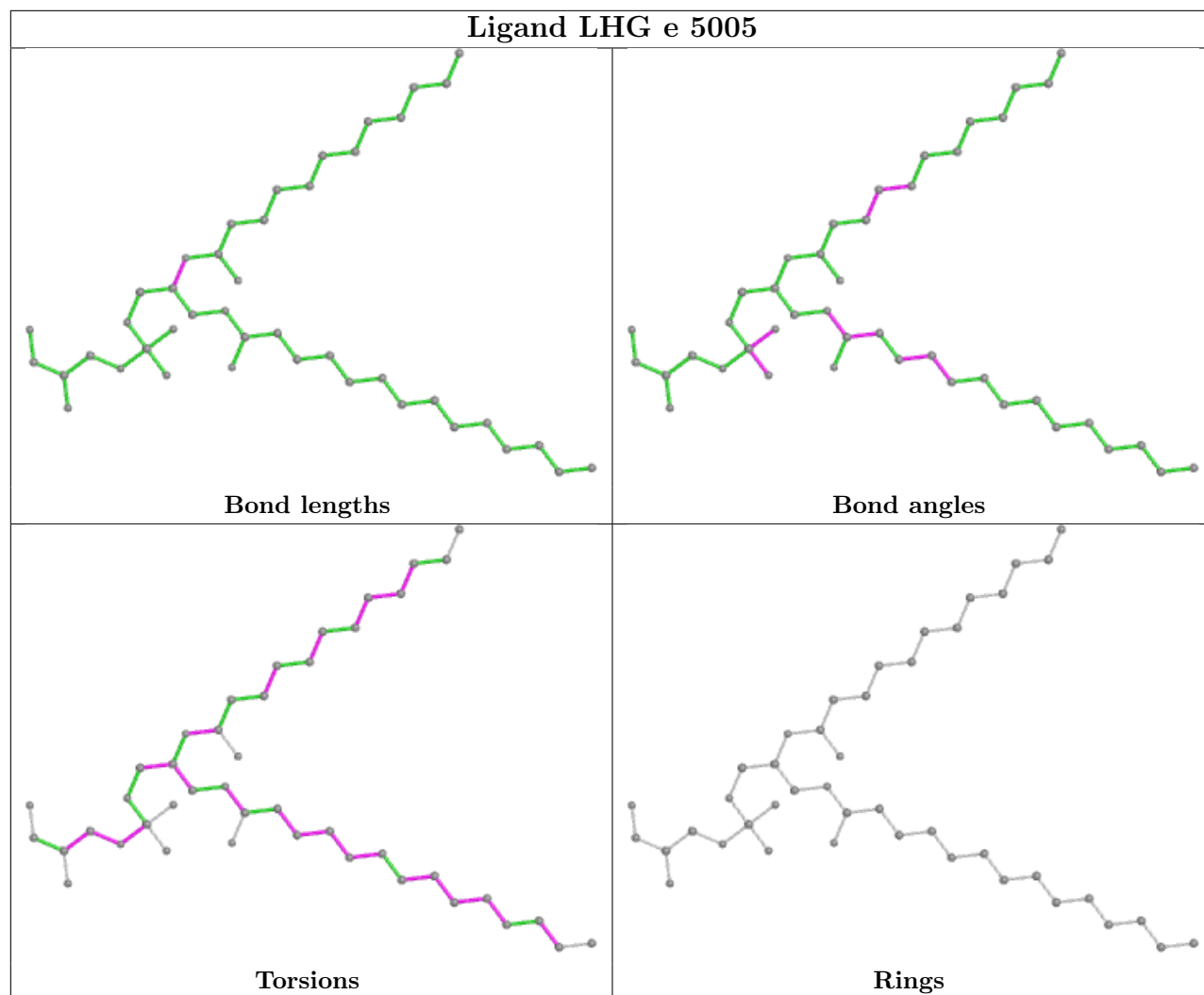
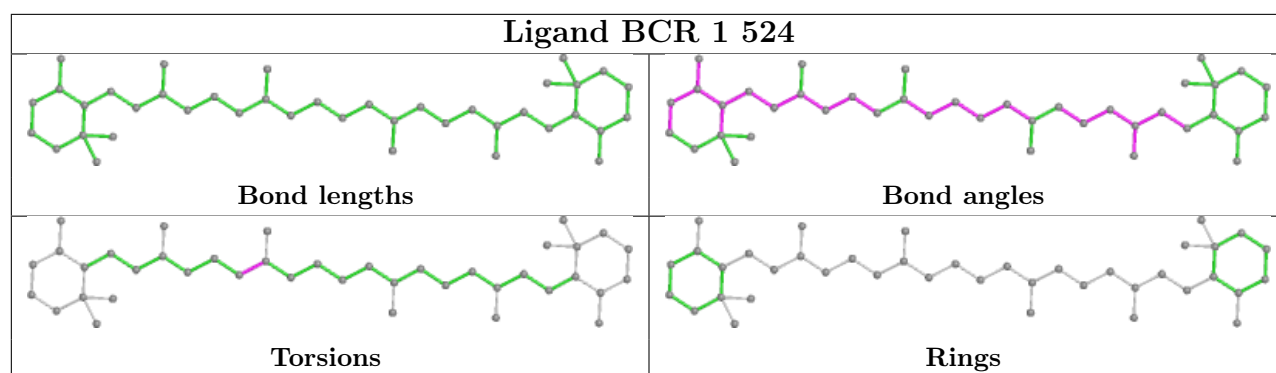
Ligand CLA t 508

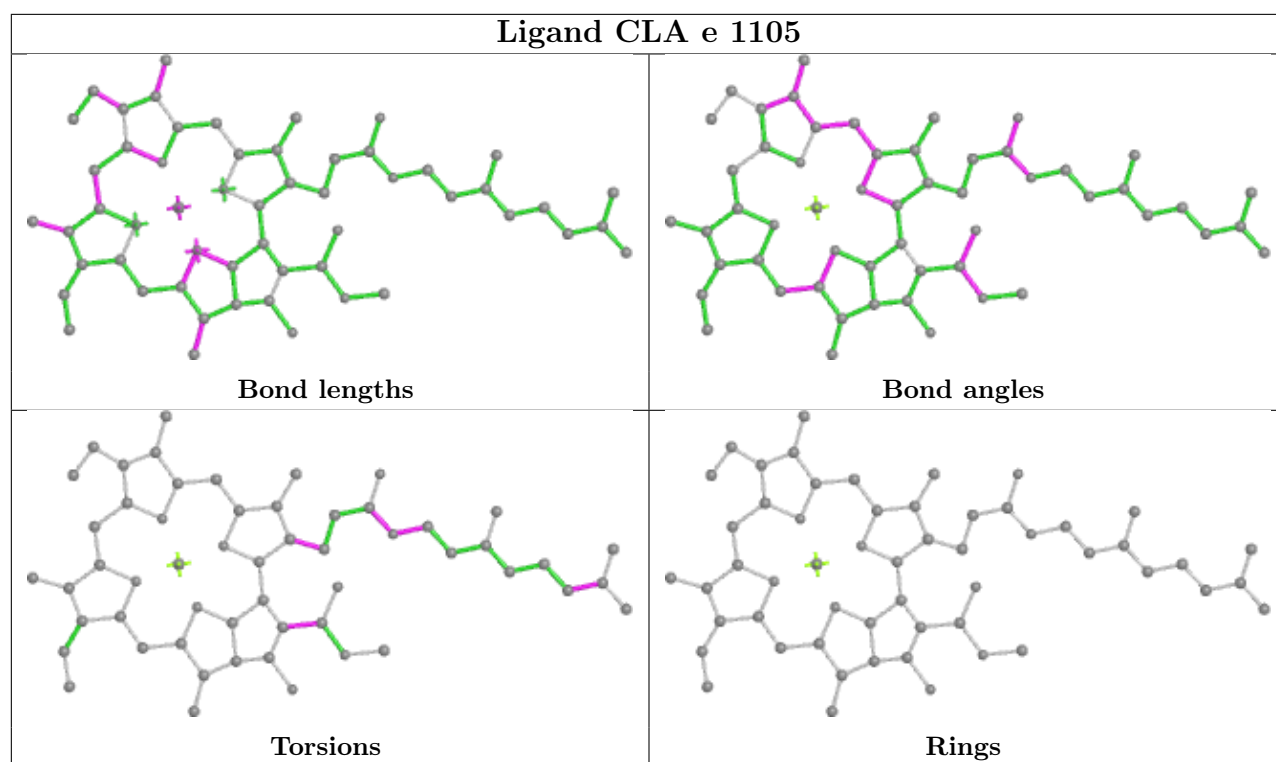


Ligand CLA H 1205

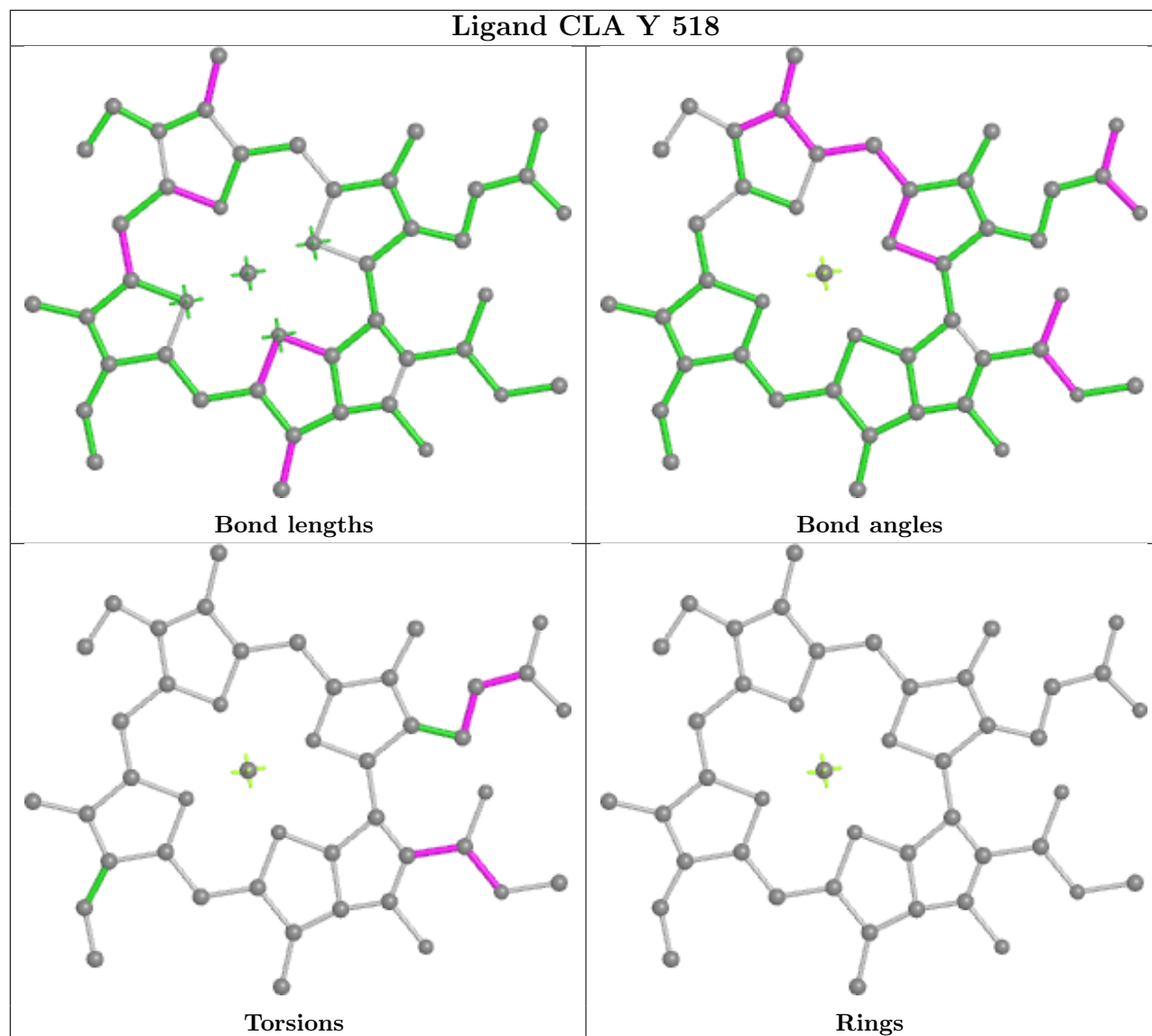


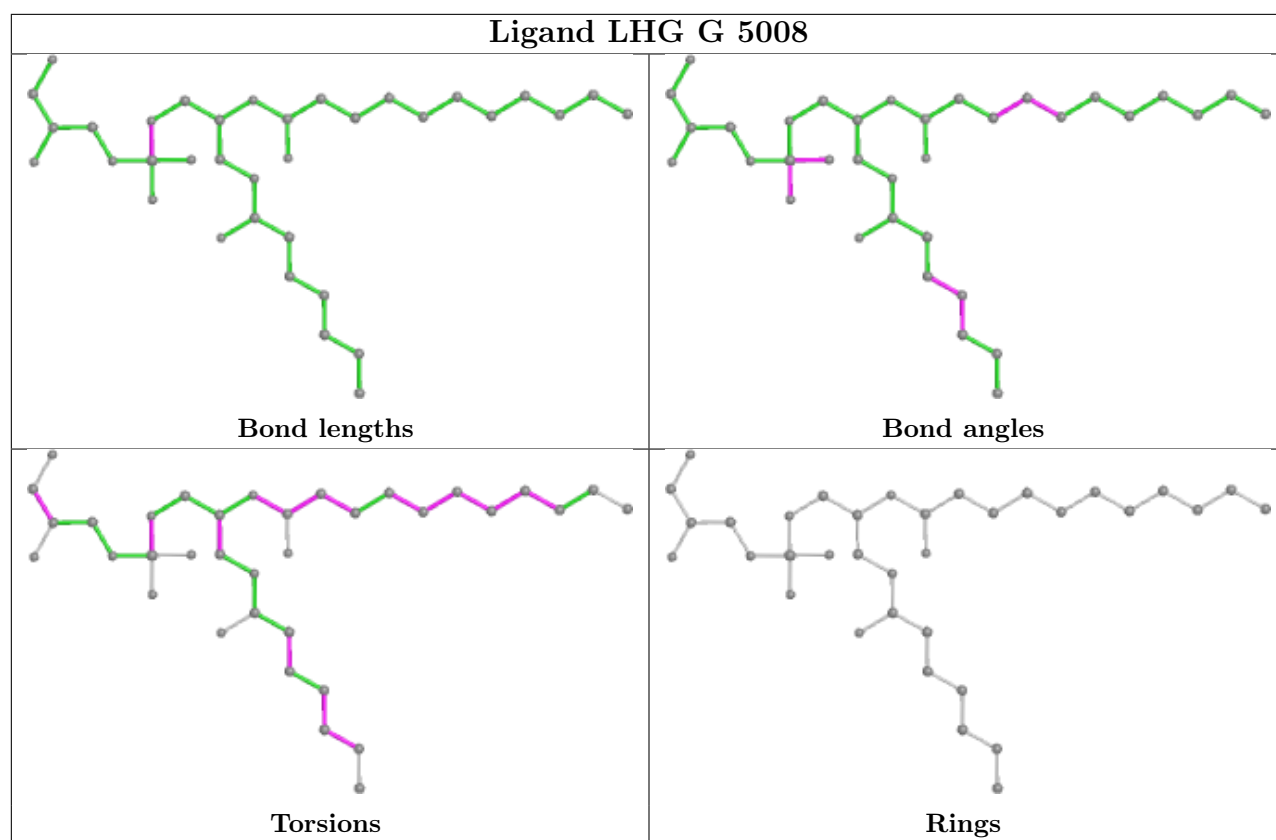


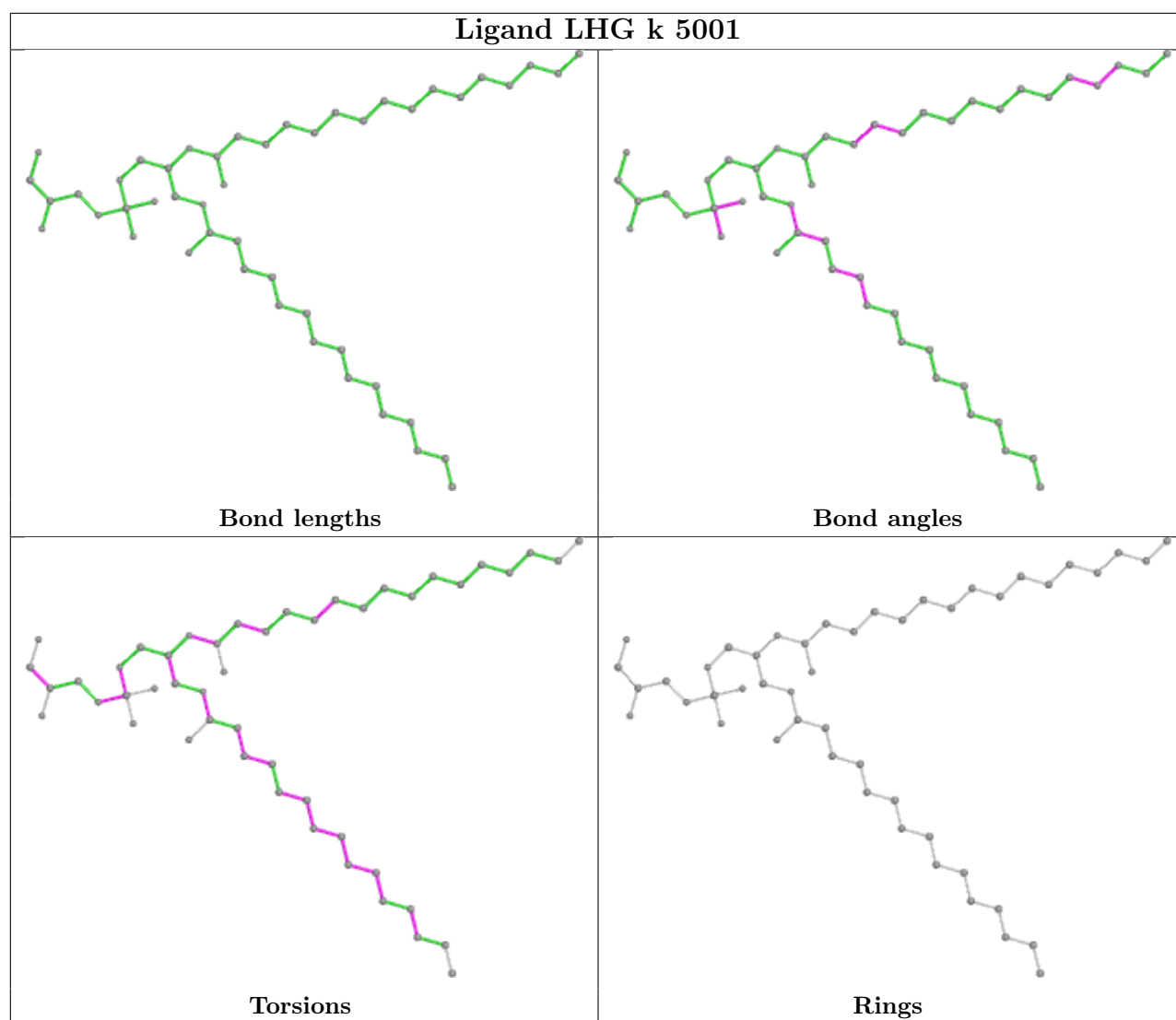


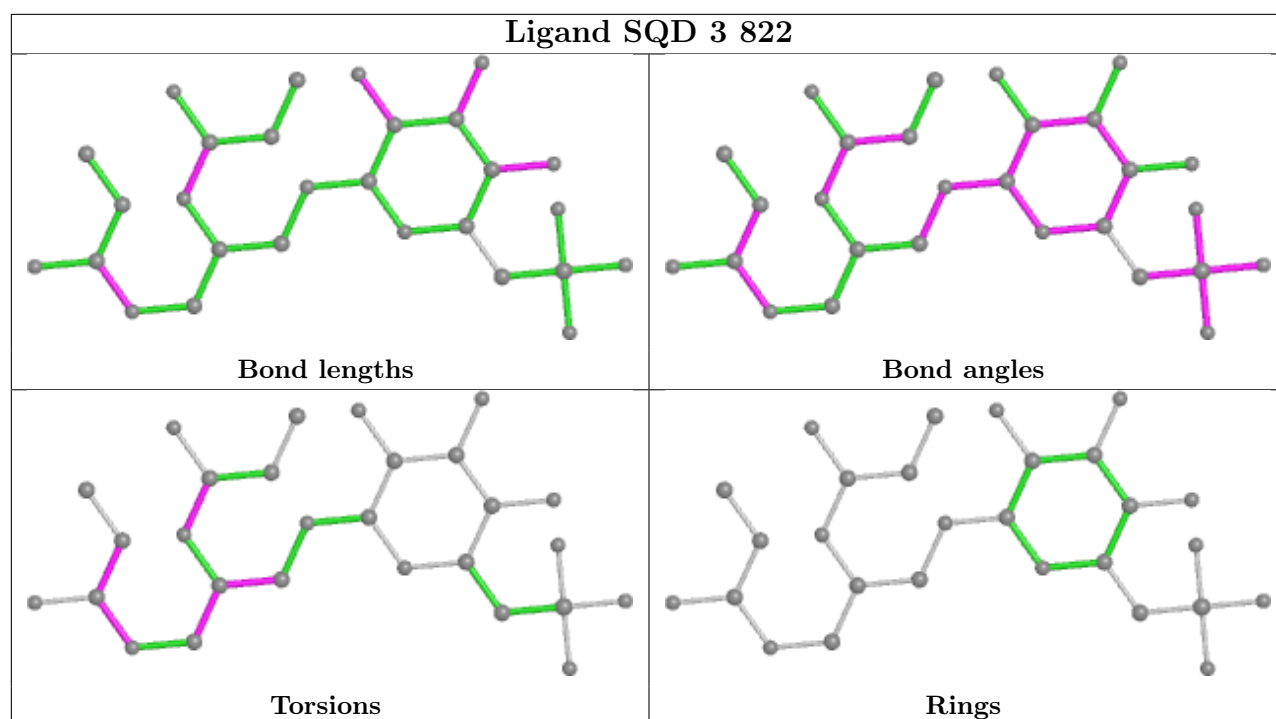


Ligand CLA Y 518

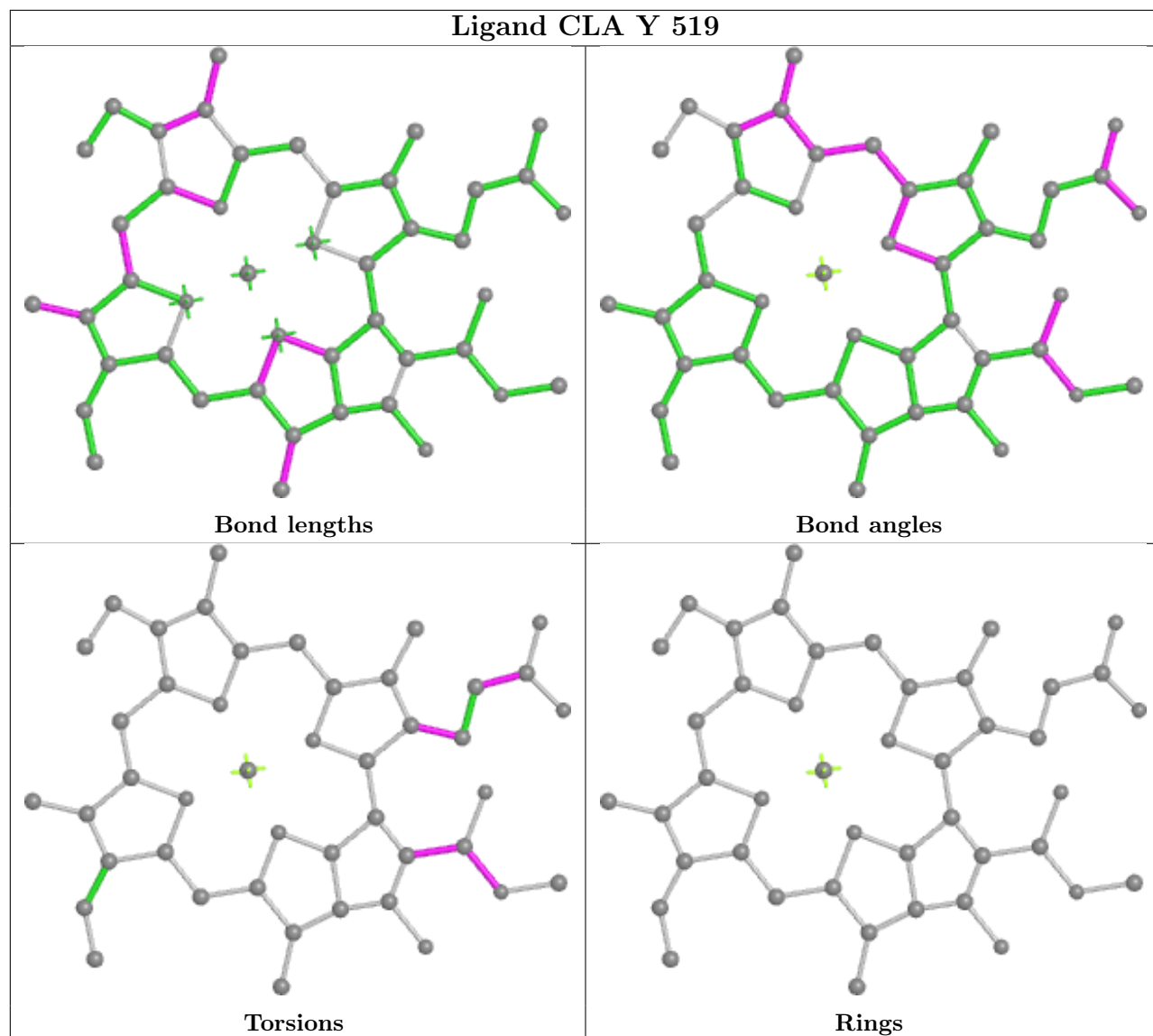




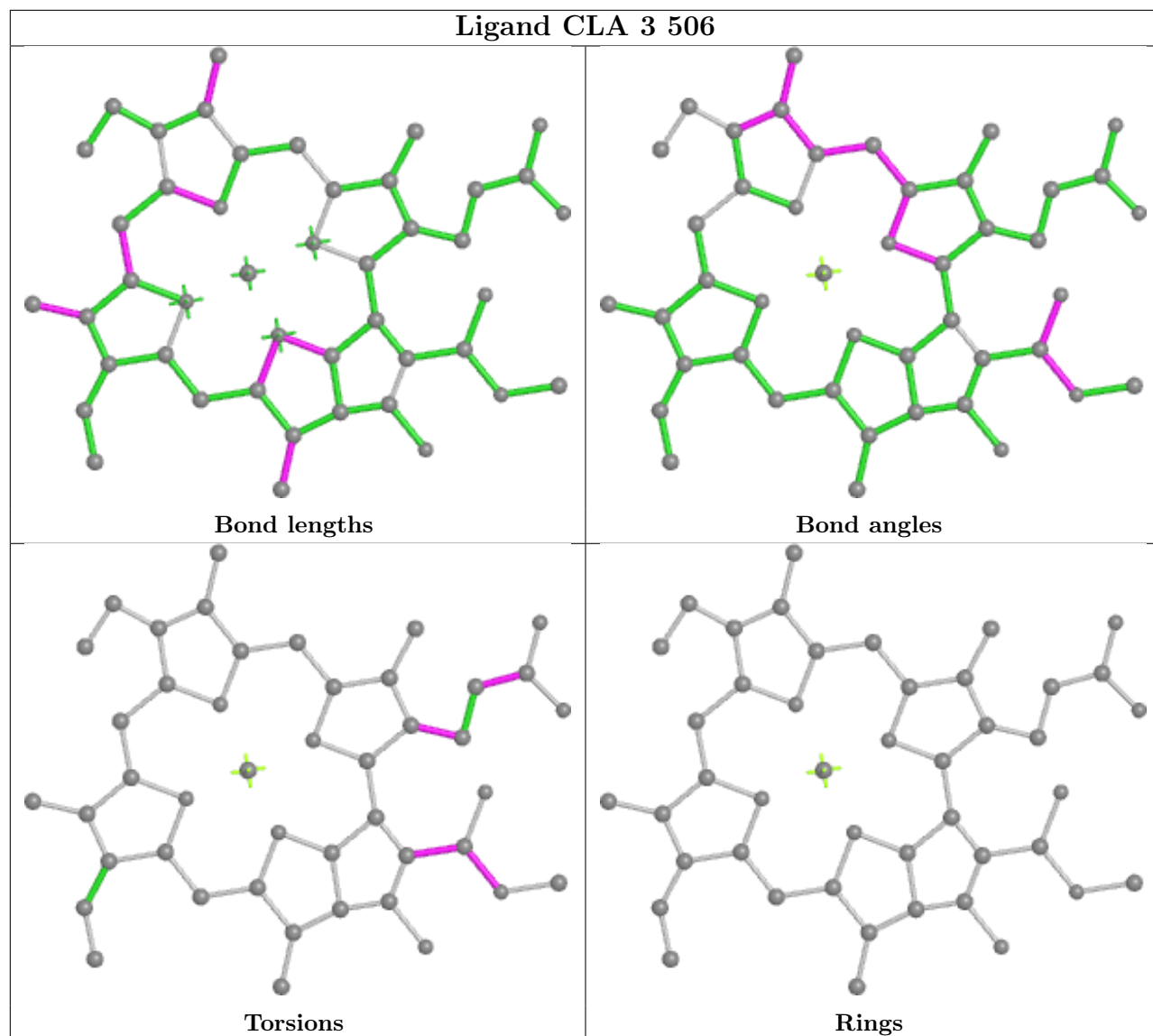


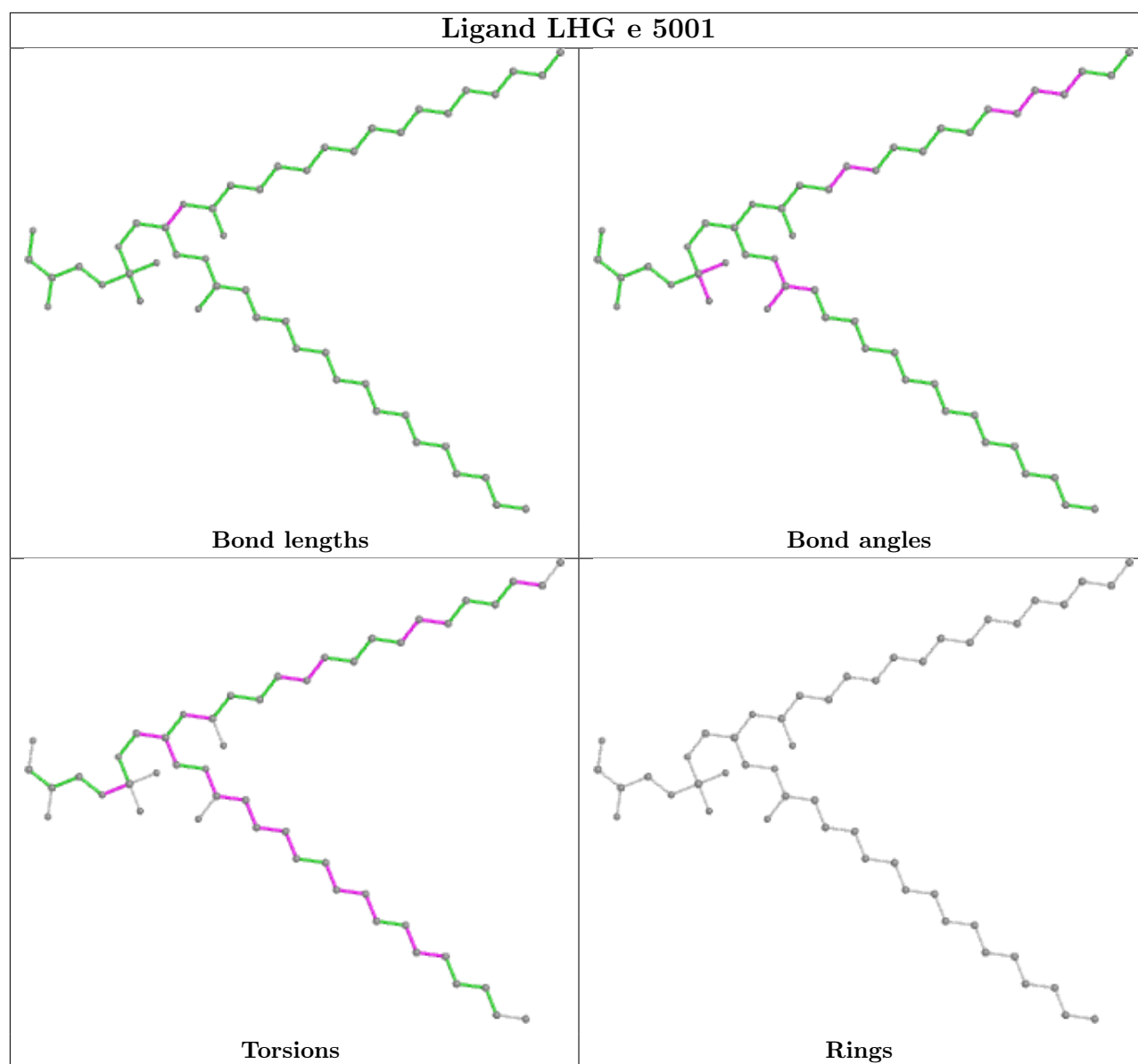


Ligand CLA Y 519

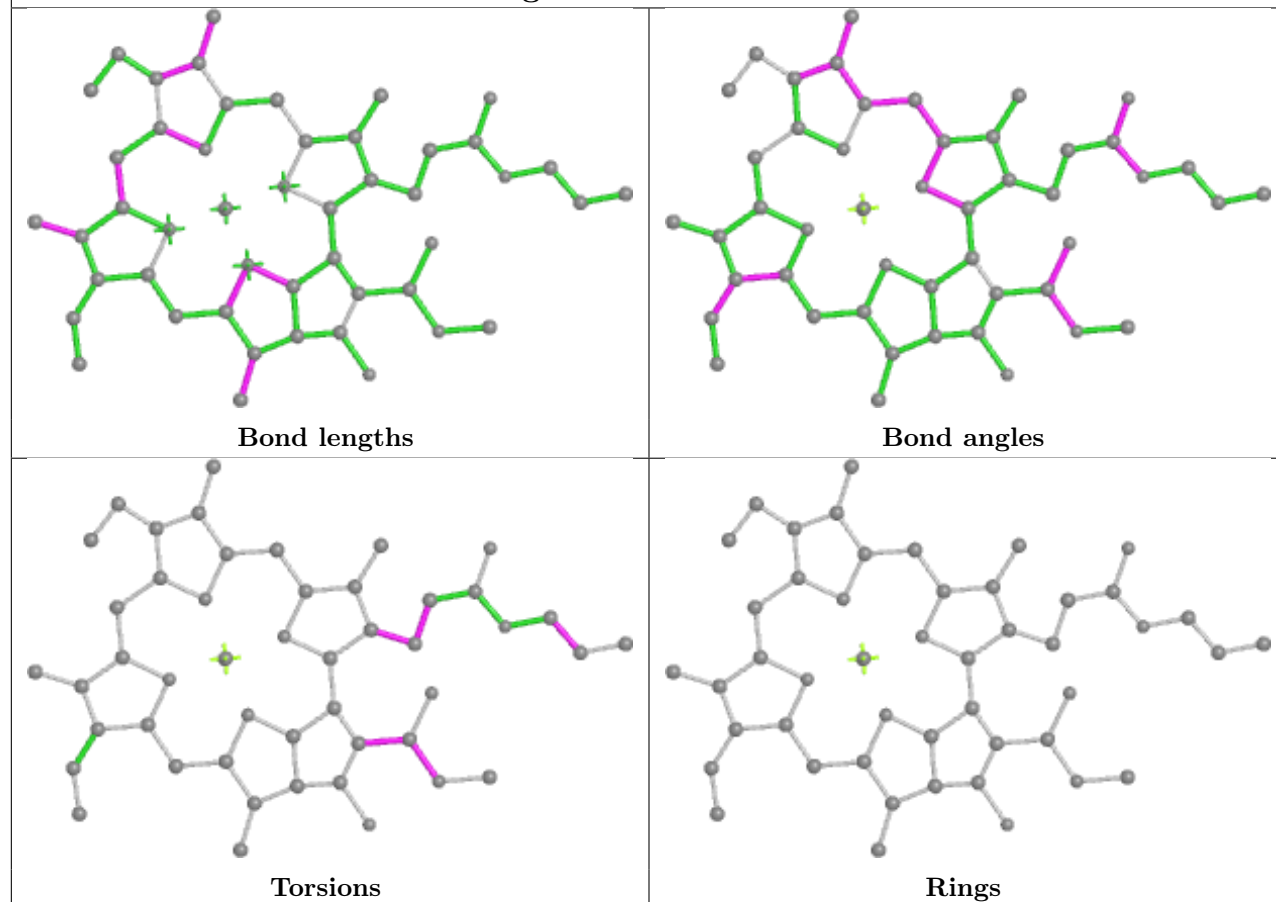


Ligand CLA 3 506

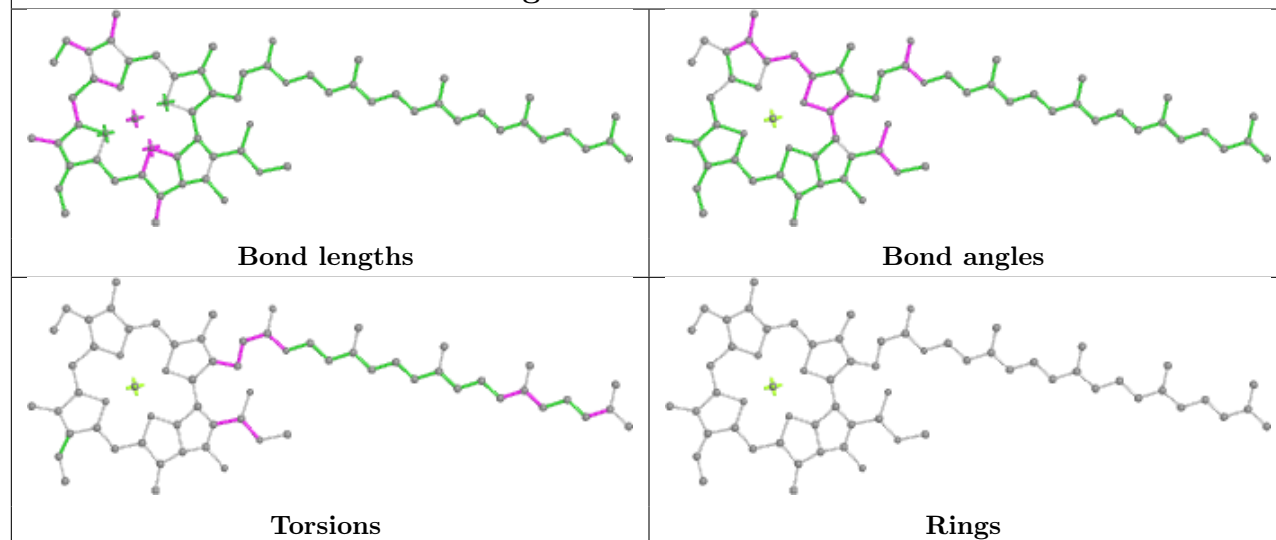


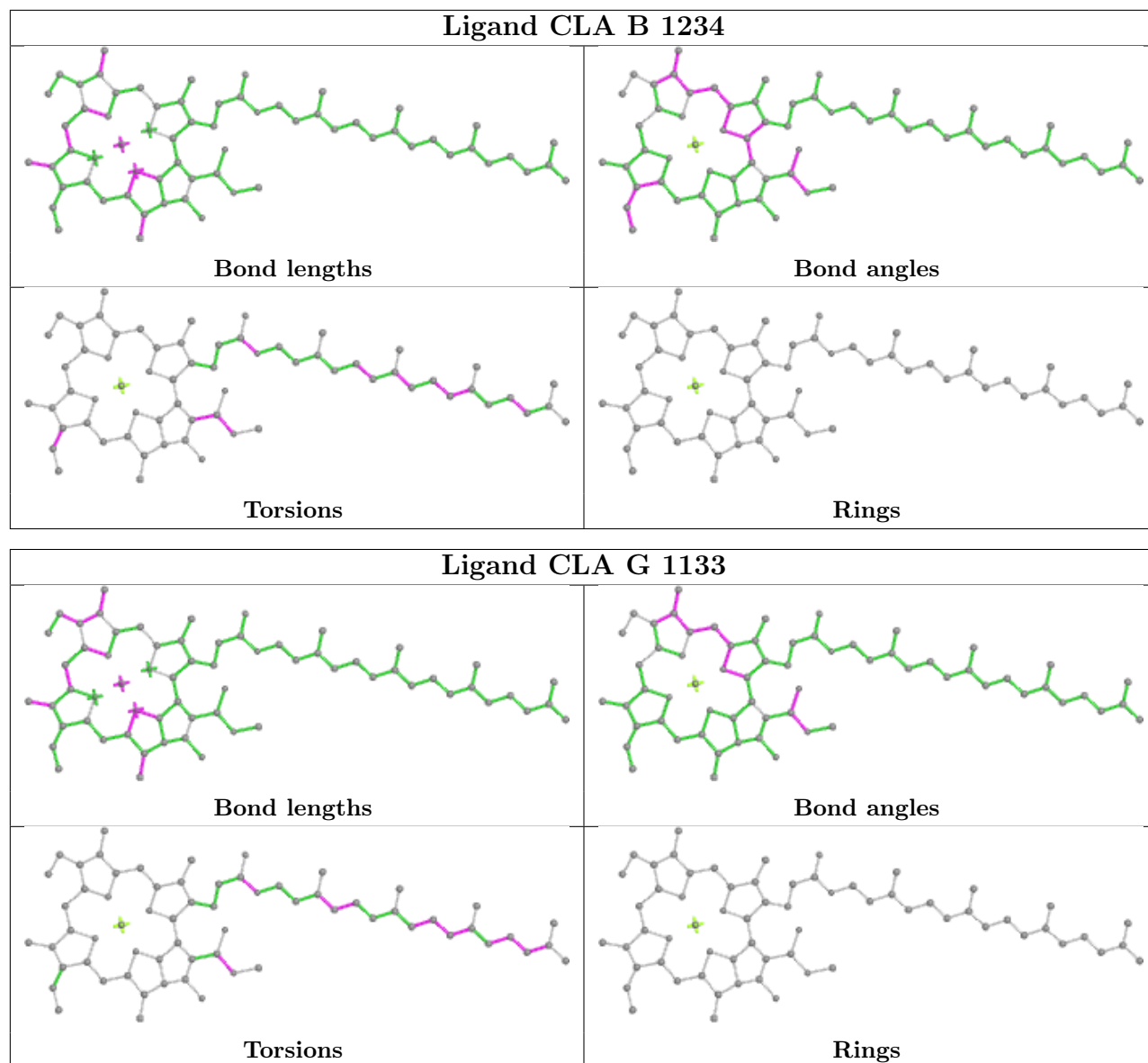


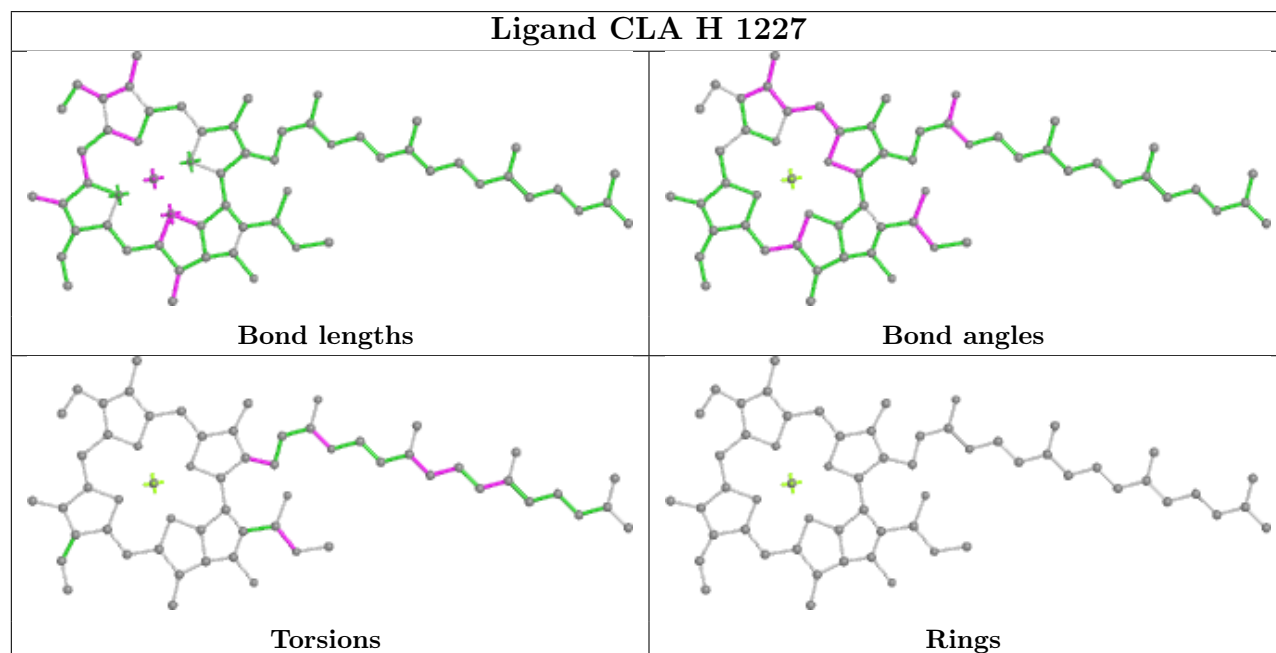
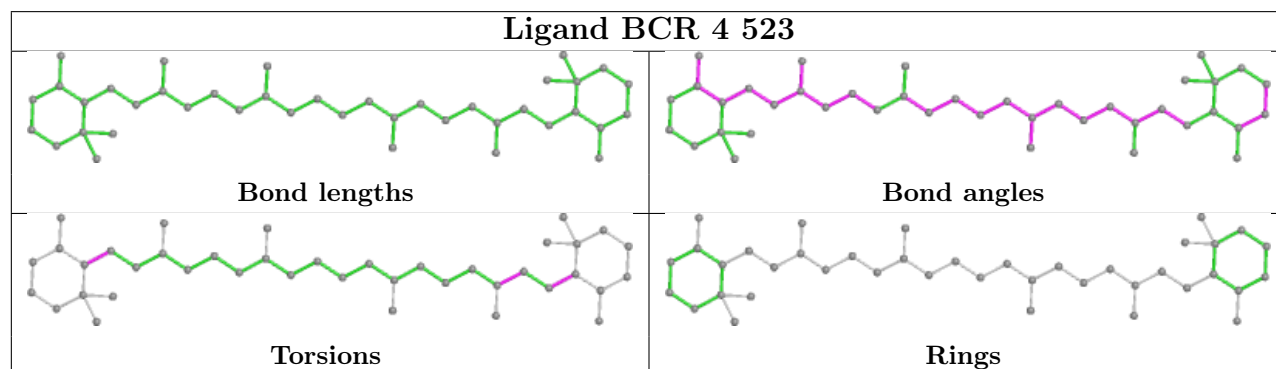
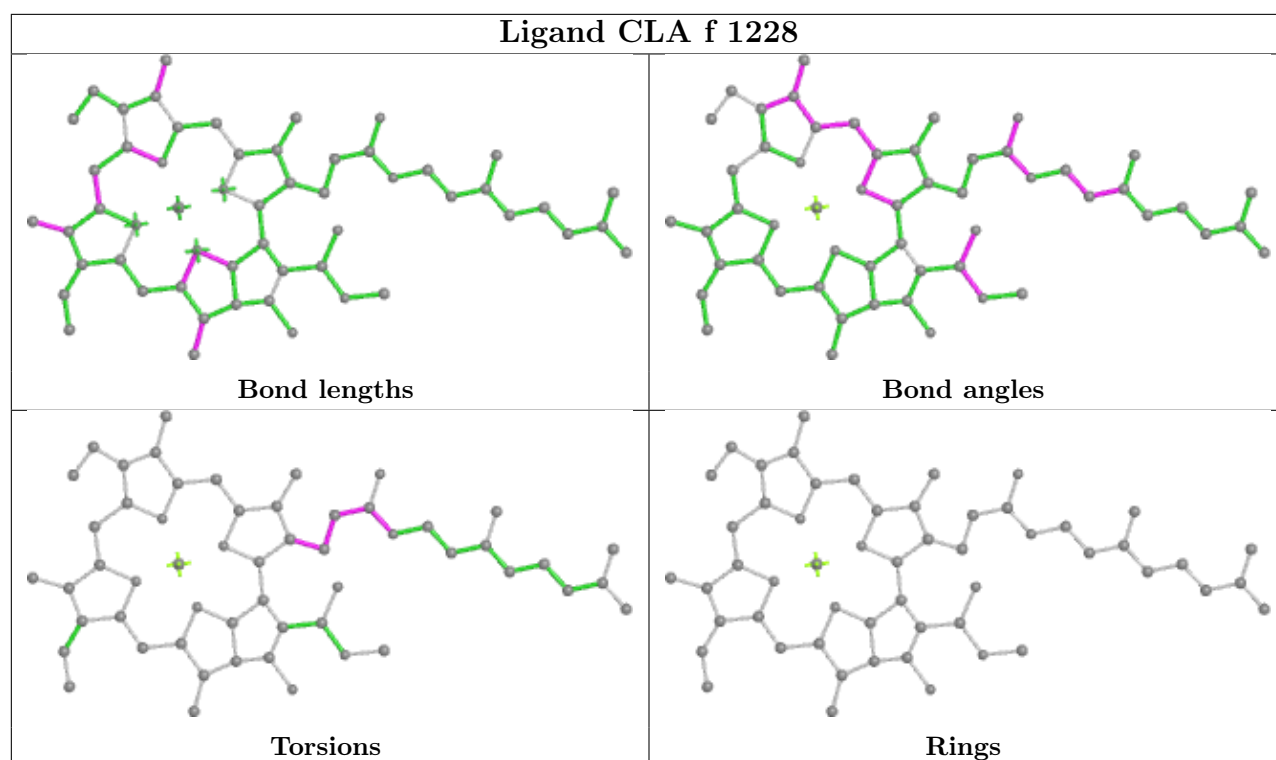
Ligand CLA U 1103



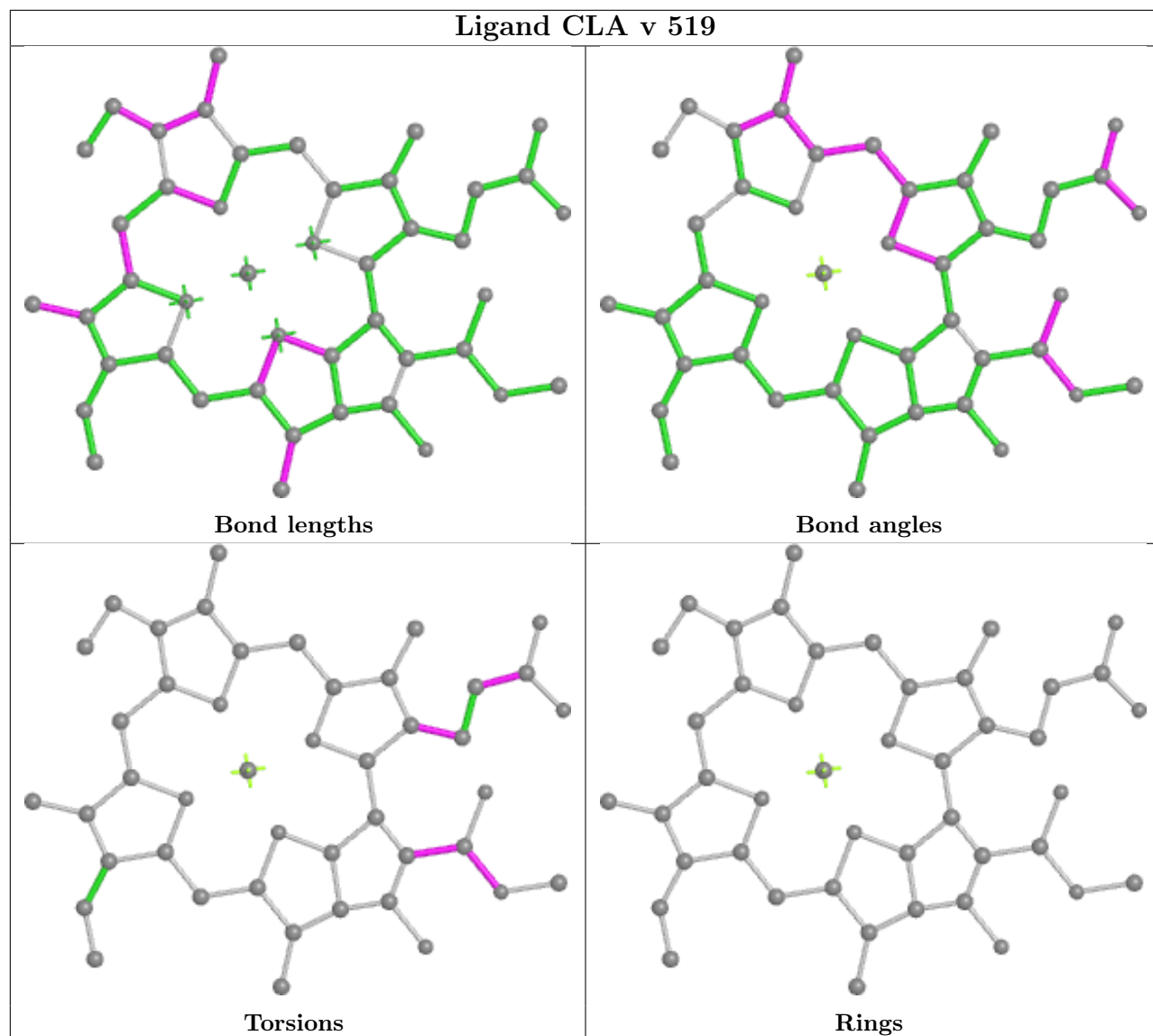
Ligand CLA A 1111



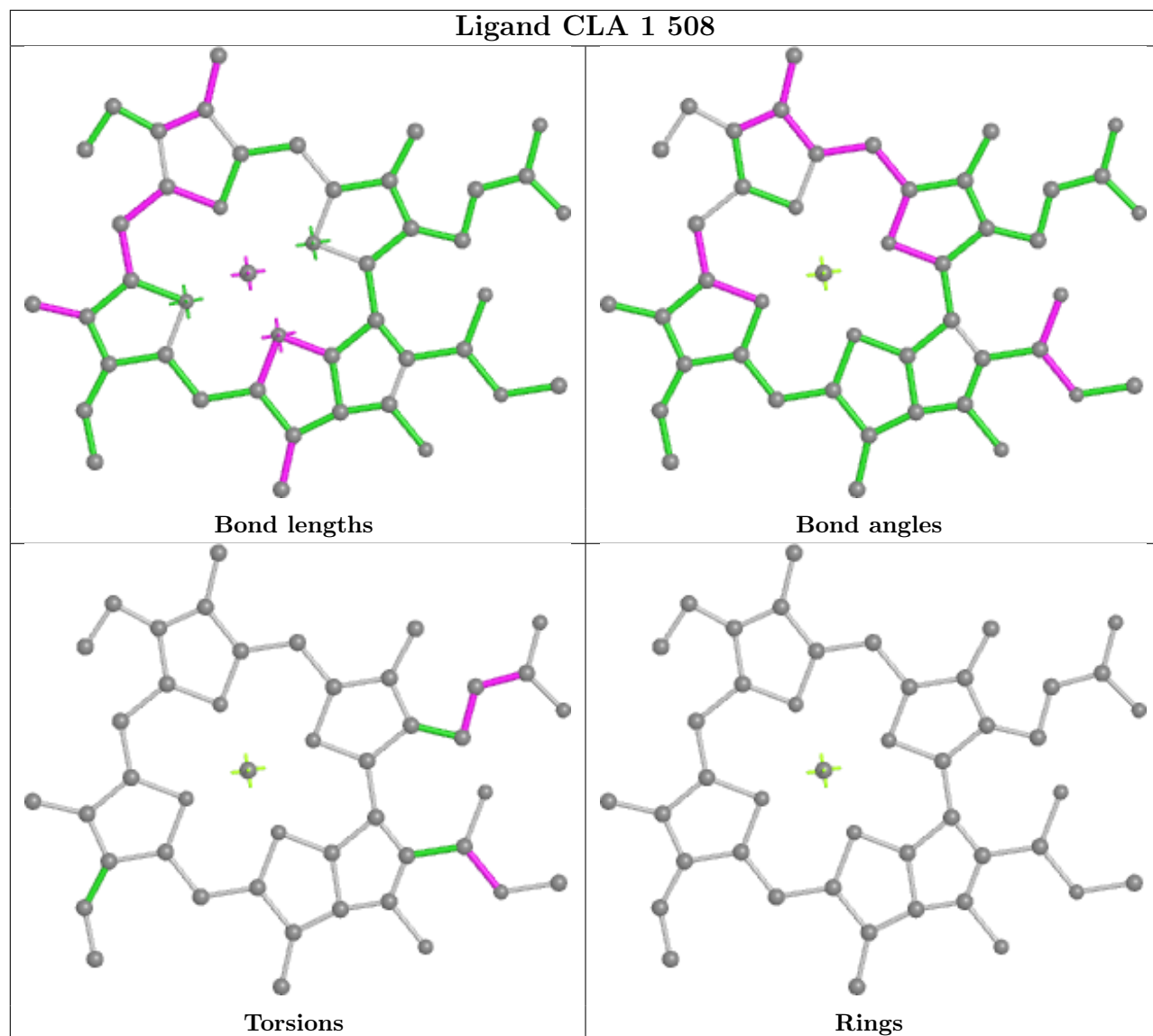




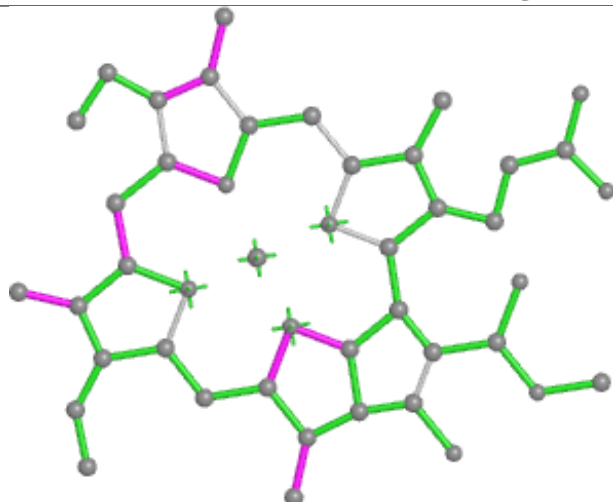
Ligand CLA v 519



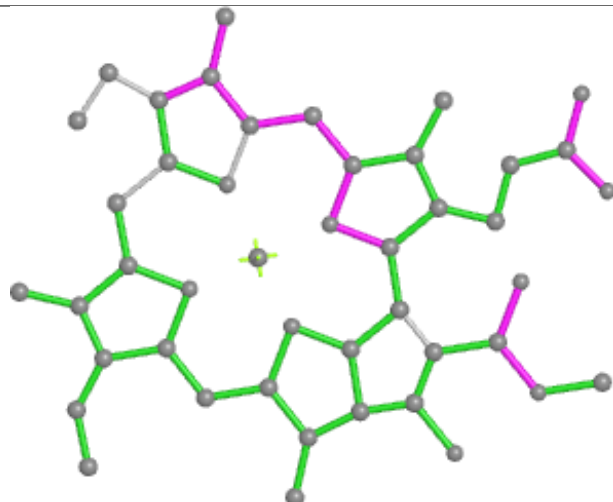
Ligand CLA 1 508



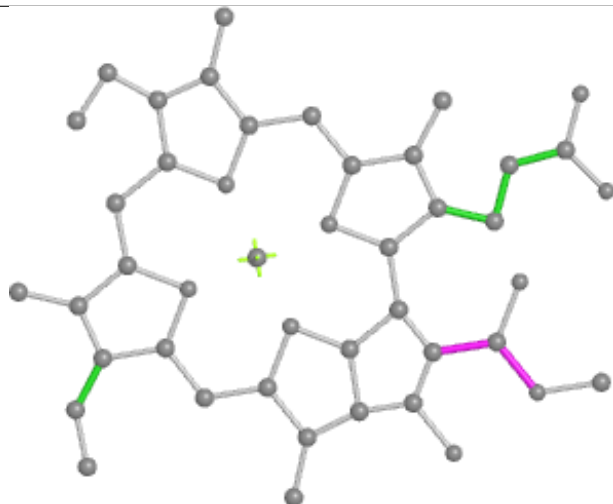
Ligand CLA Z 506



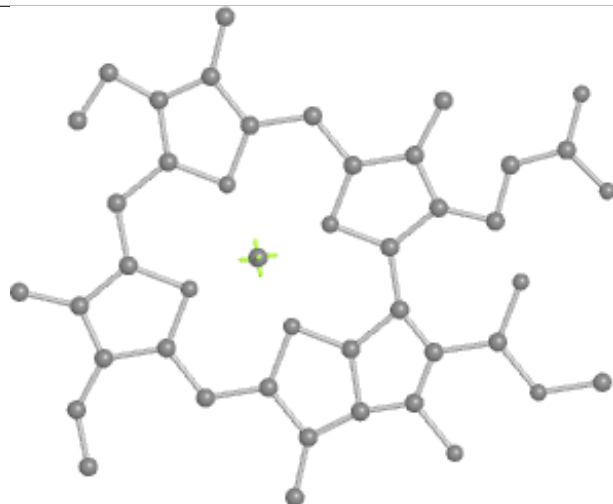
Bond lengths



Bond angles

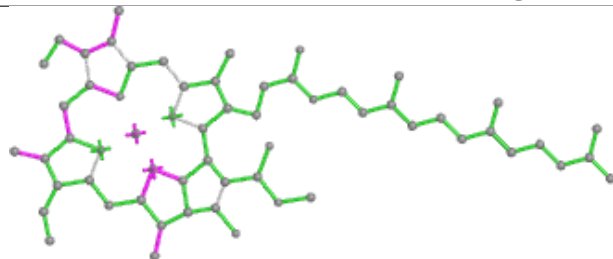


Torsions

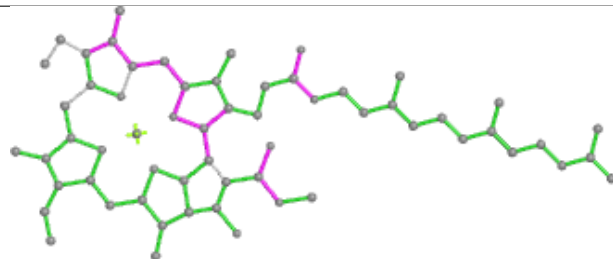


Rings

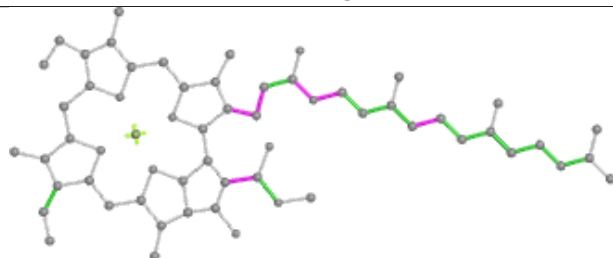
Ligand CLA e 1118



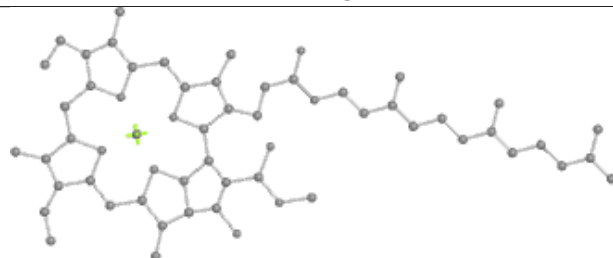
Bond lengths



Bond angles

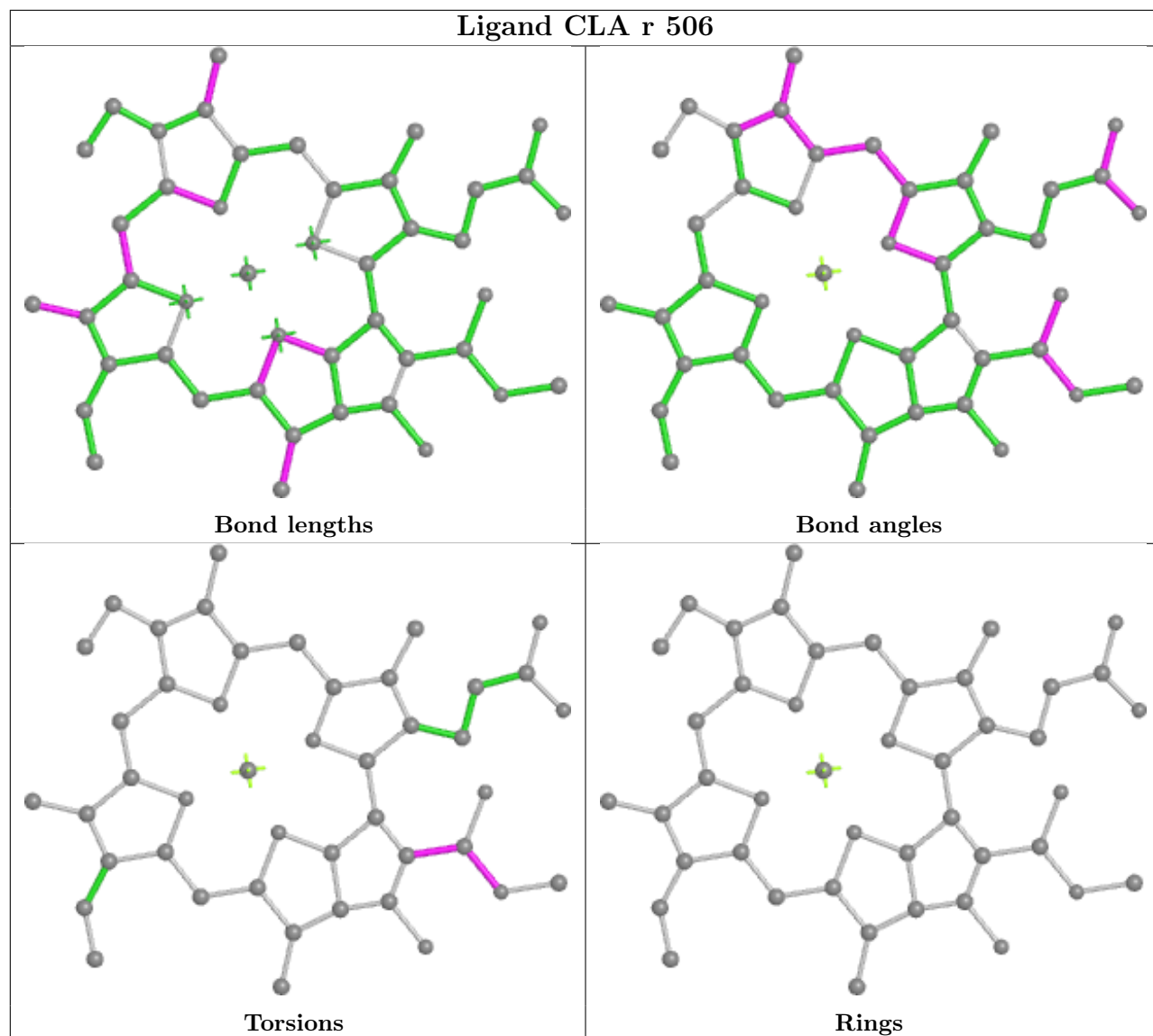


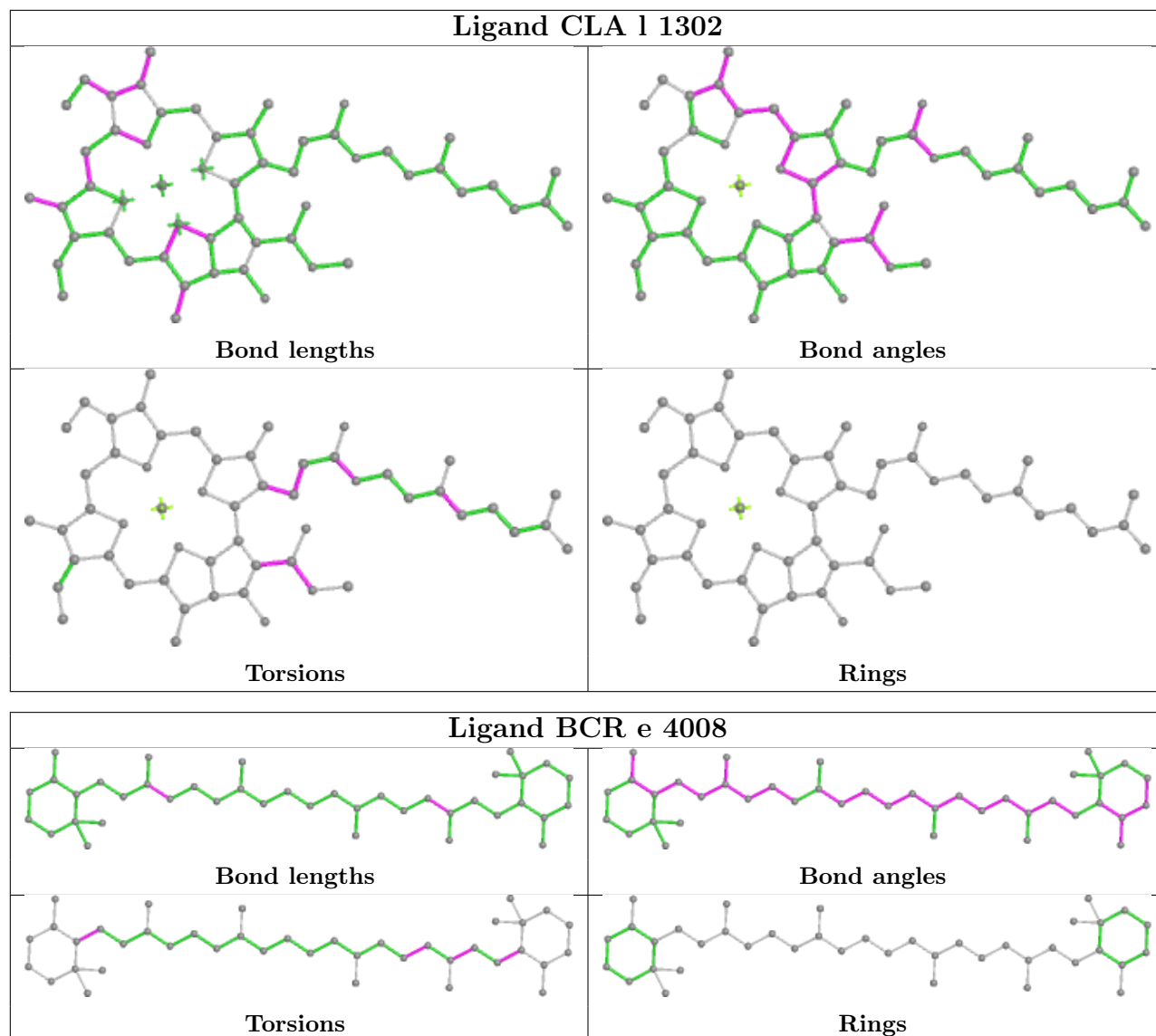
Torsions

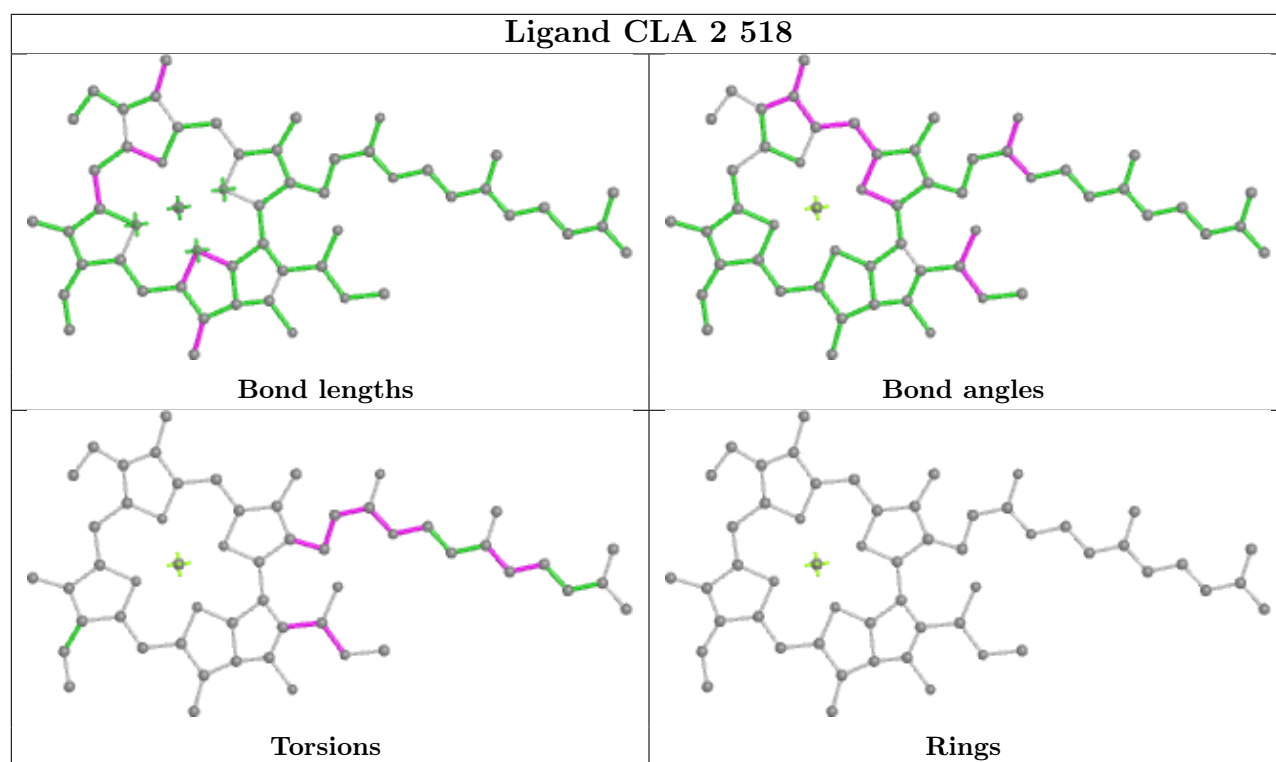


Rings

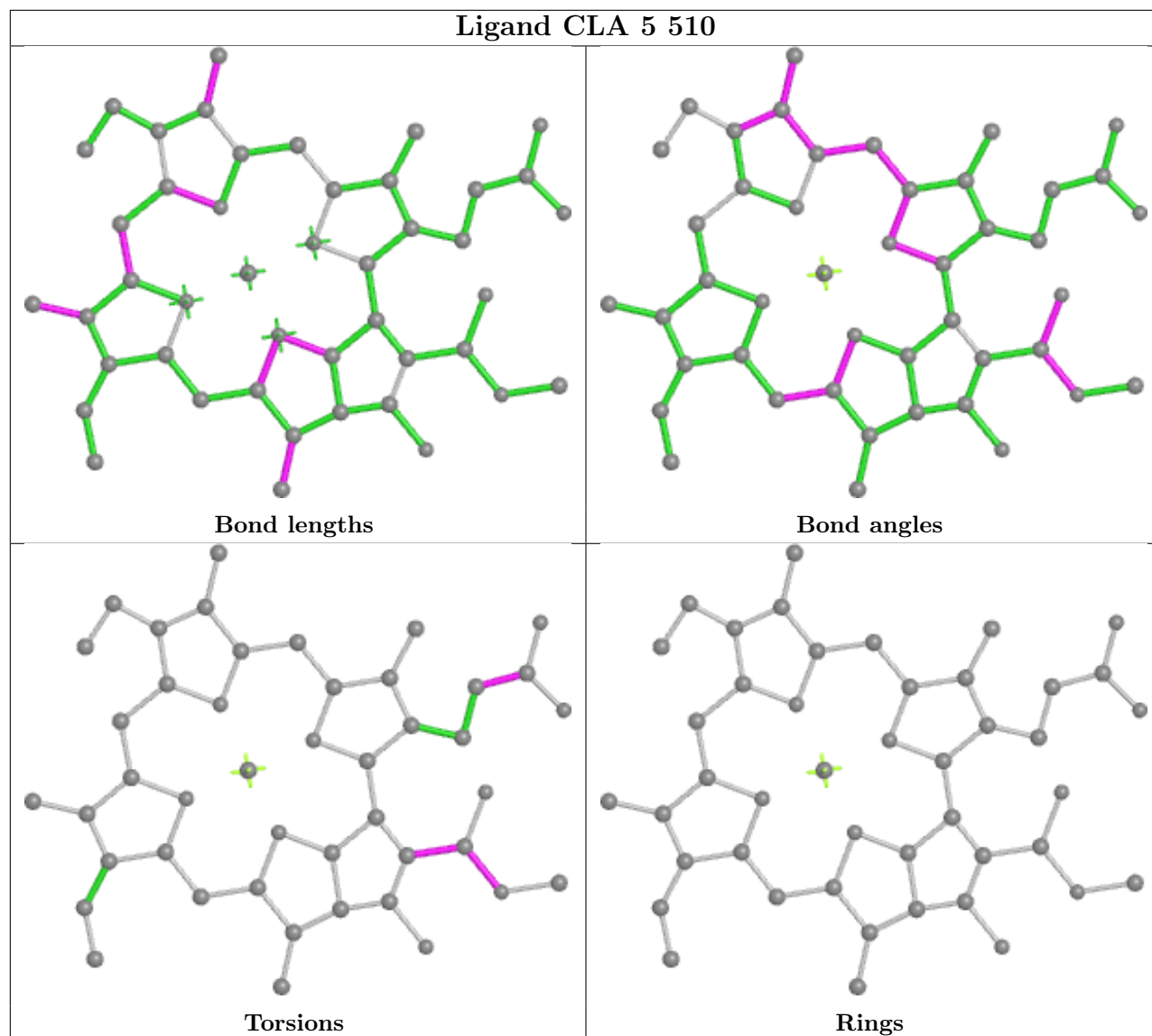
Ligand CLA r 506



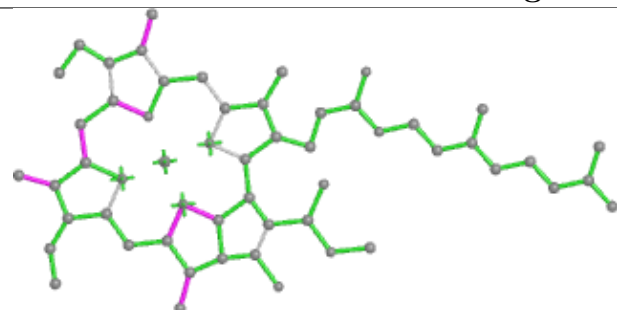




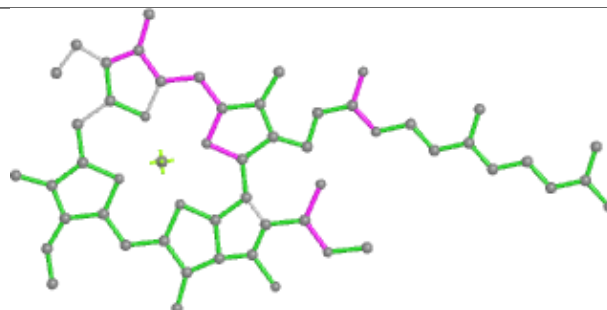
Ligand CLA 5 510



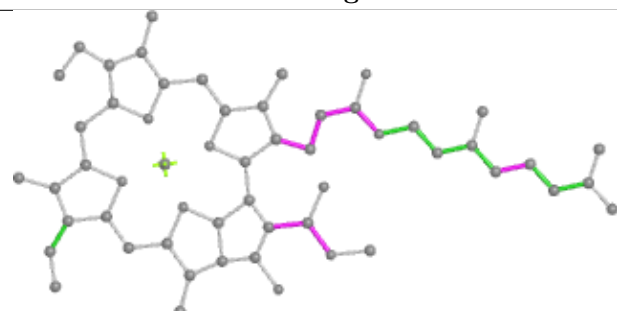
Ligand CLA s 518



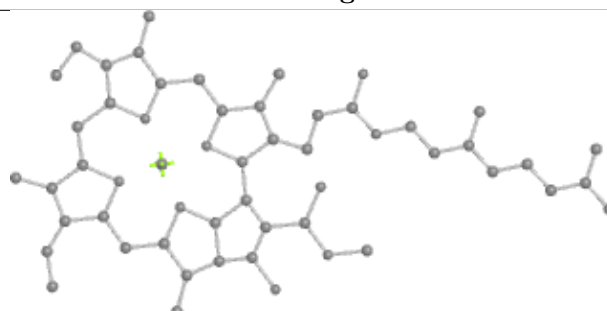
Bond lengths



Bond angles

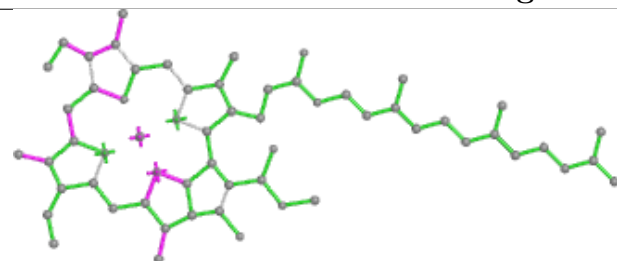


Torsions

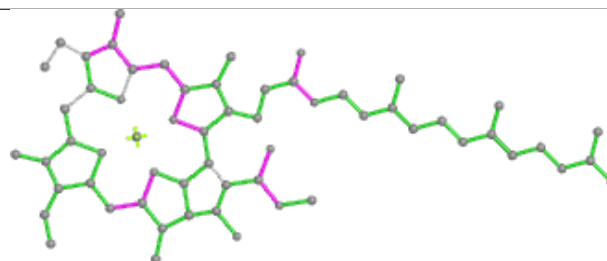


Rings

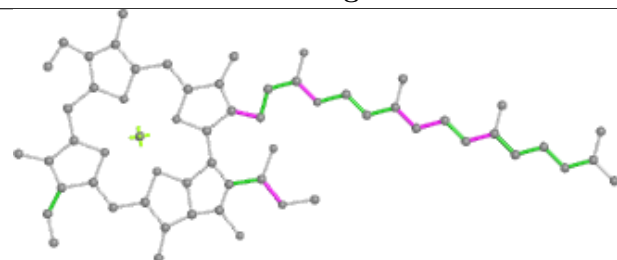
Ligand CLA f 1227



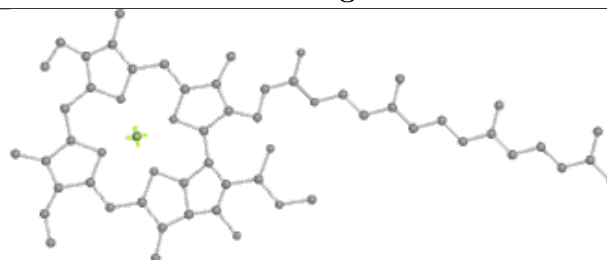
Bond lengths



Bond angles

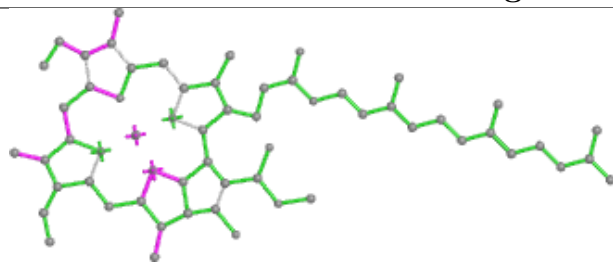


Torsions

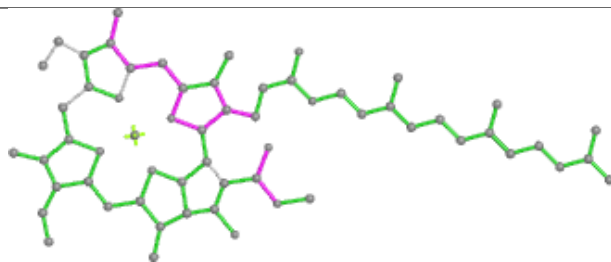


Rings

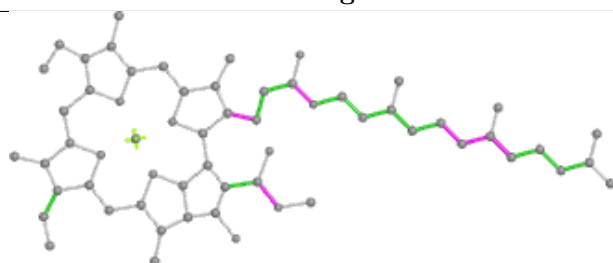
Ligand CLA H 1230



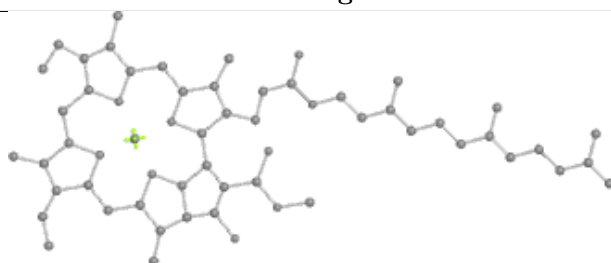
Bond lengths



Bond angles

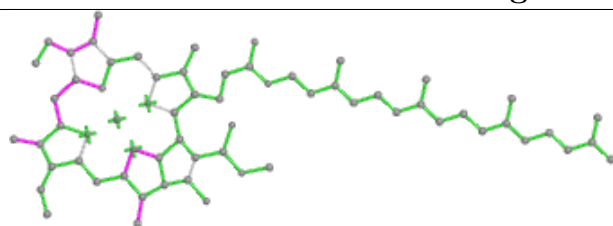


Torsions

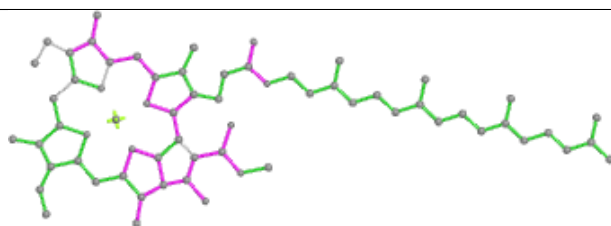


Rings

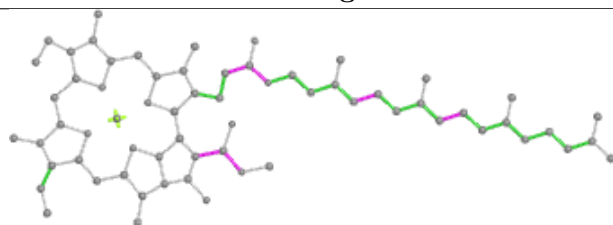
Ligand CLA e 1011



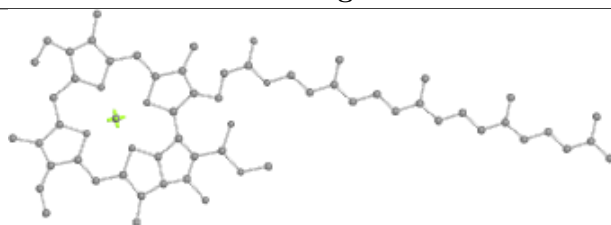
Bond lengths



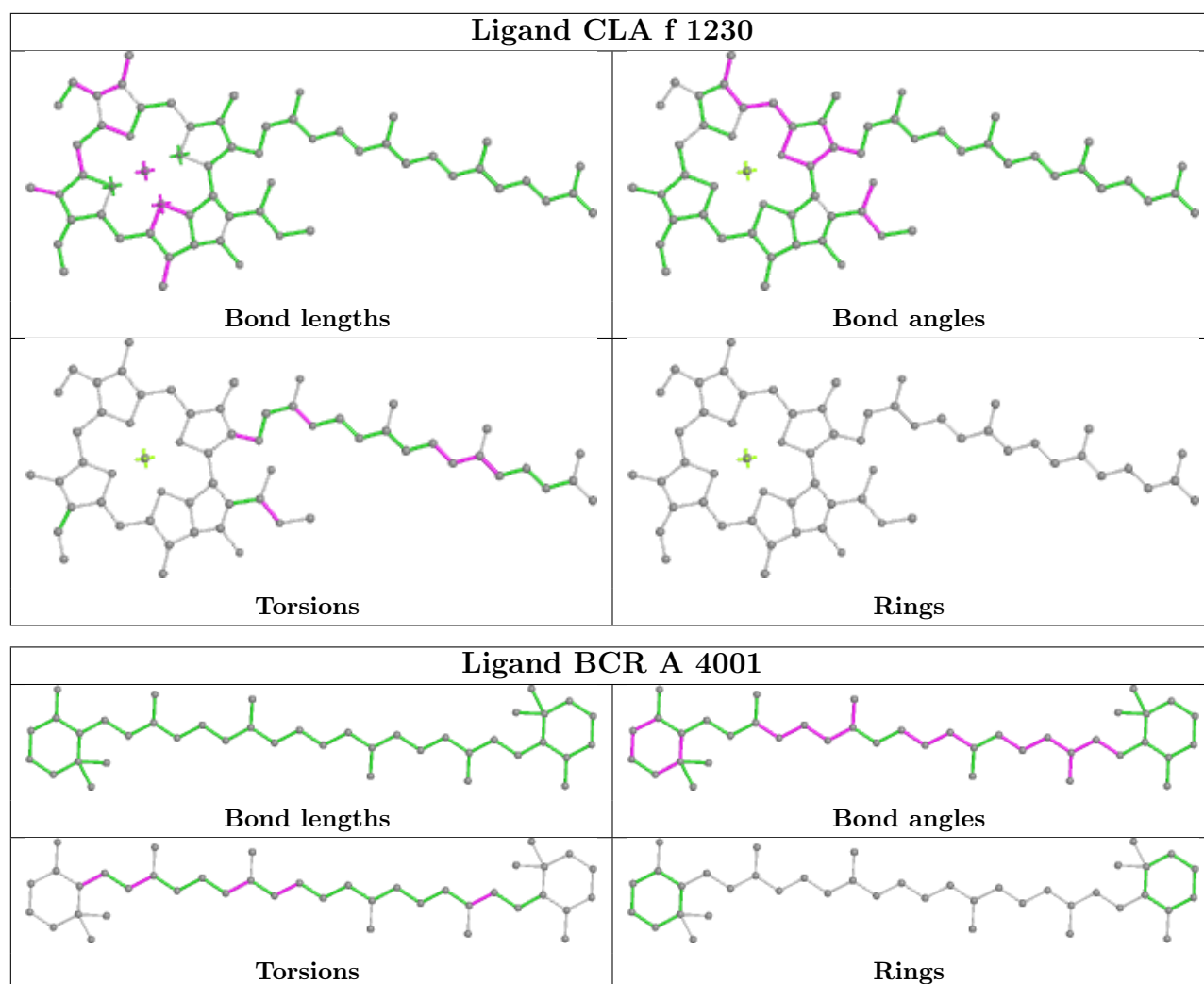
Bond angles



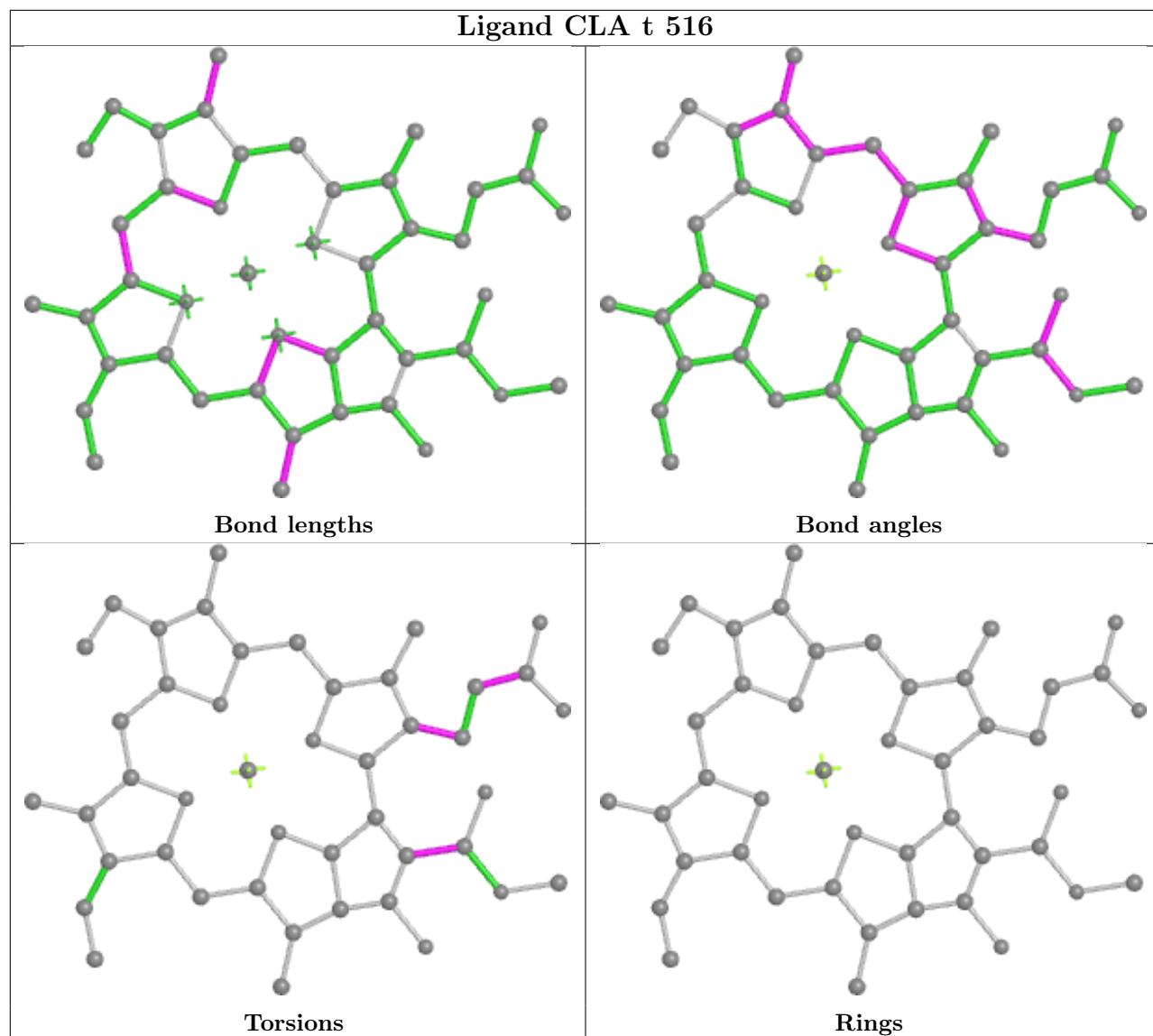
Torsions



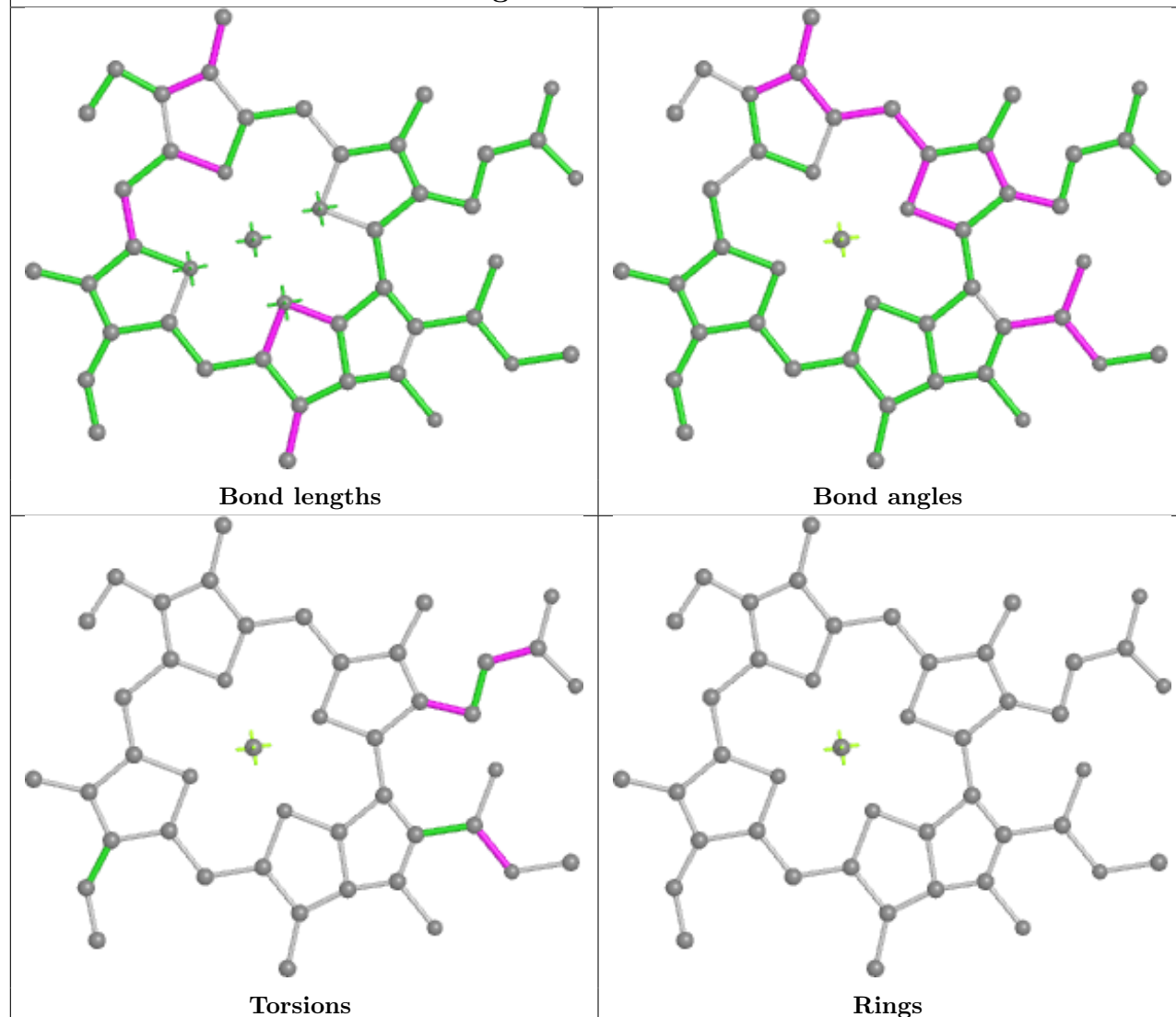
Rings



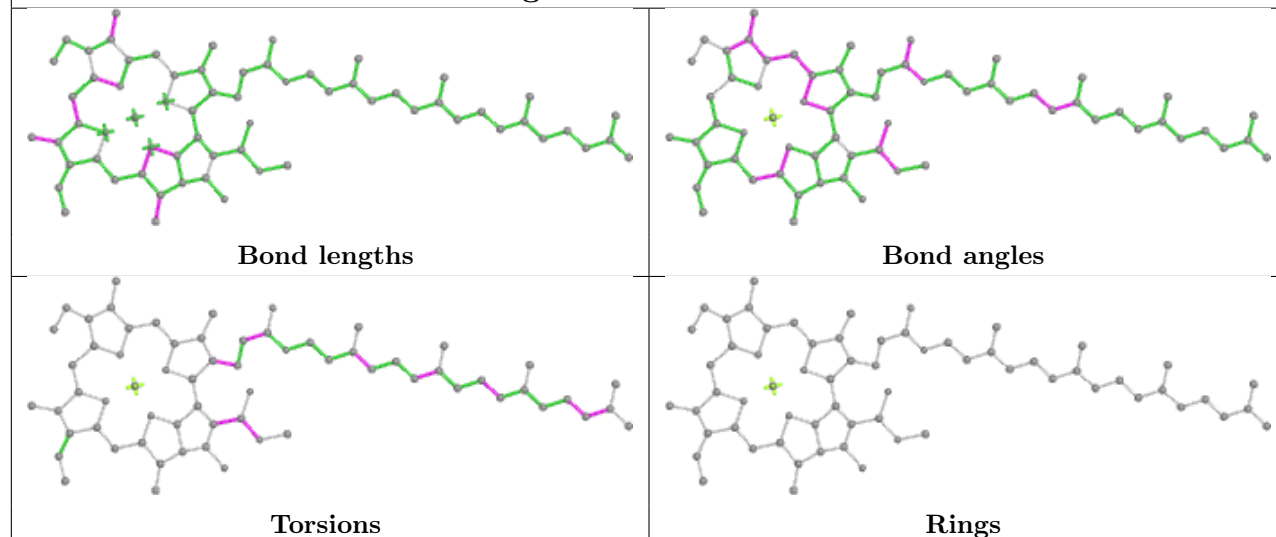
Ligand CLA t 516

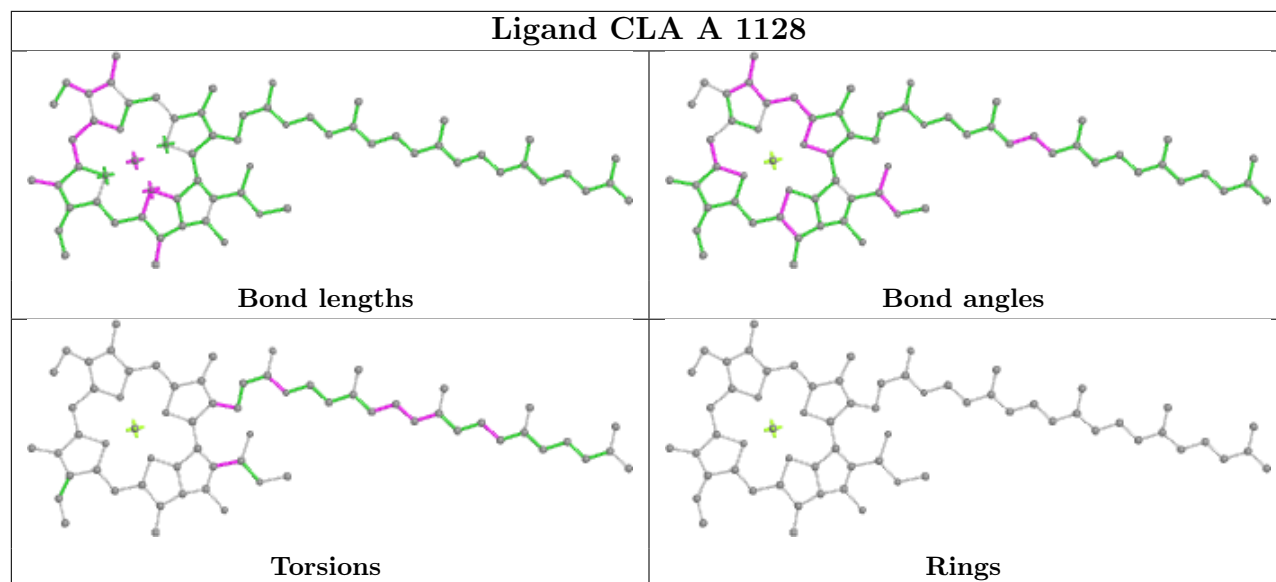
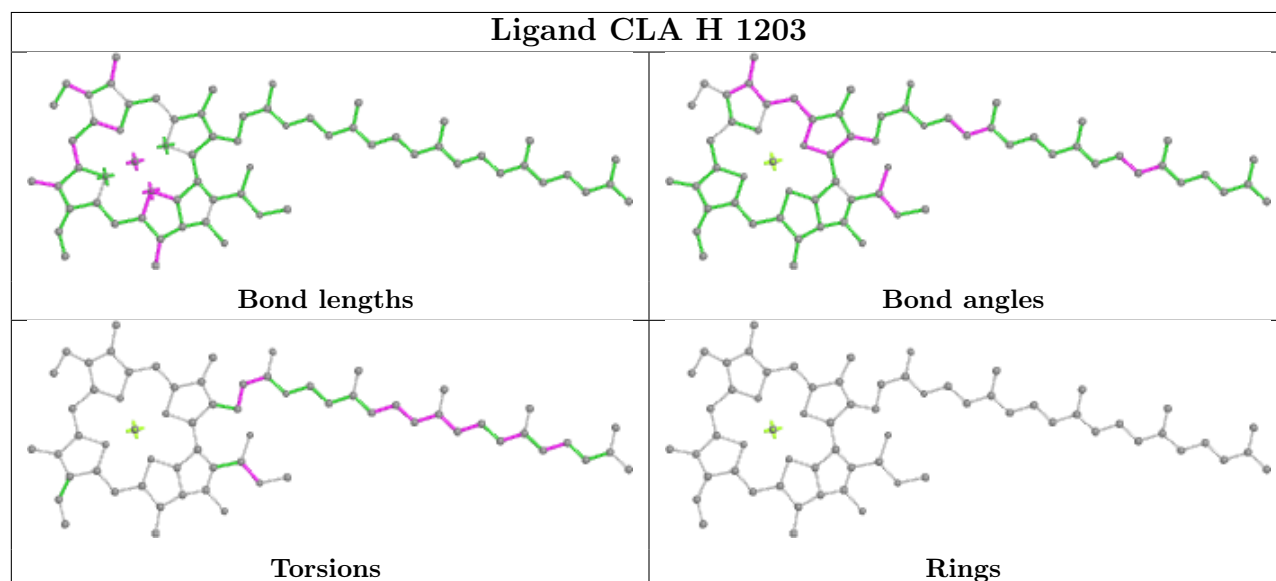


Ligand CLA Z 516

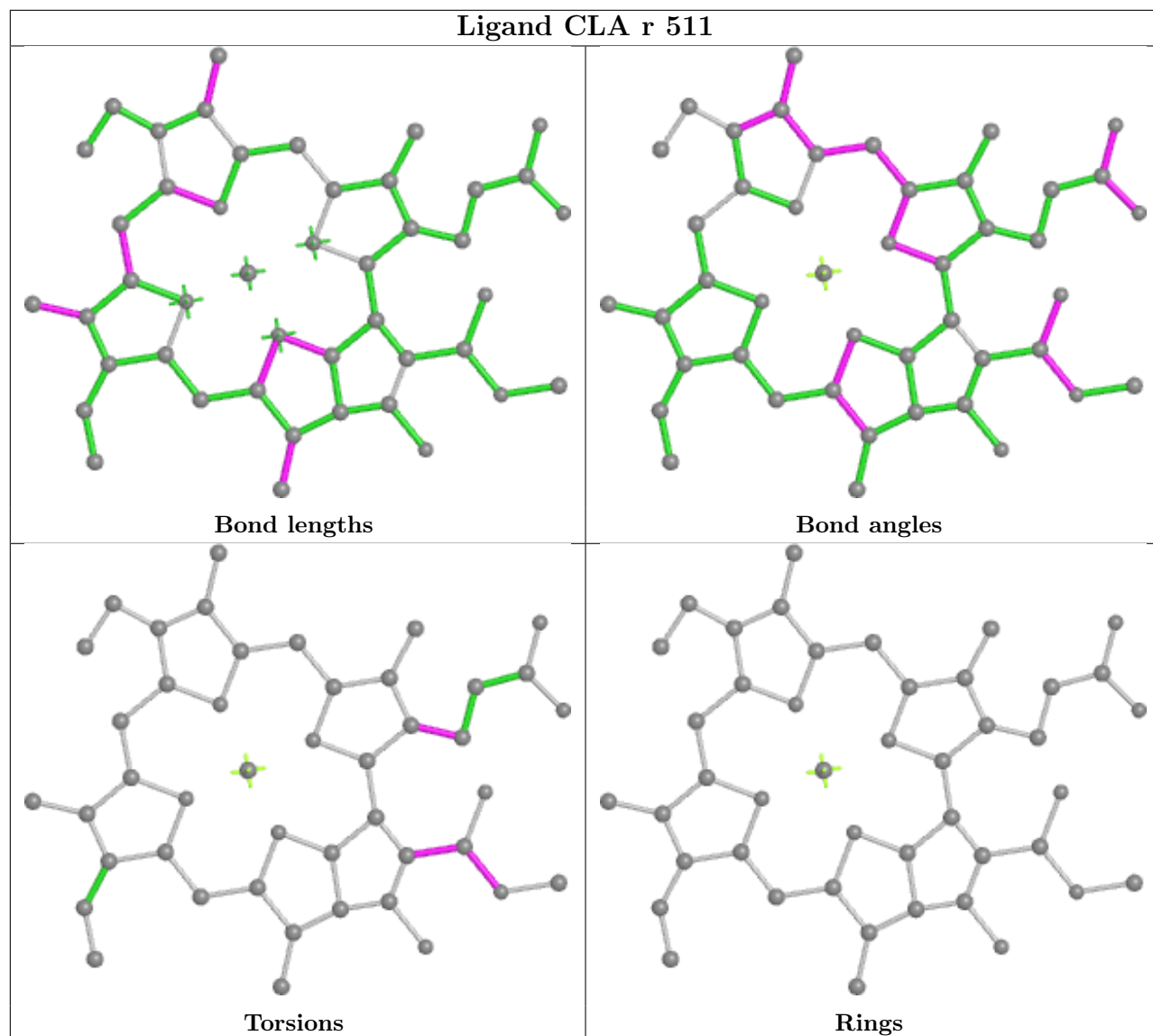


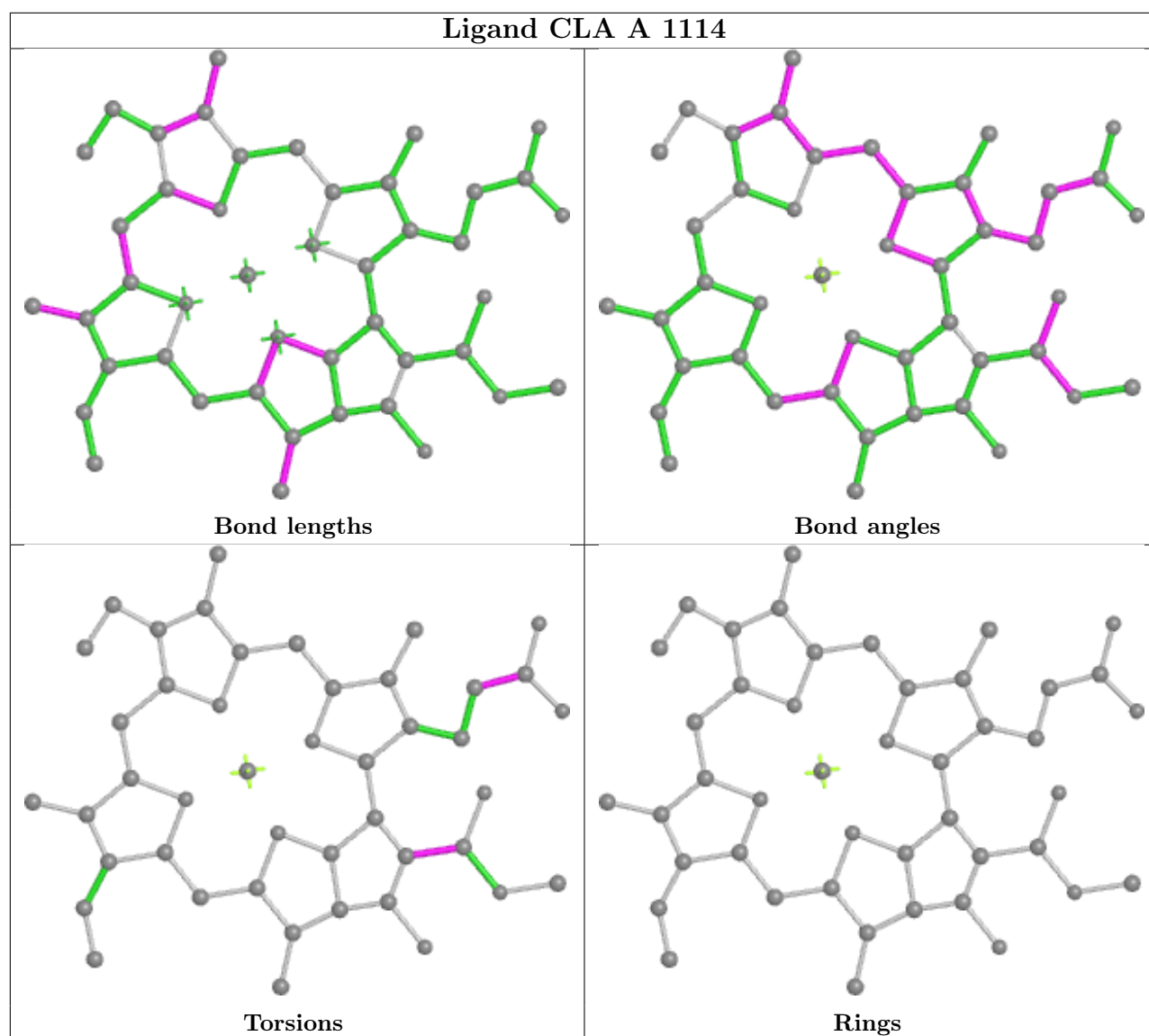
Ligand CLA H 1229



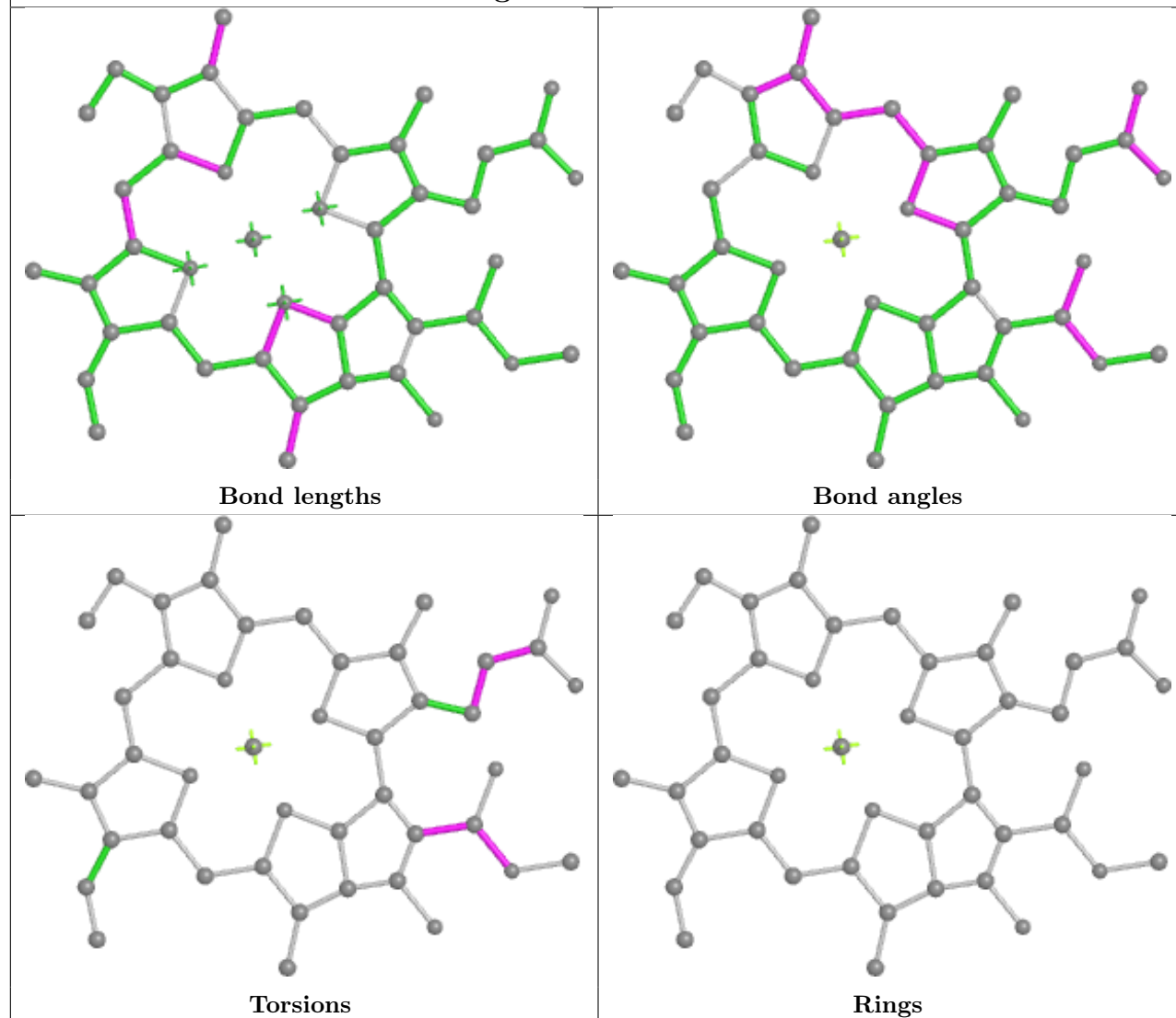
Ligand CLA A 1128**Ligand CLA H 1203**

Ligand CLA r 511

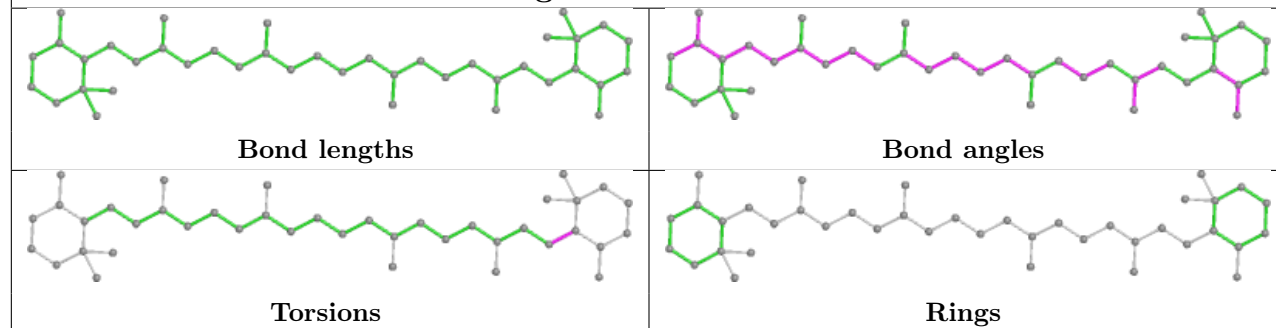


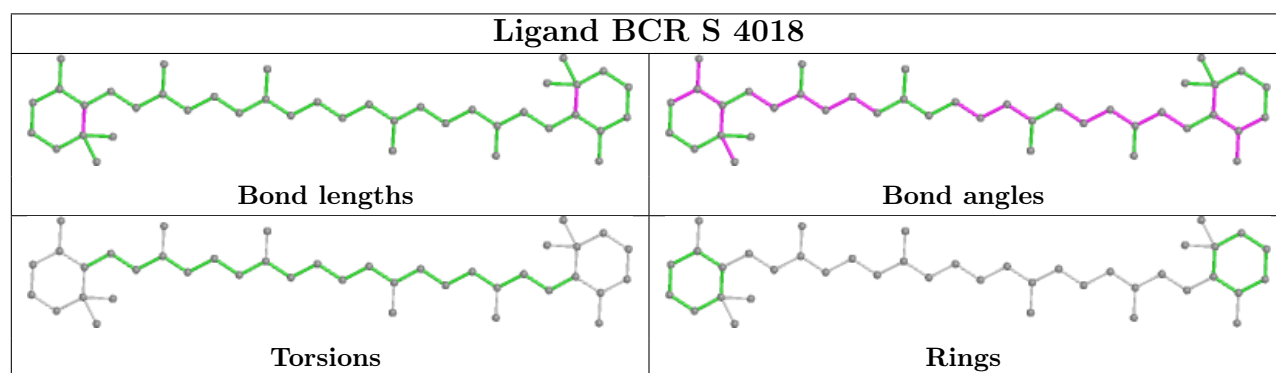
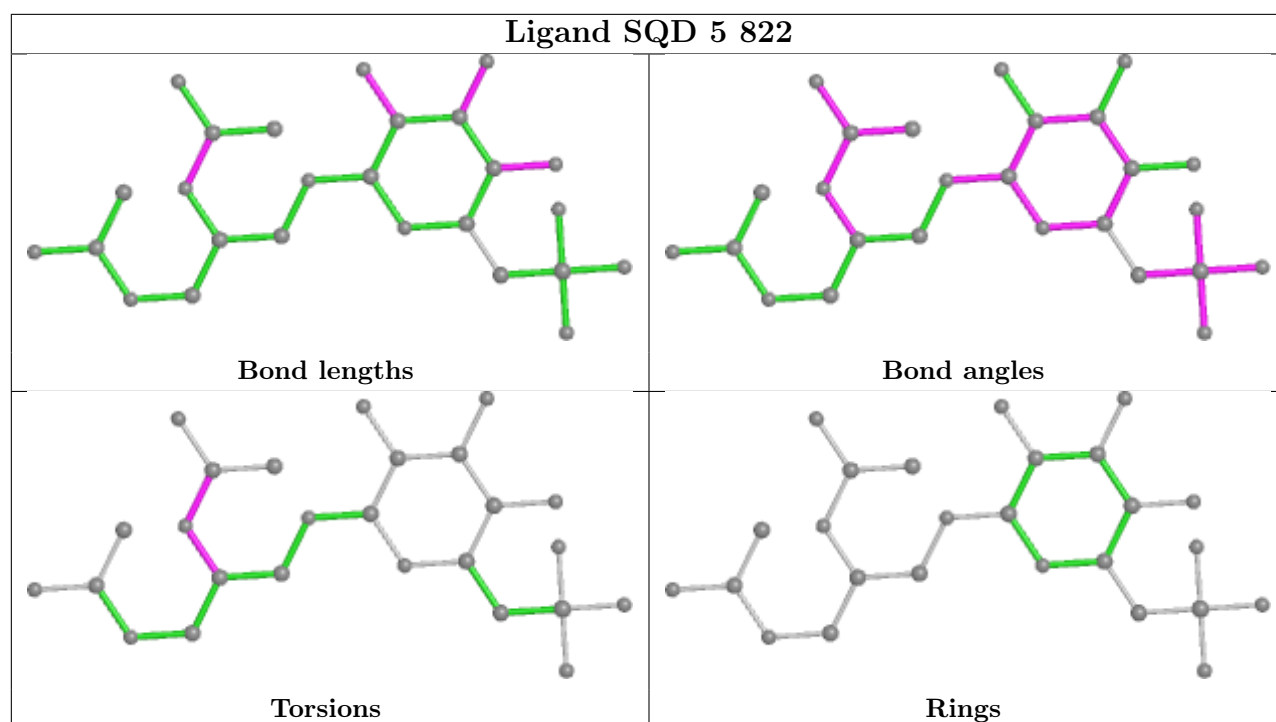


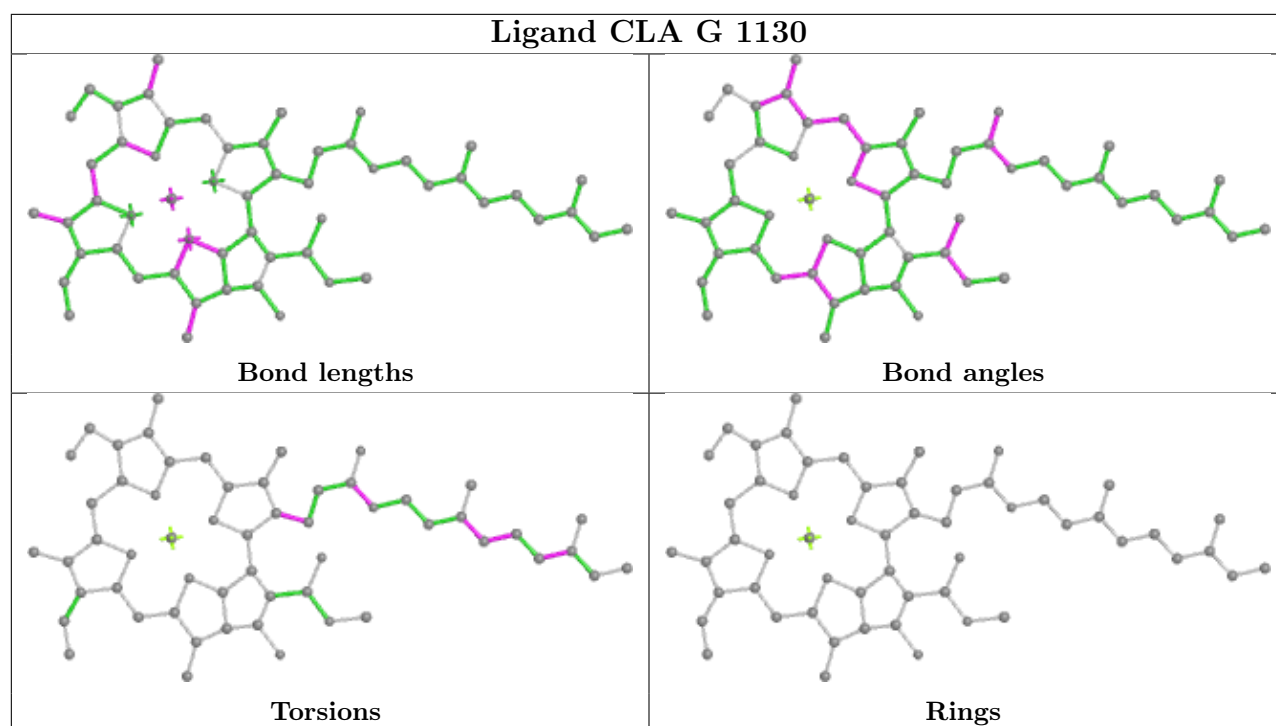
Ligand CLA 1 518



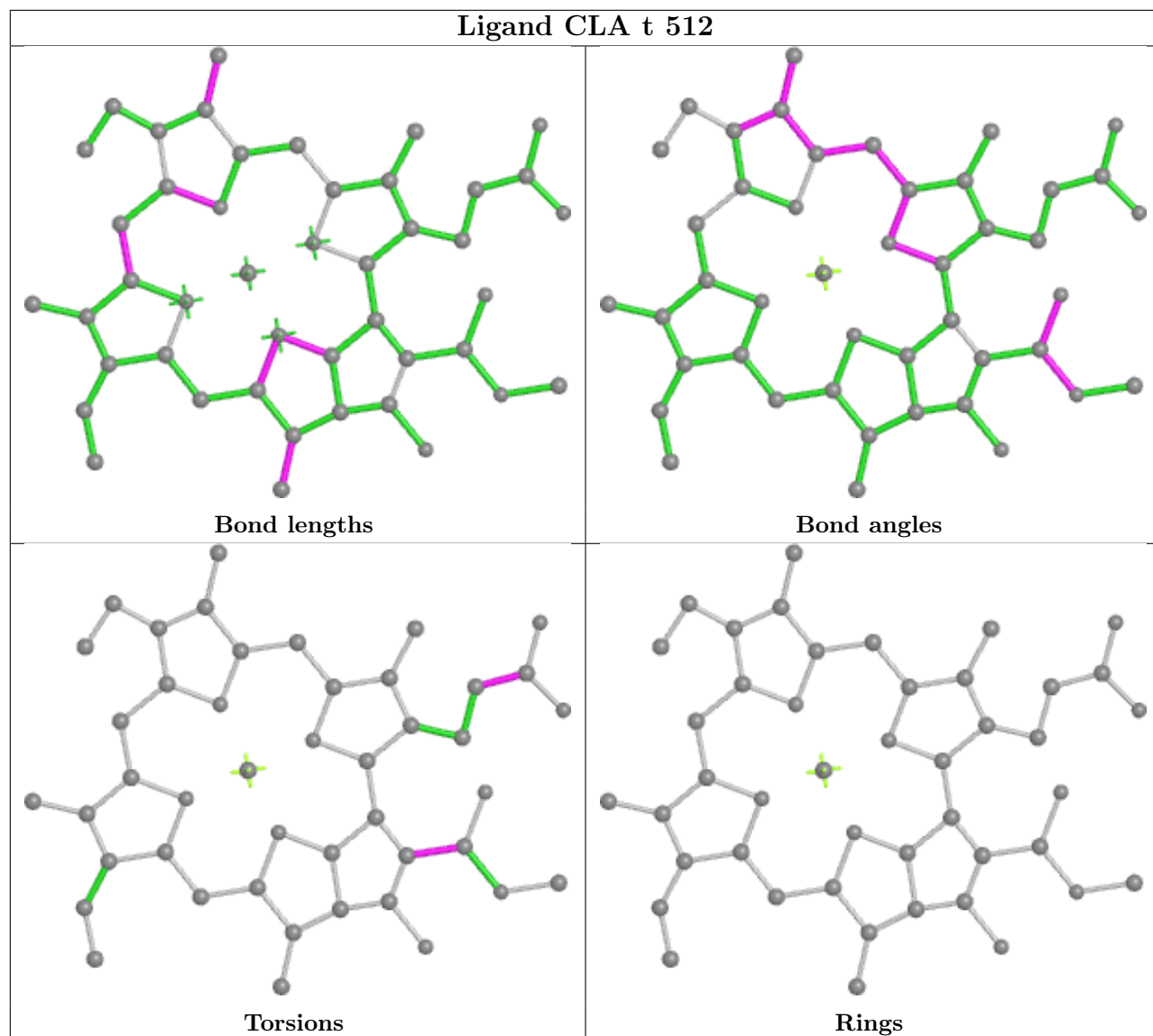
Ligand BCR c 524

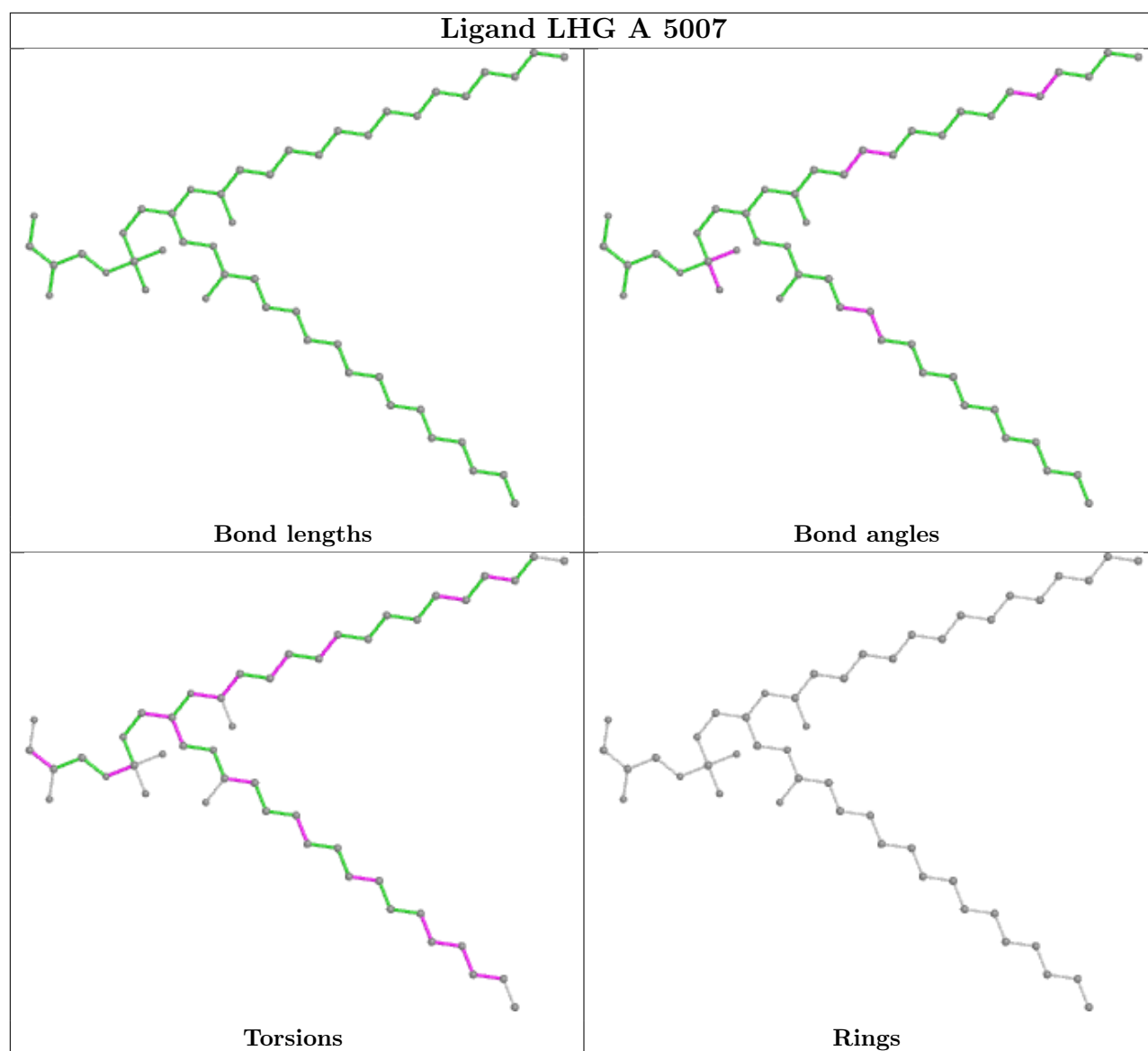




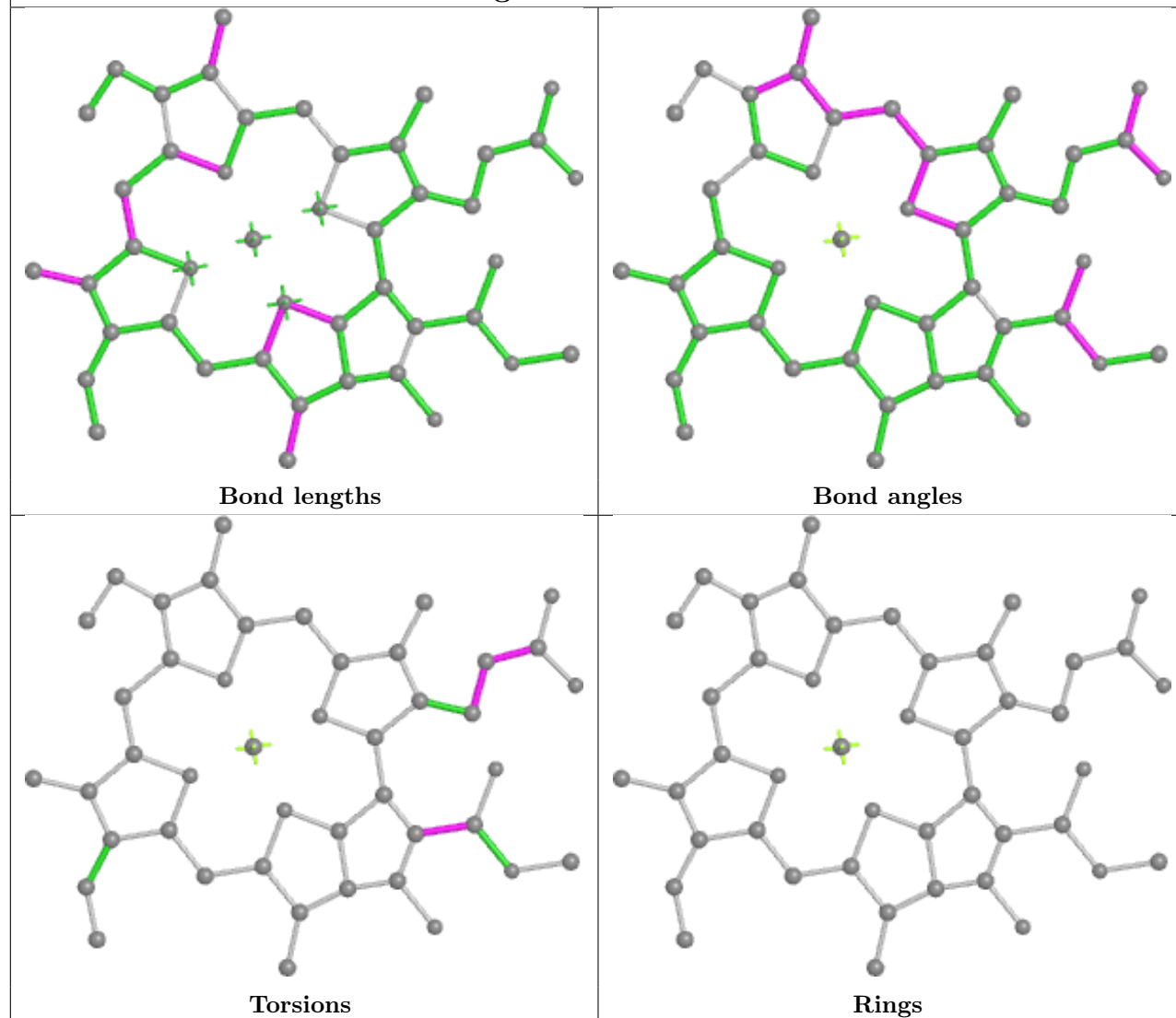


Ligand CLA t 512

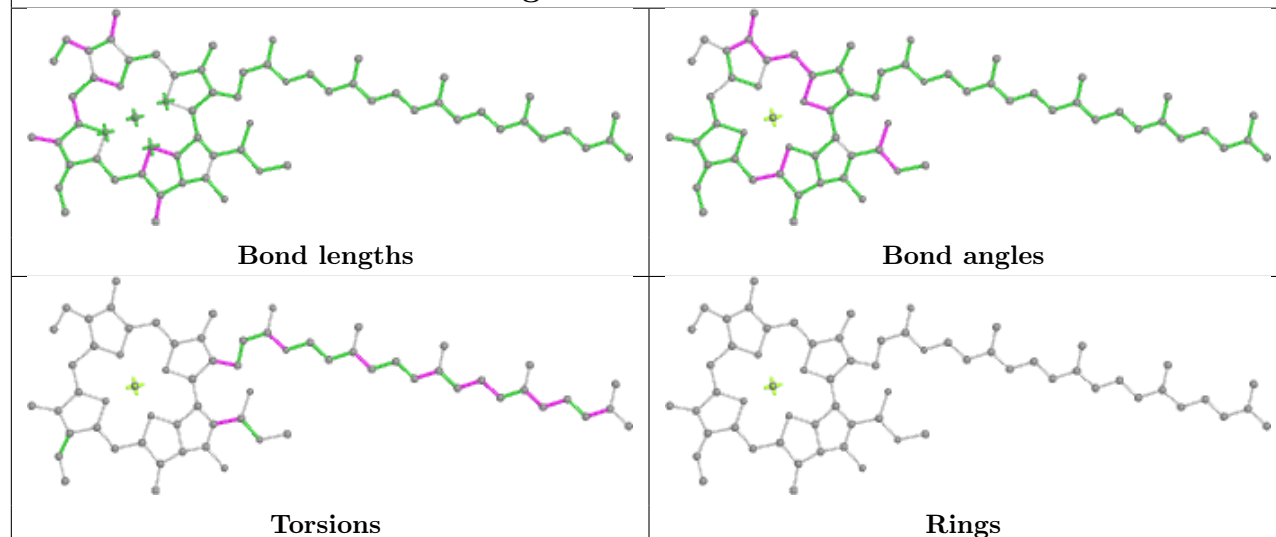




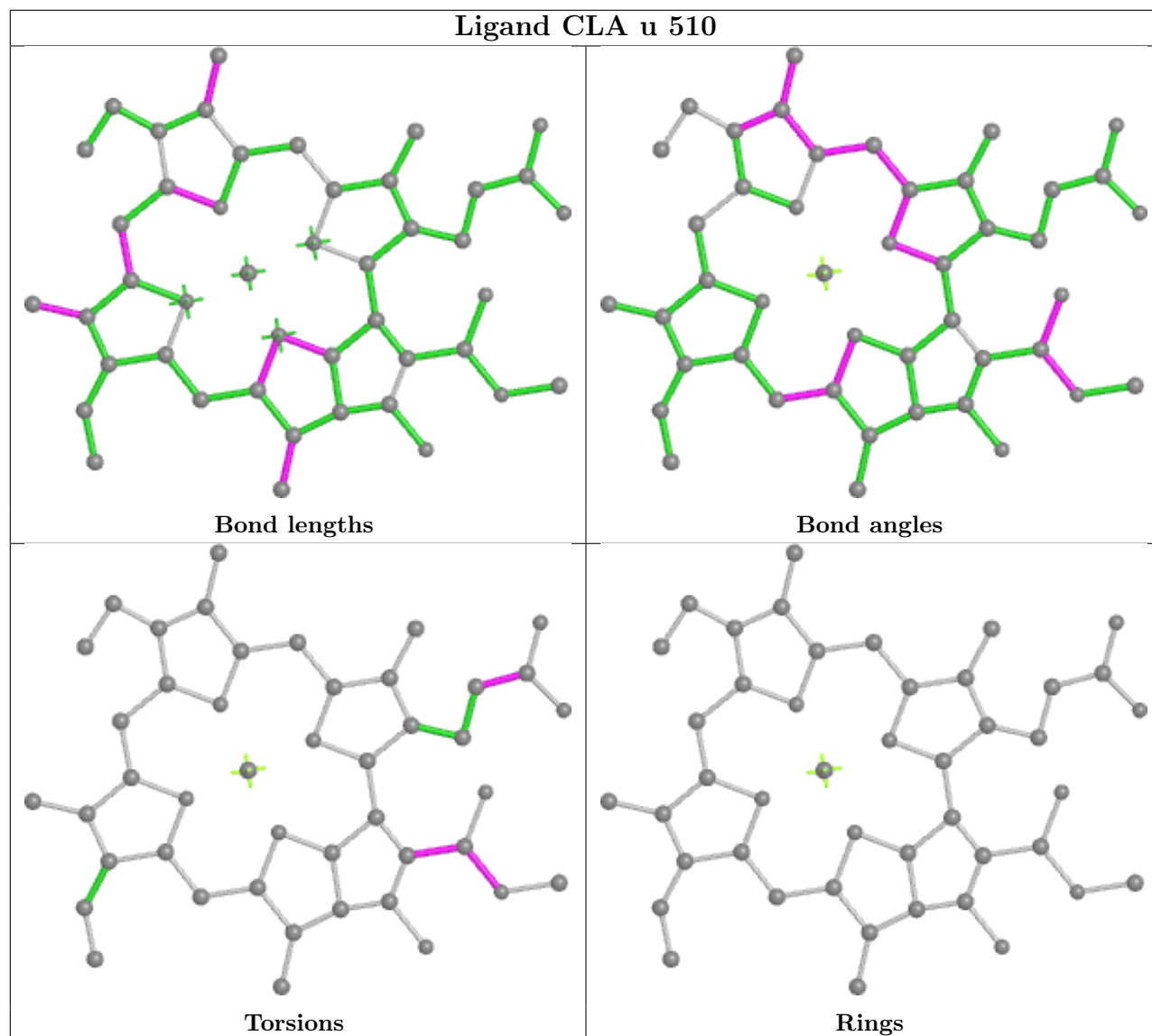
Ligand CLA 1 513

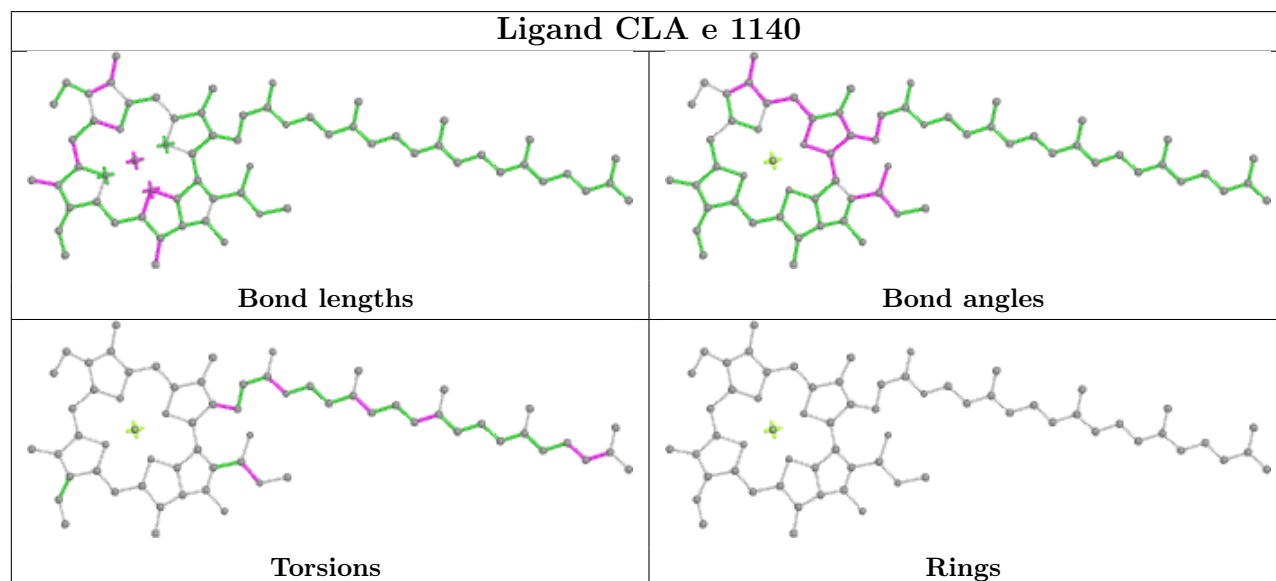
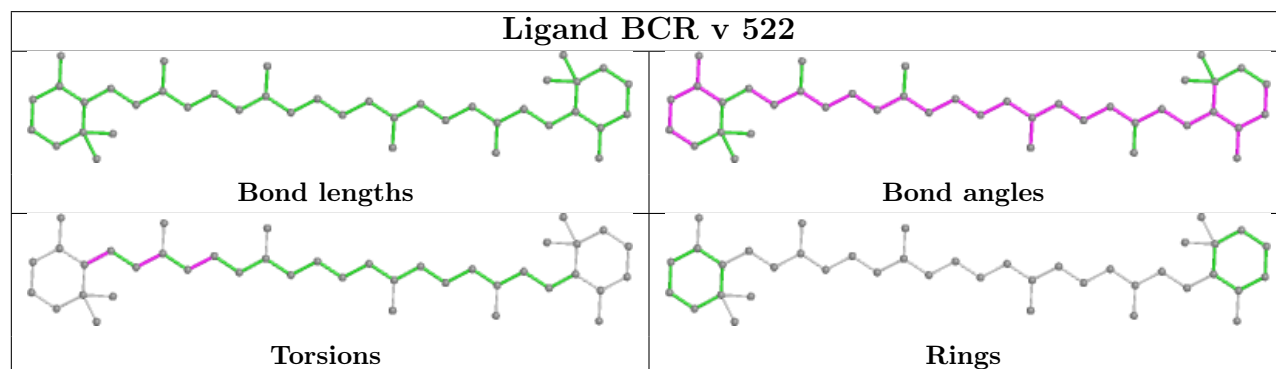
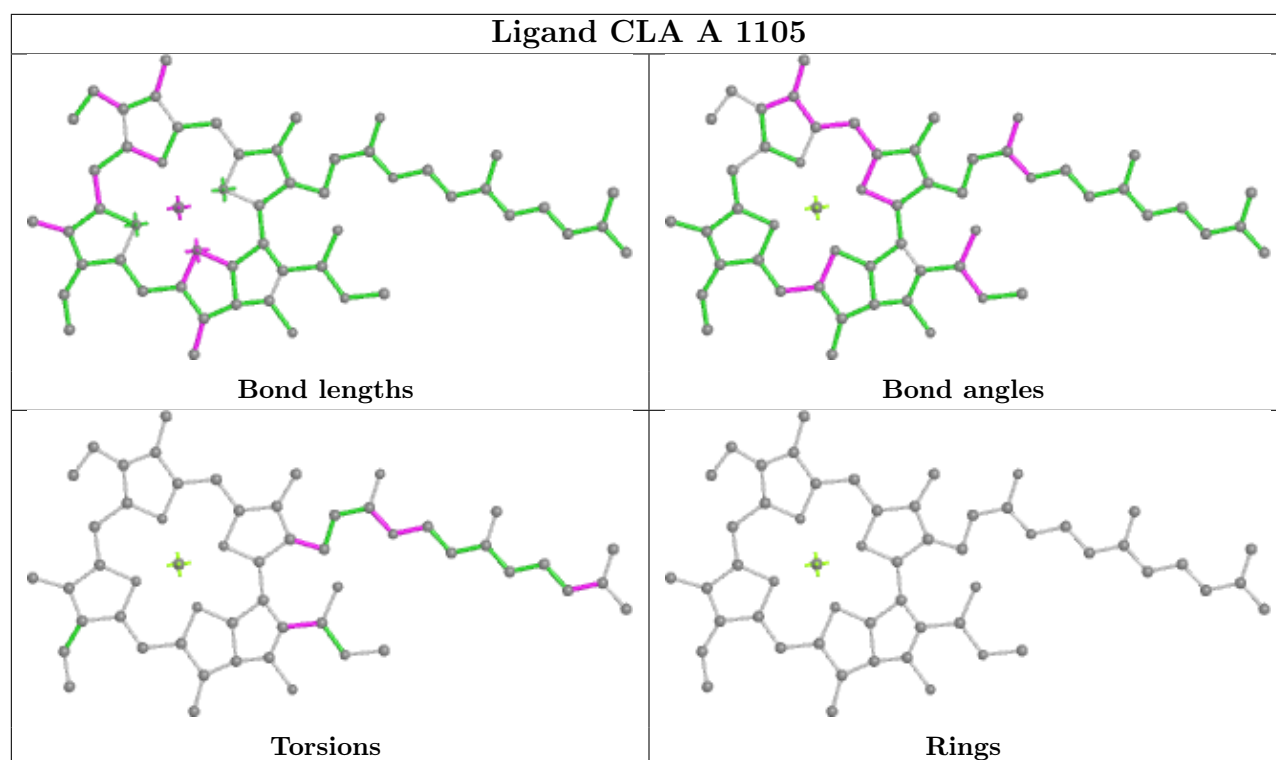


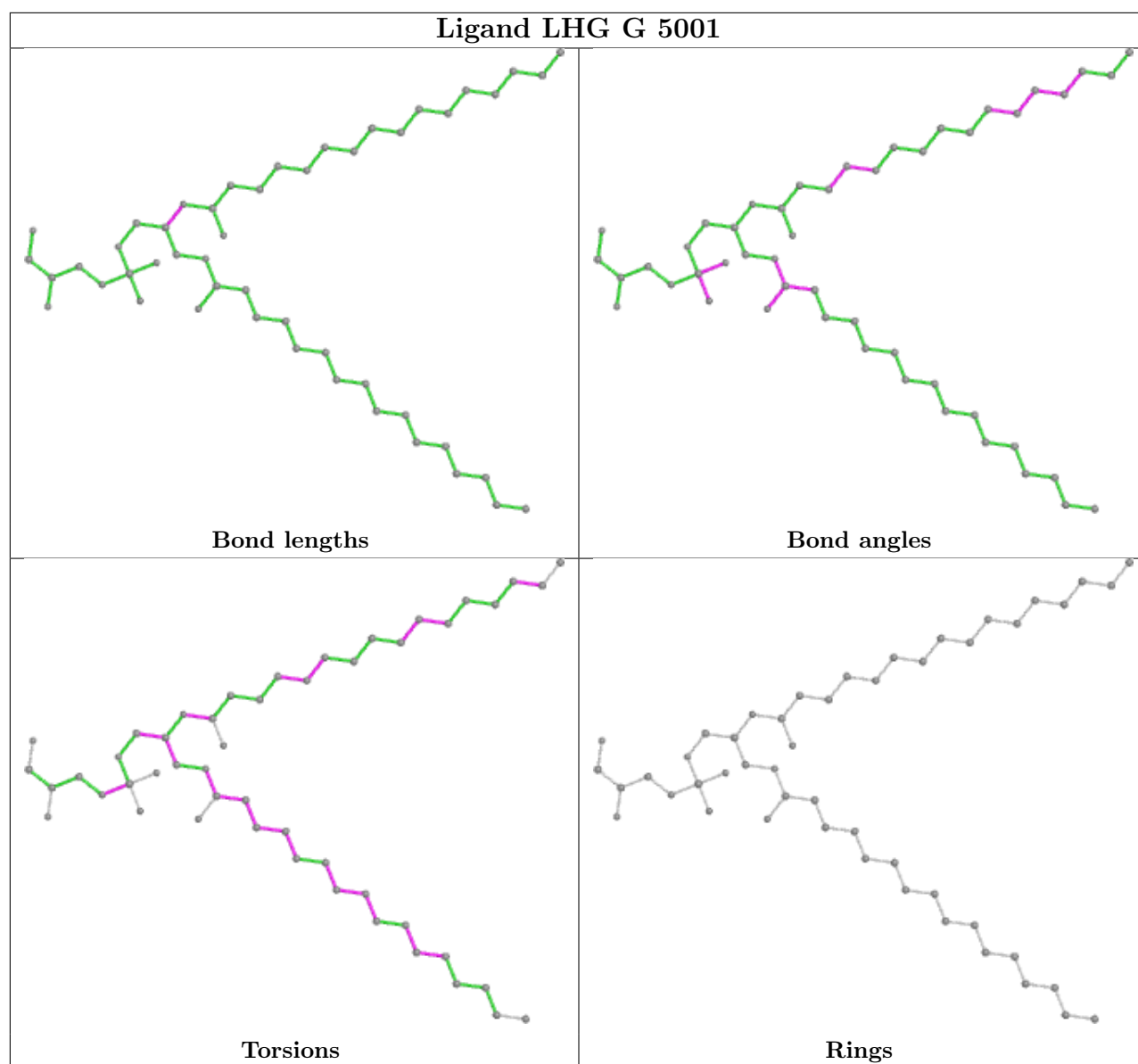
Ligand CLA H 1208



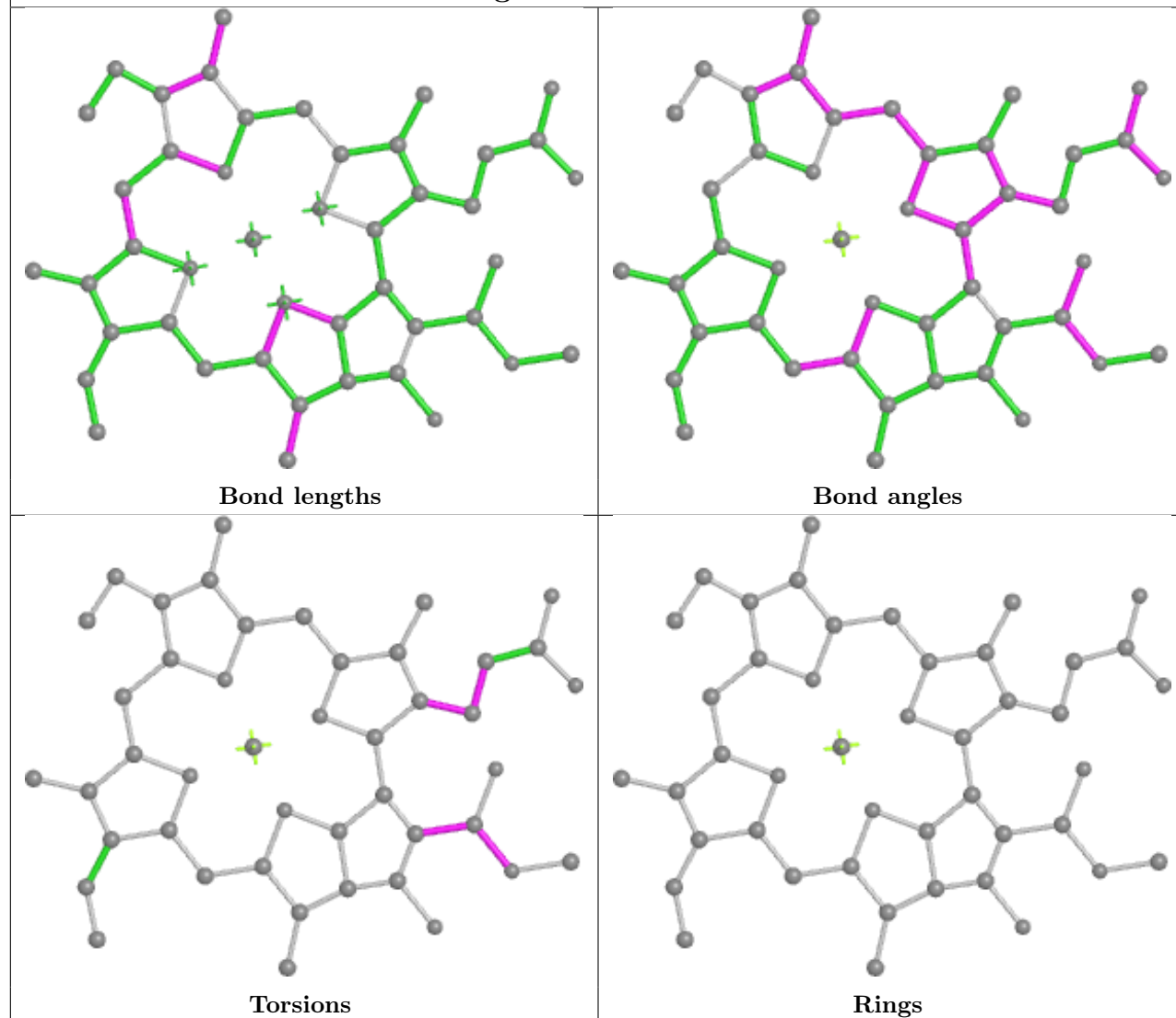
Ligand CLA u 510



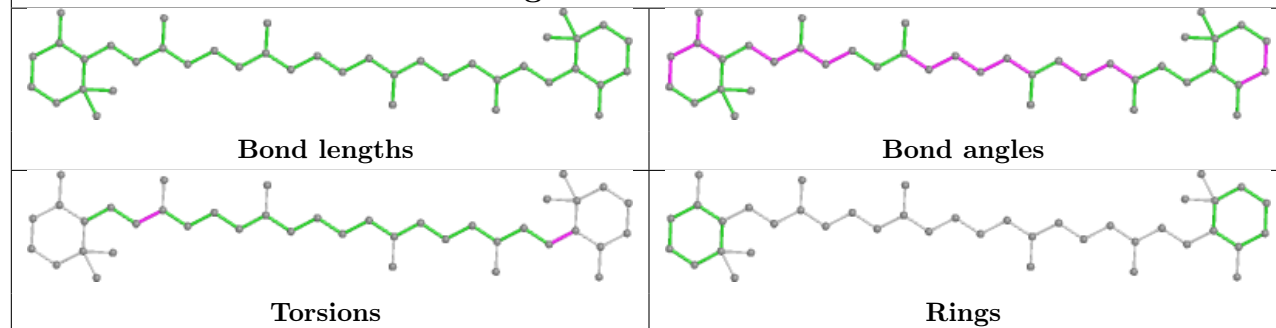


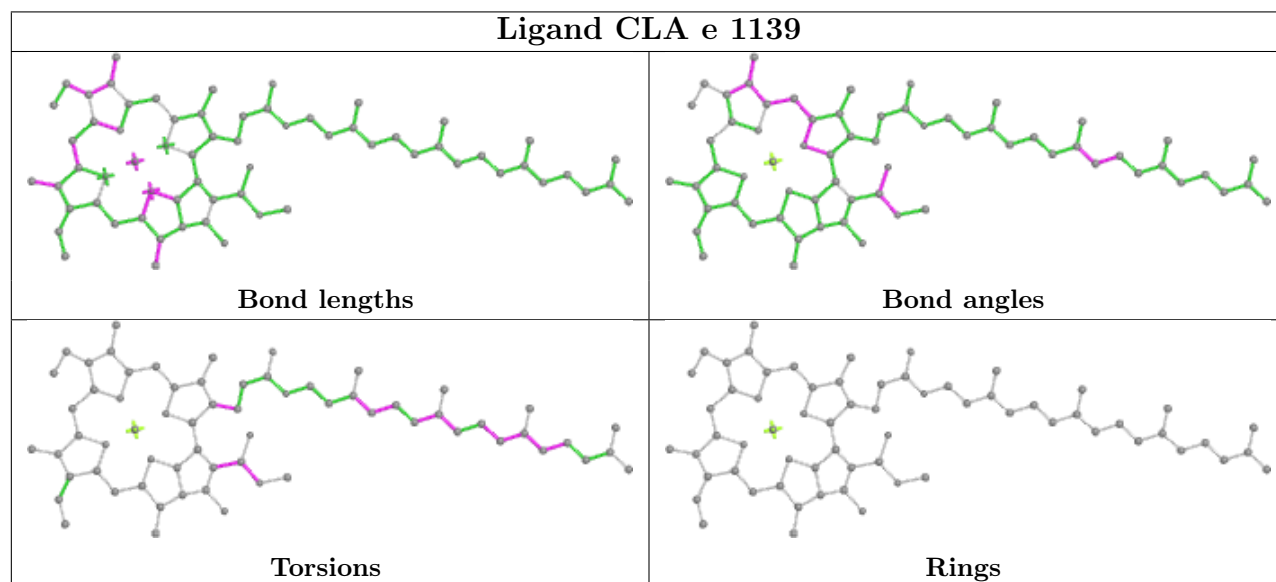
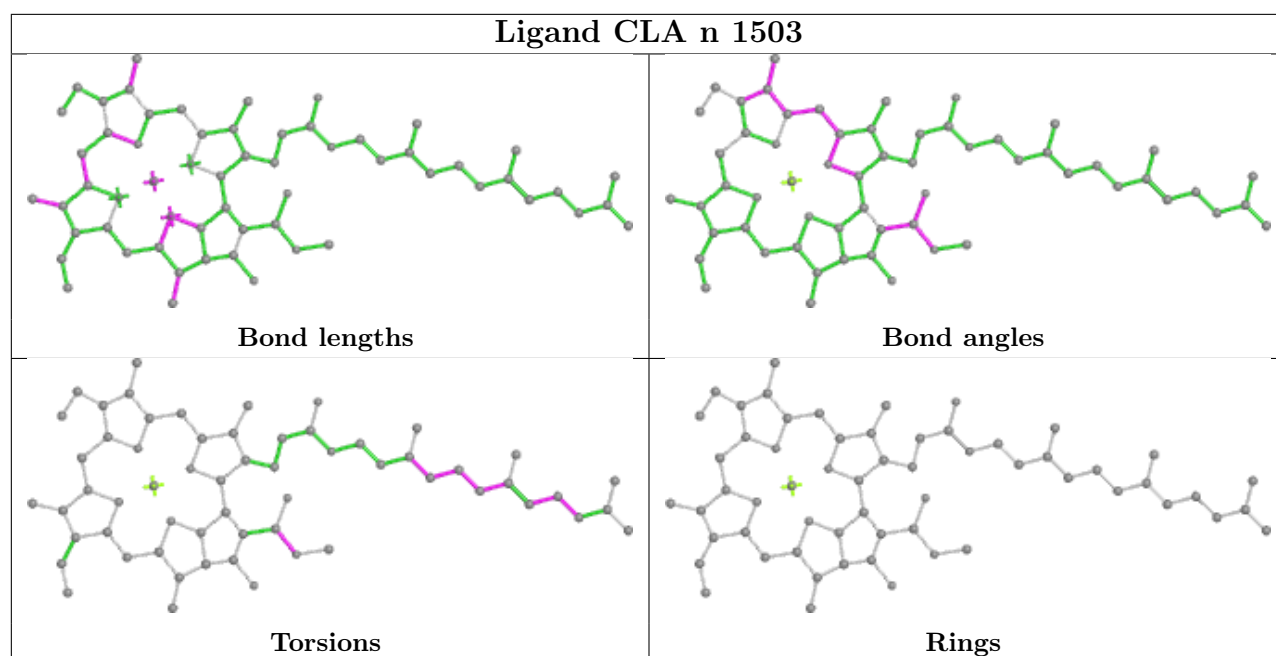


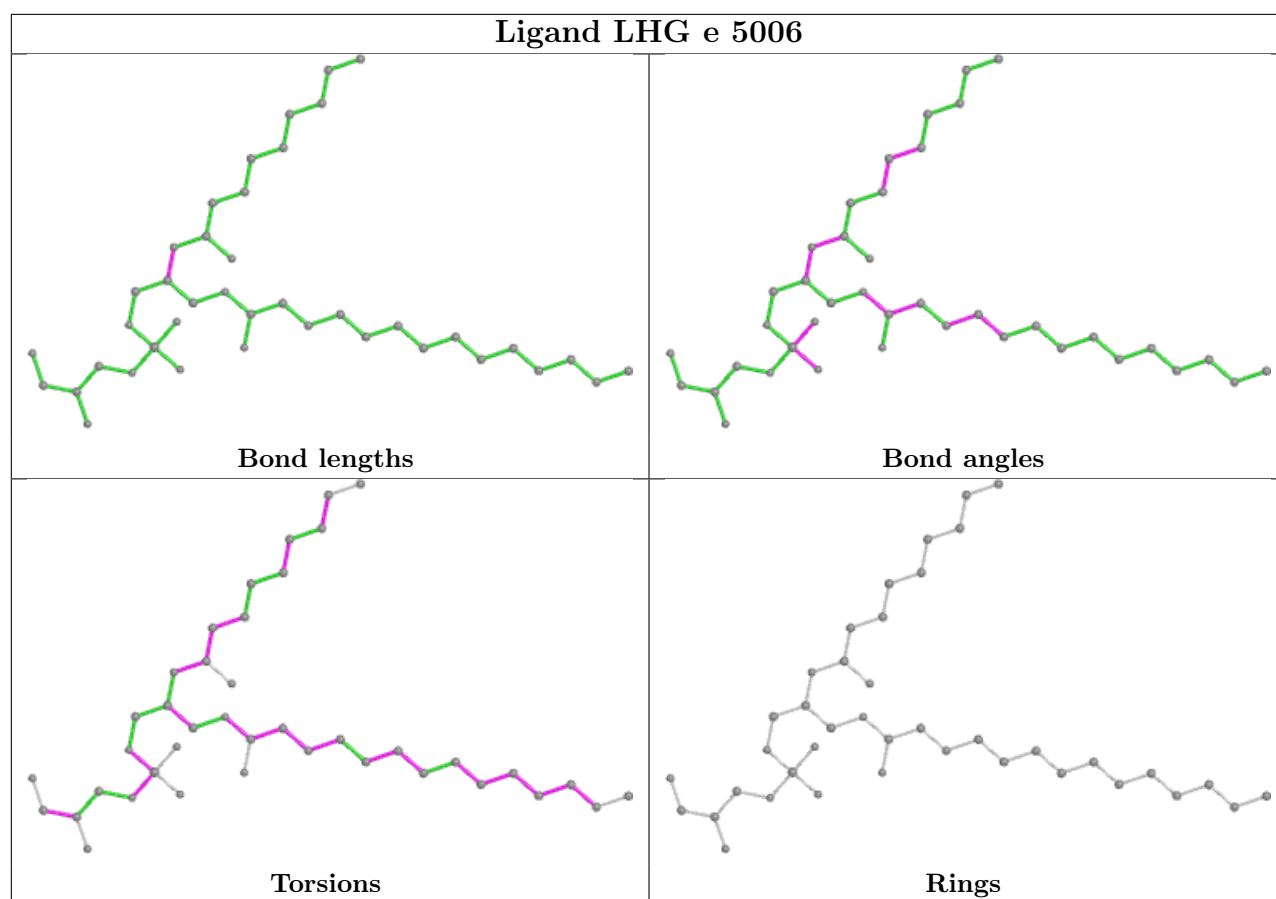
Ligand CLA 5 503



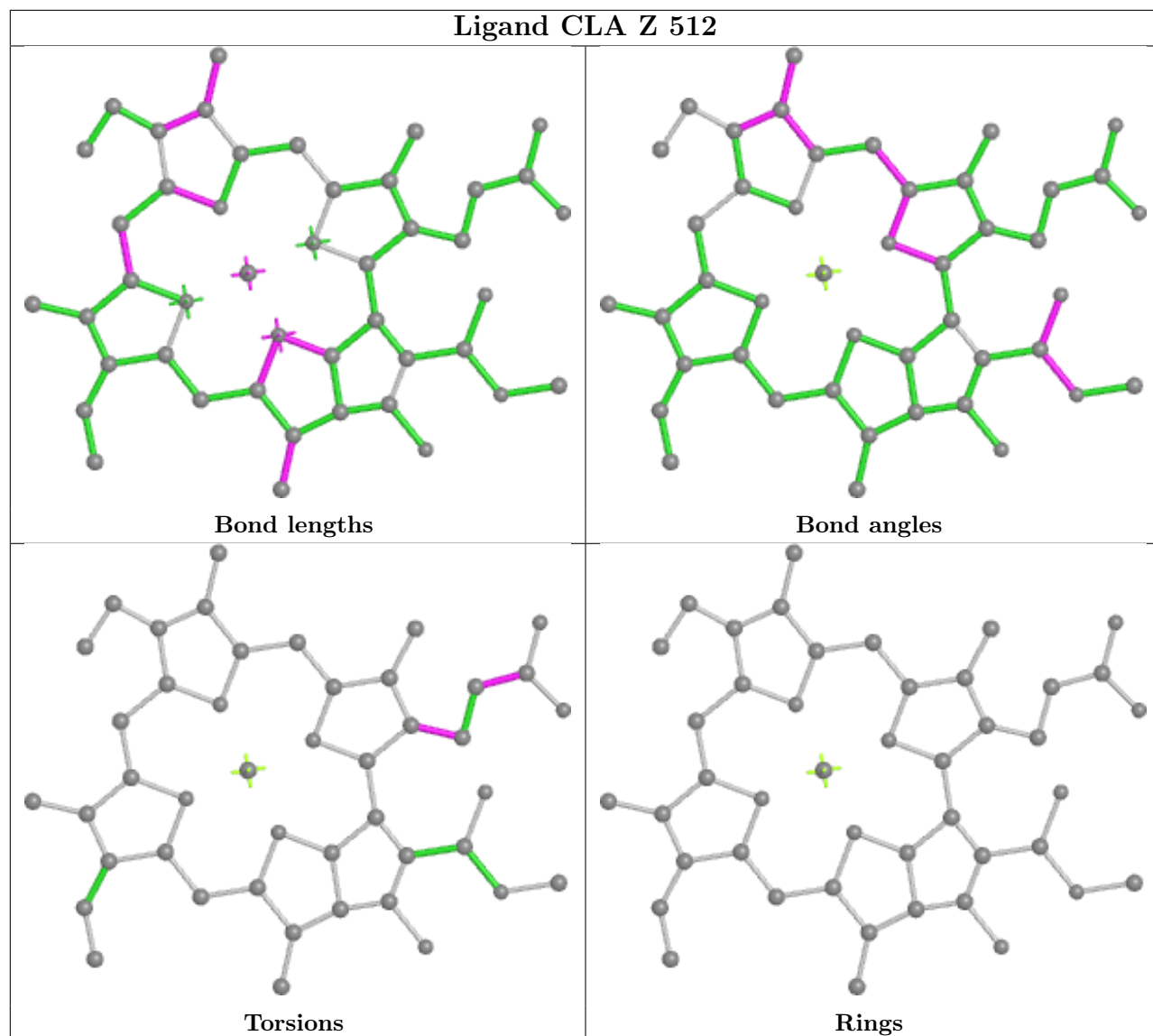
Ligand BCR n 4022



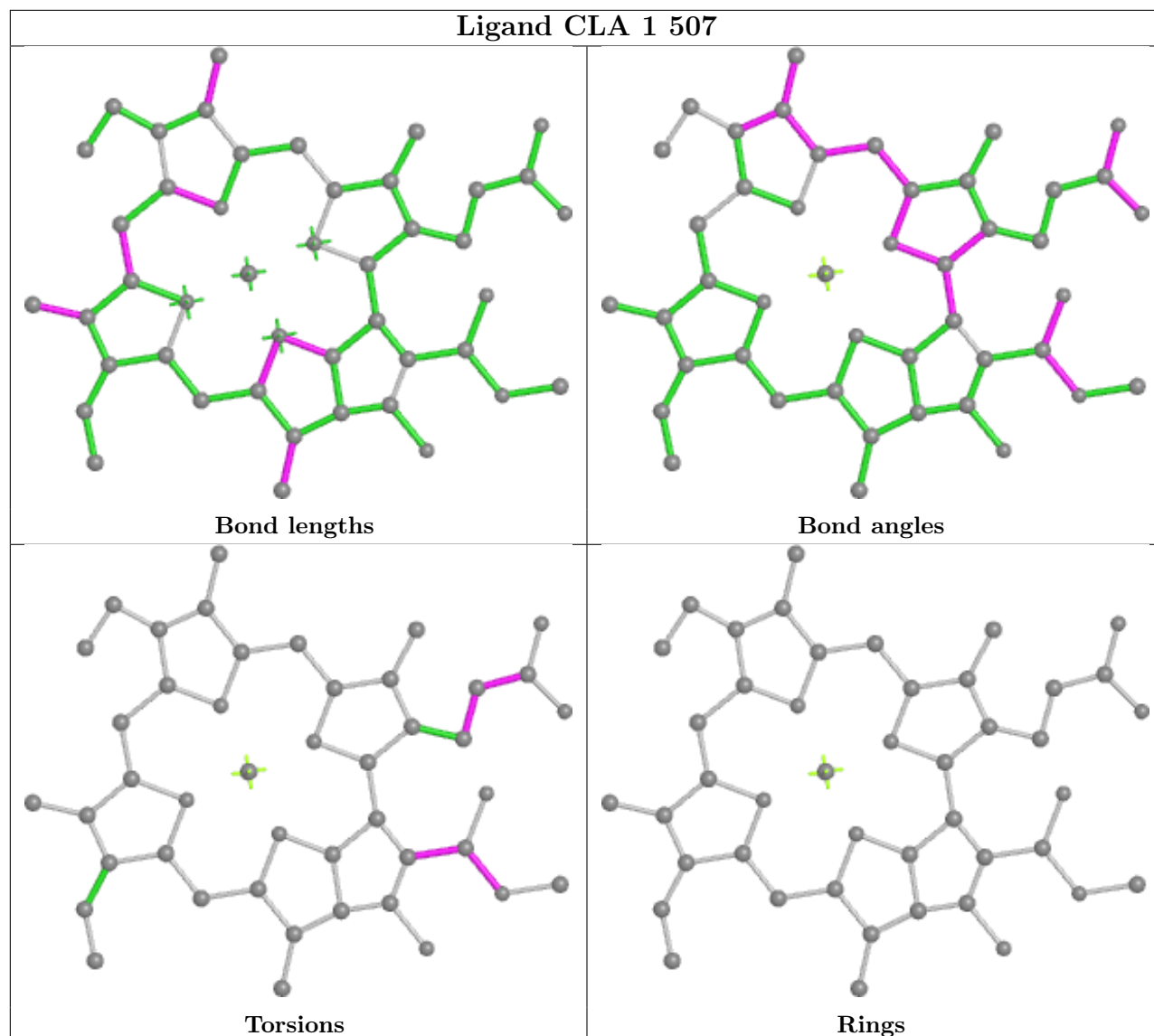


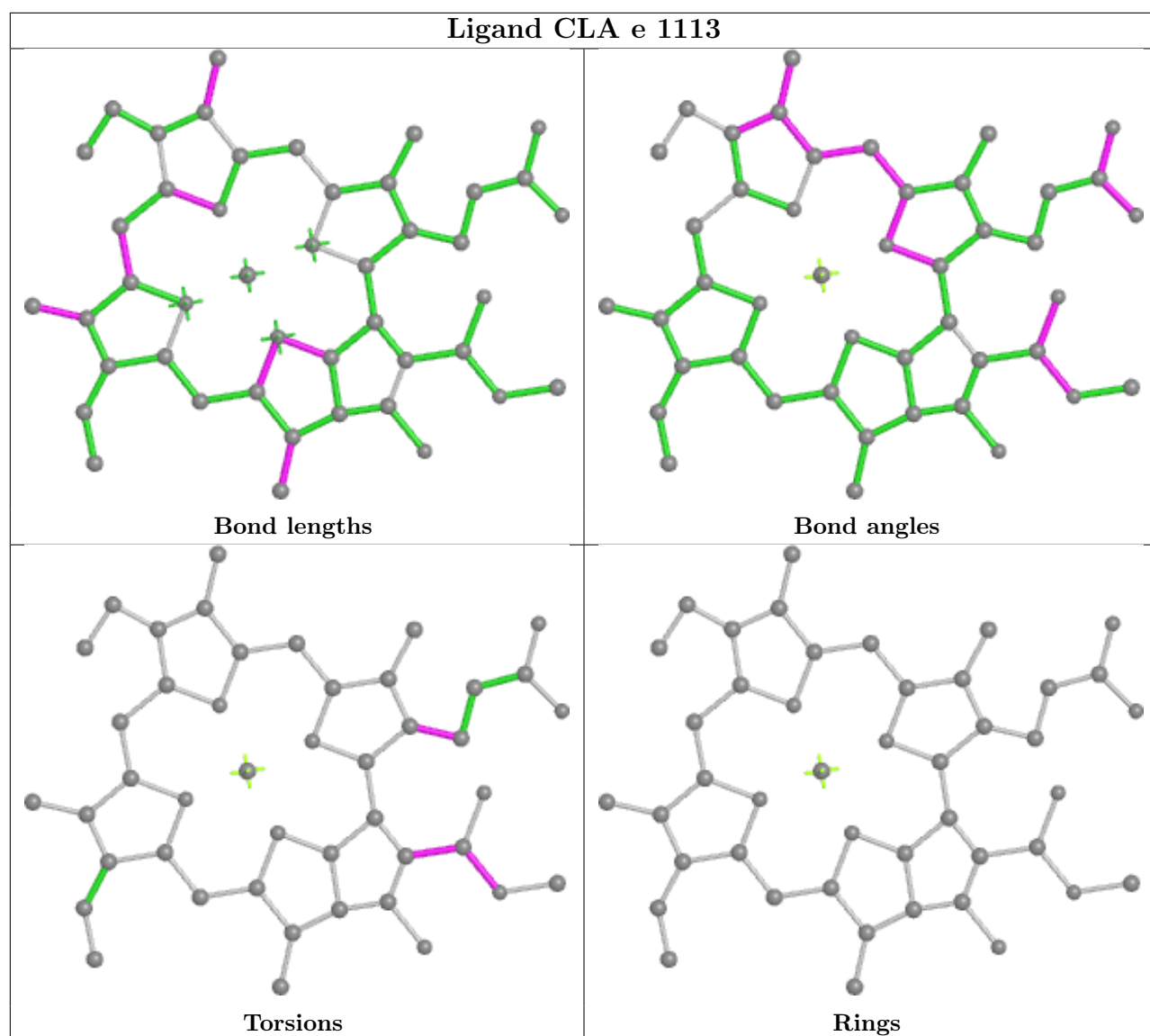


Ligand CLA Z 512

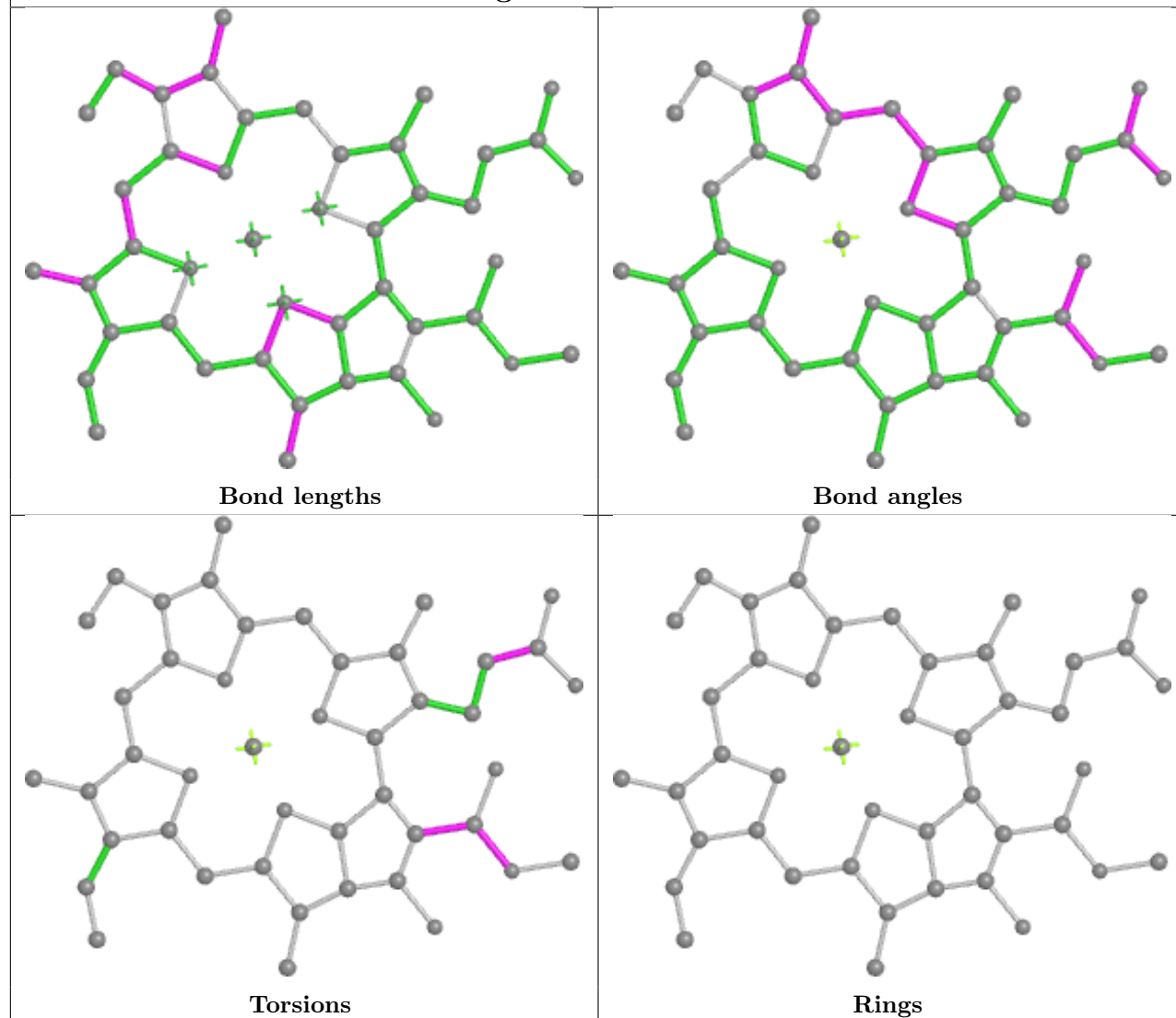


Ligand CLA 1 507

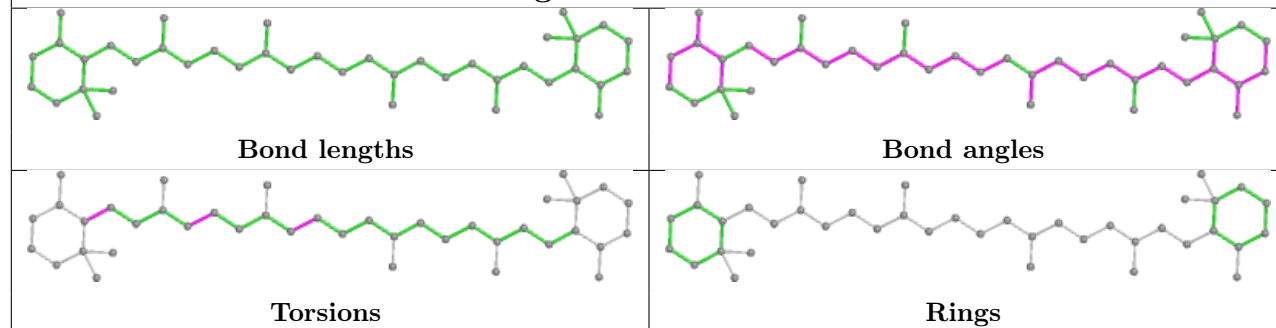




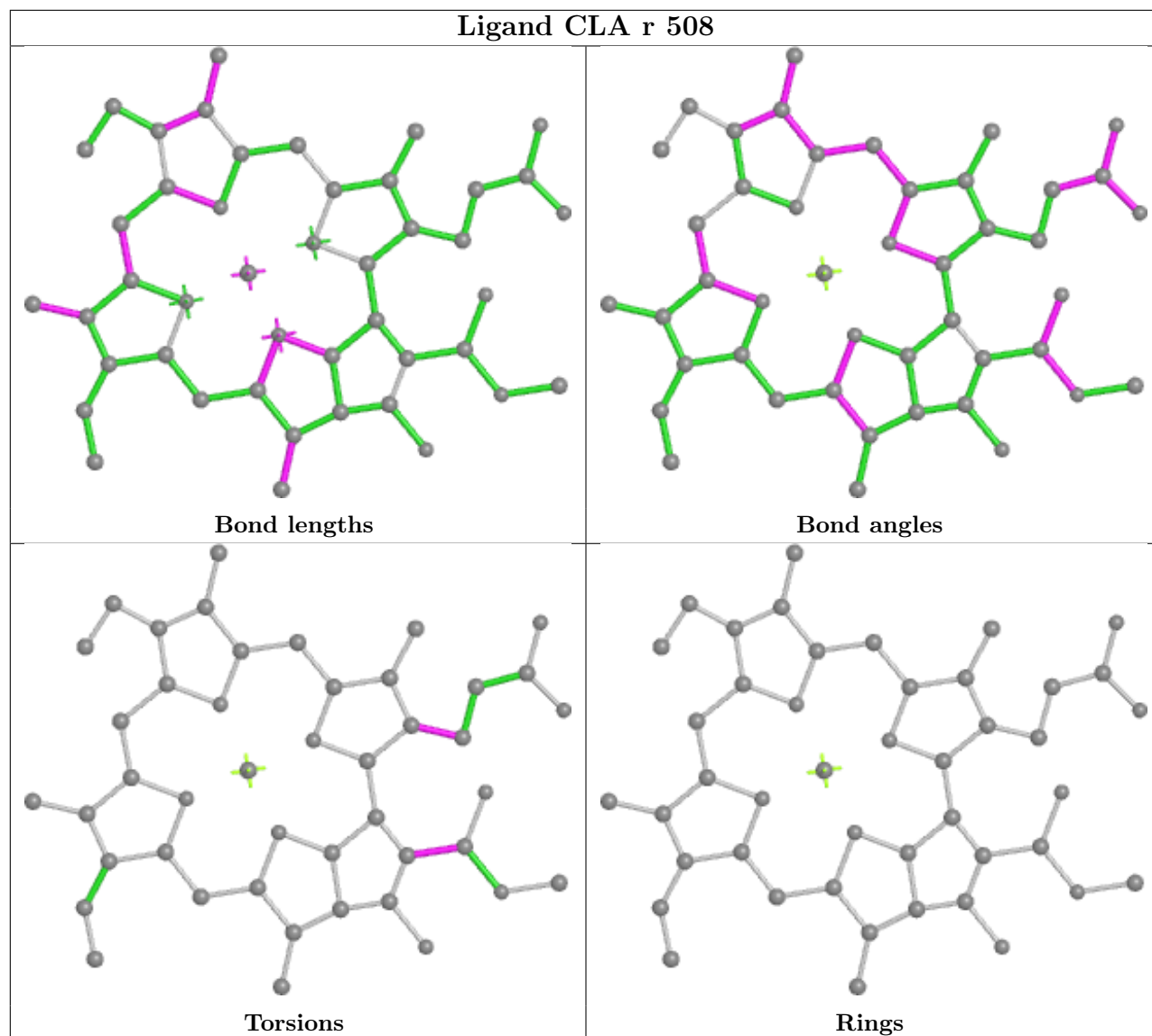
Ligand CLA s 519

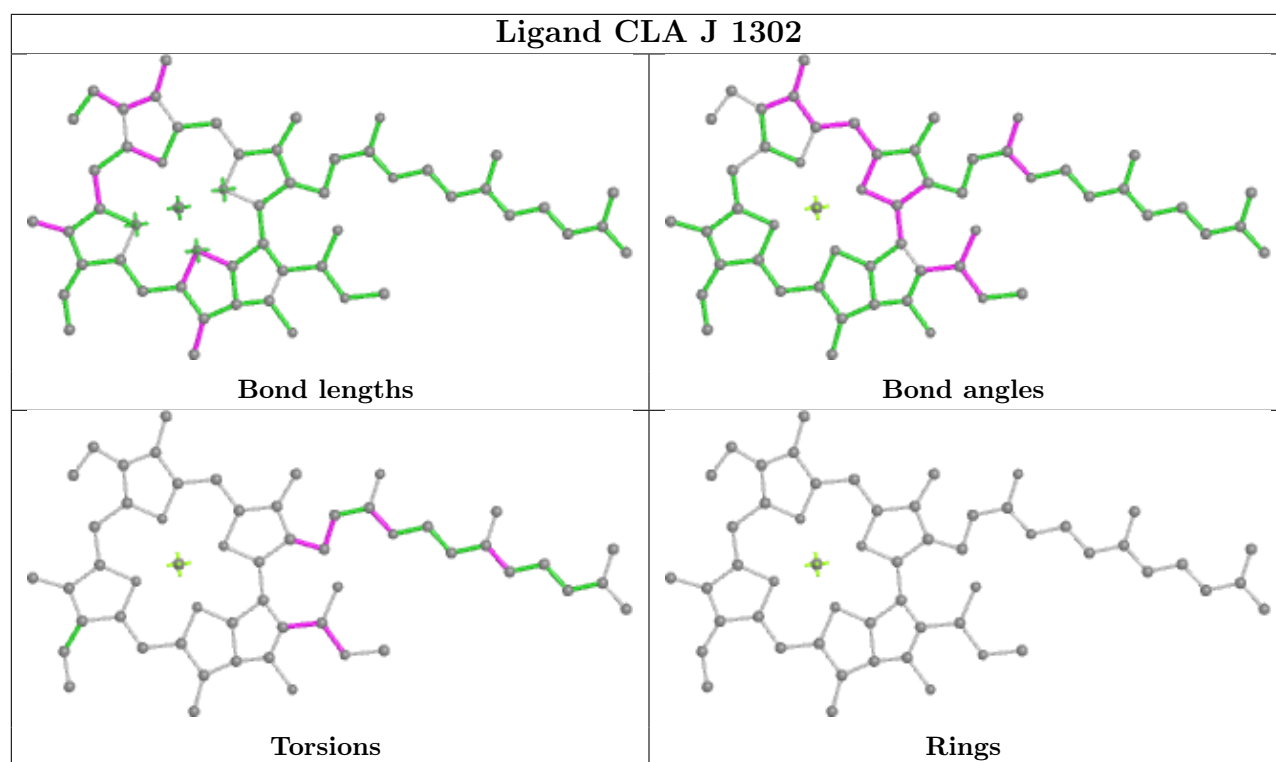


Ligand BCR 4 522

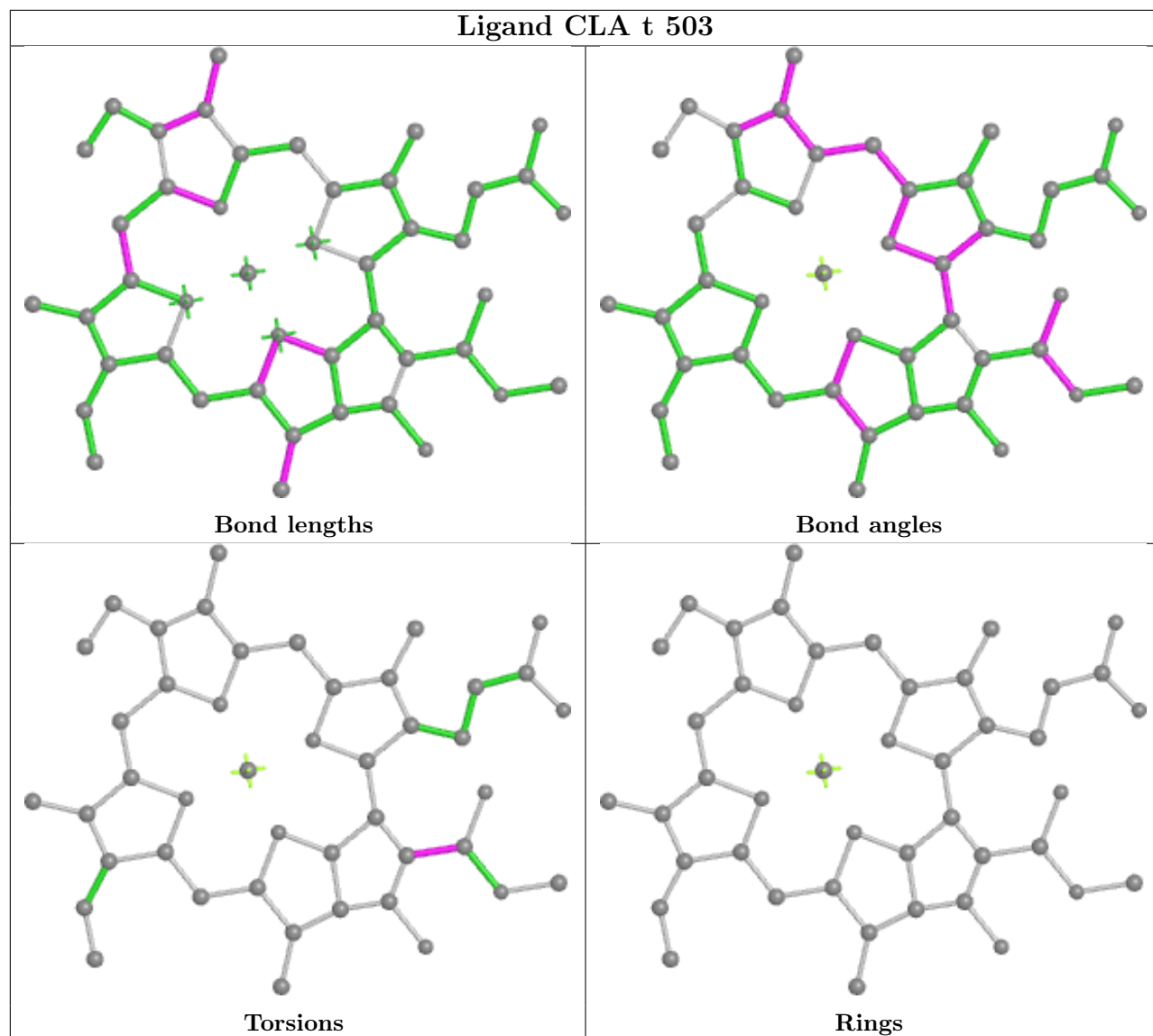


Ligand CLA r 508

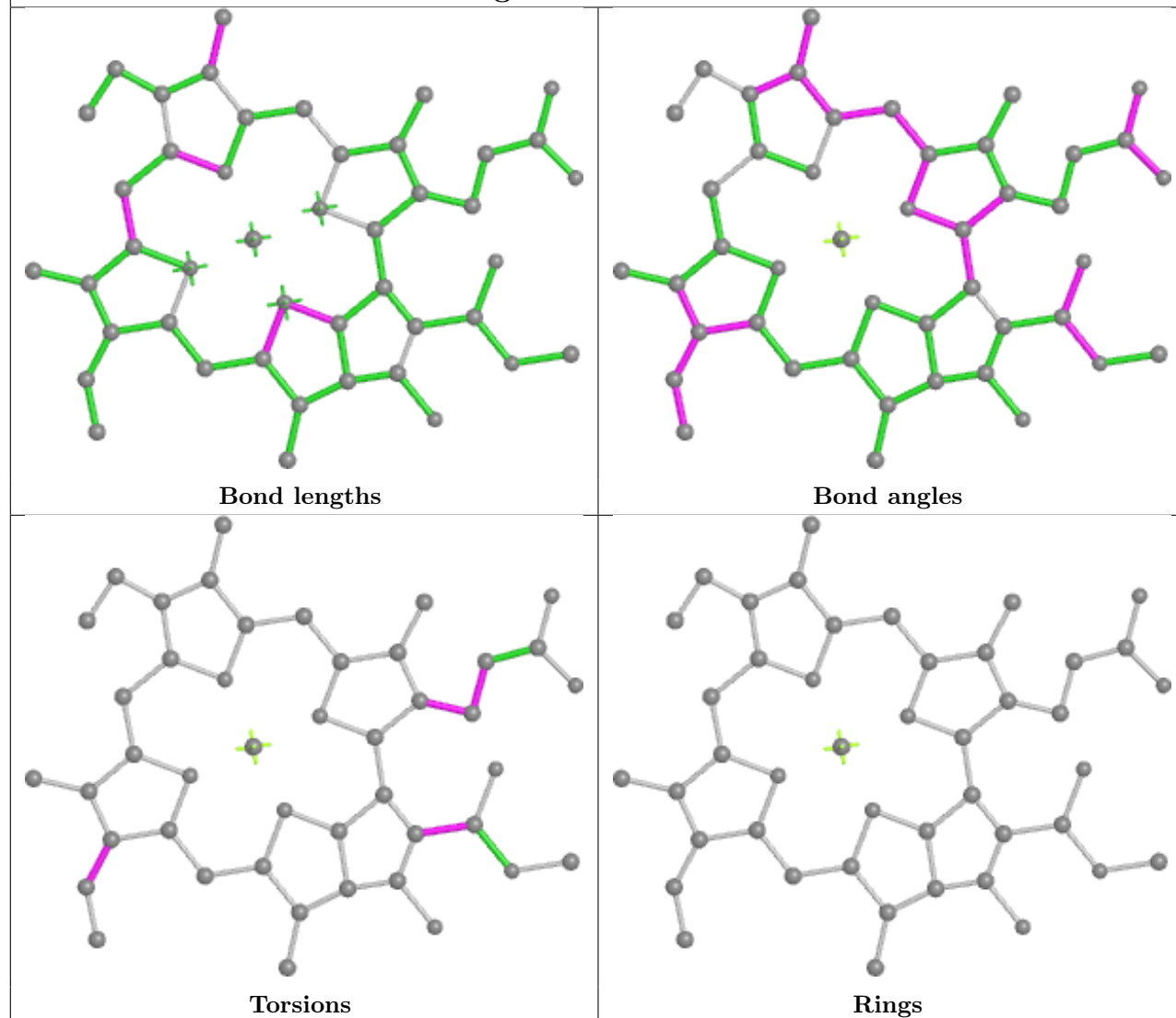




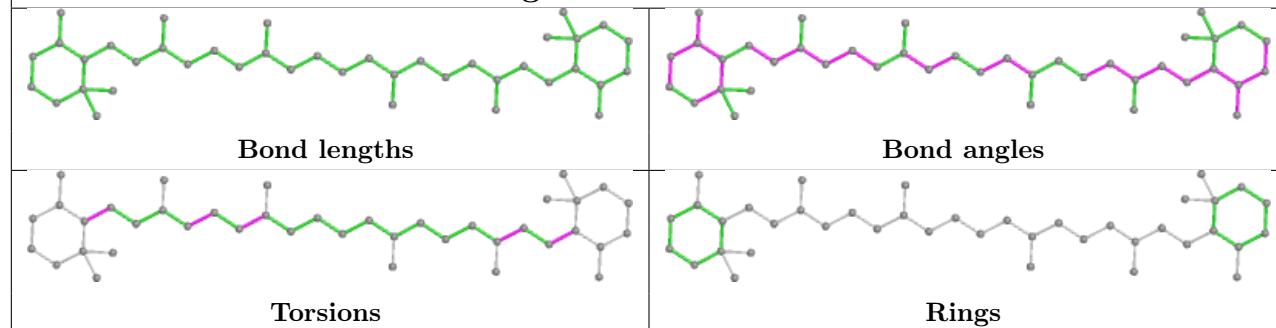
Ligand CLA t 503



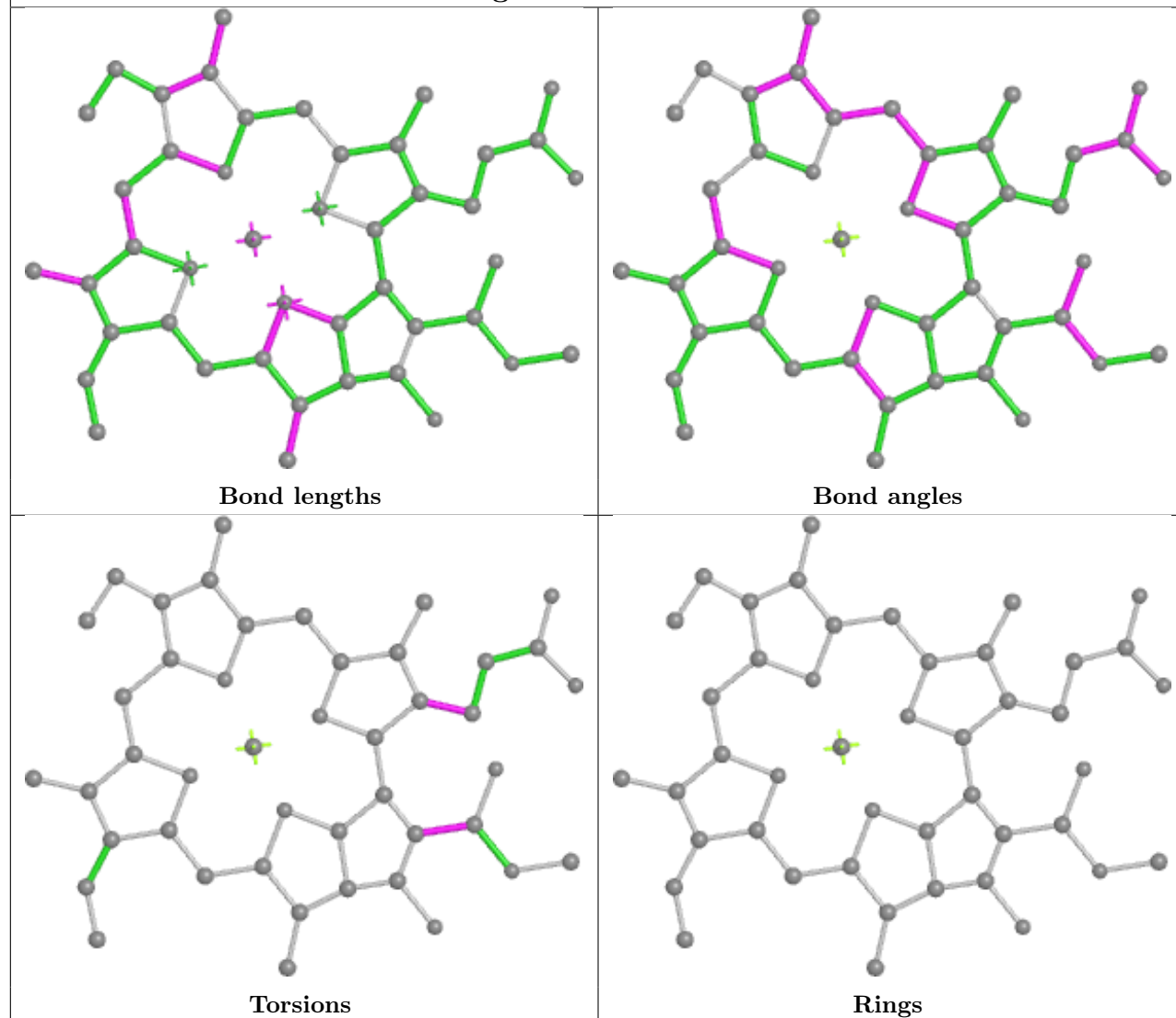
Ligand CLA 3 516



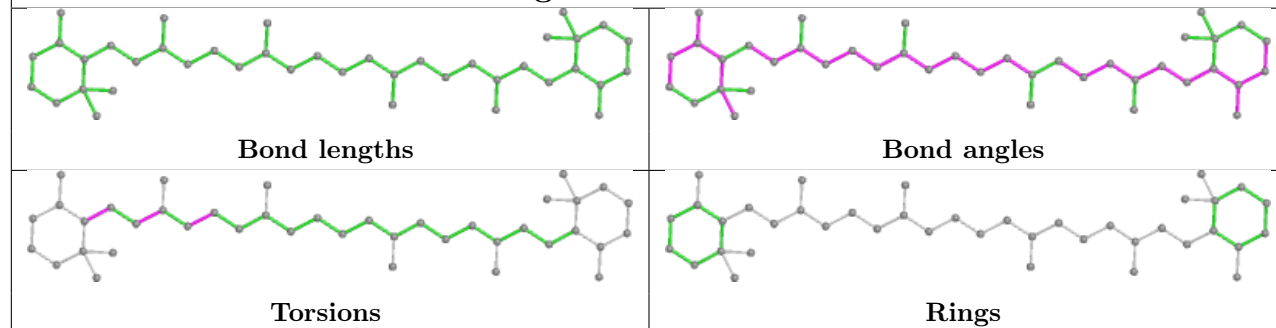
Ligand BCR T 4012

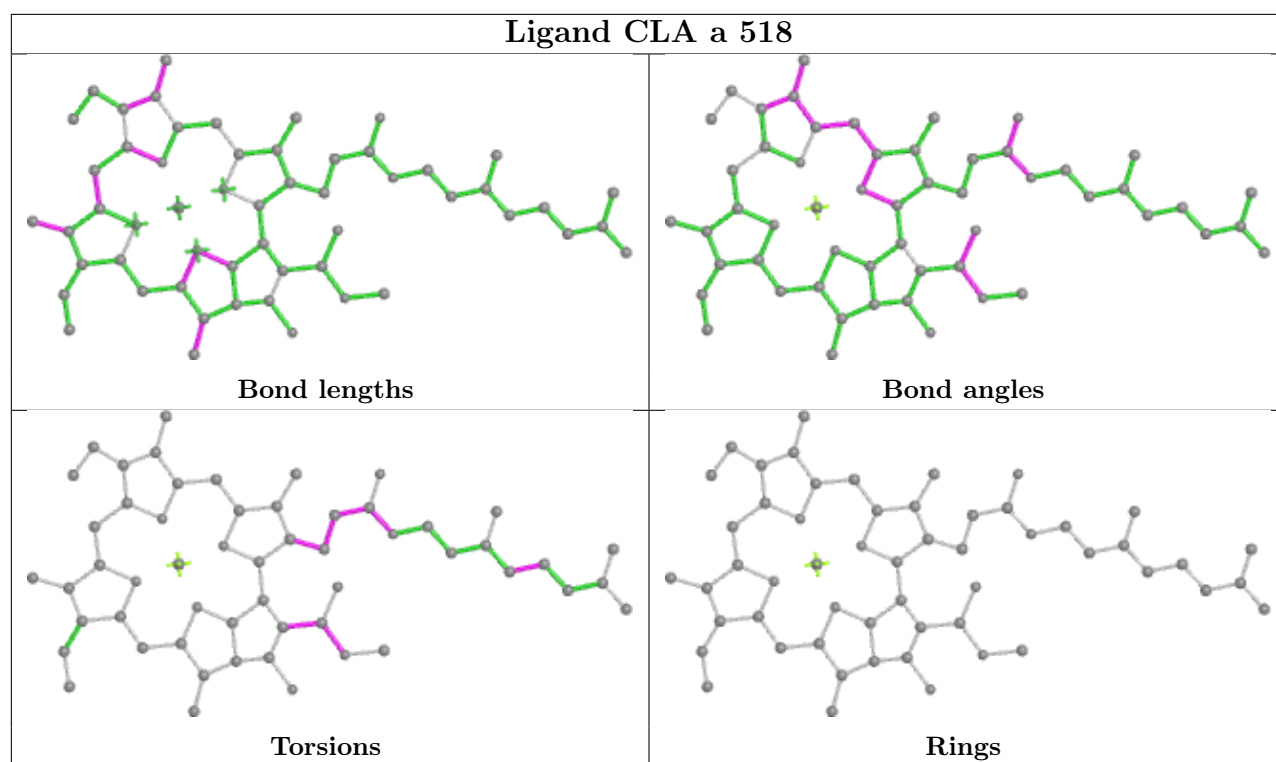


Ligand CLA Z 508

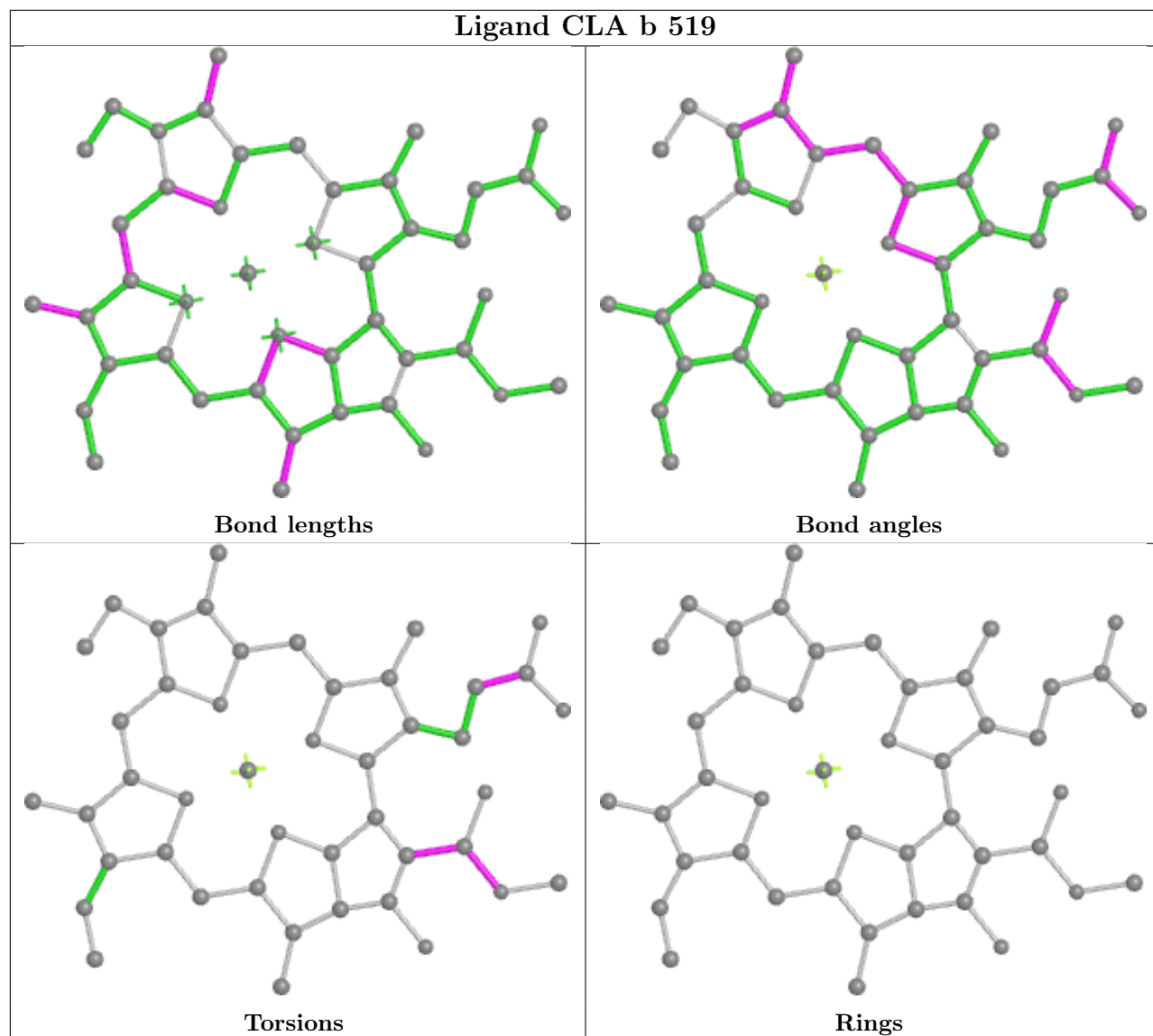


Ligand BCR a 522

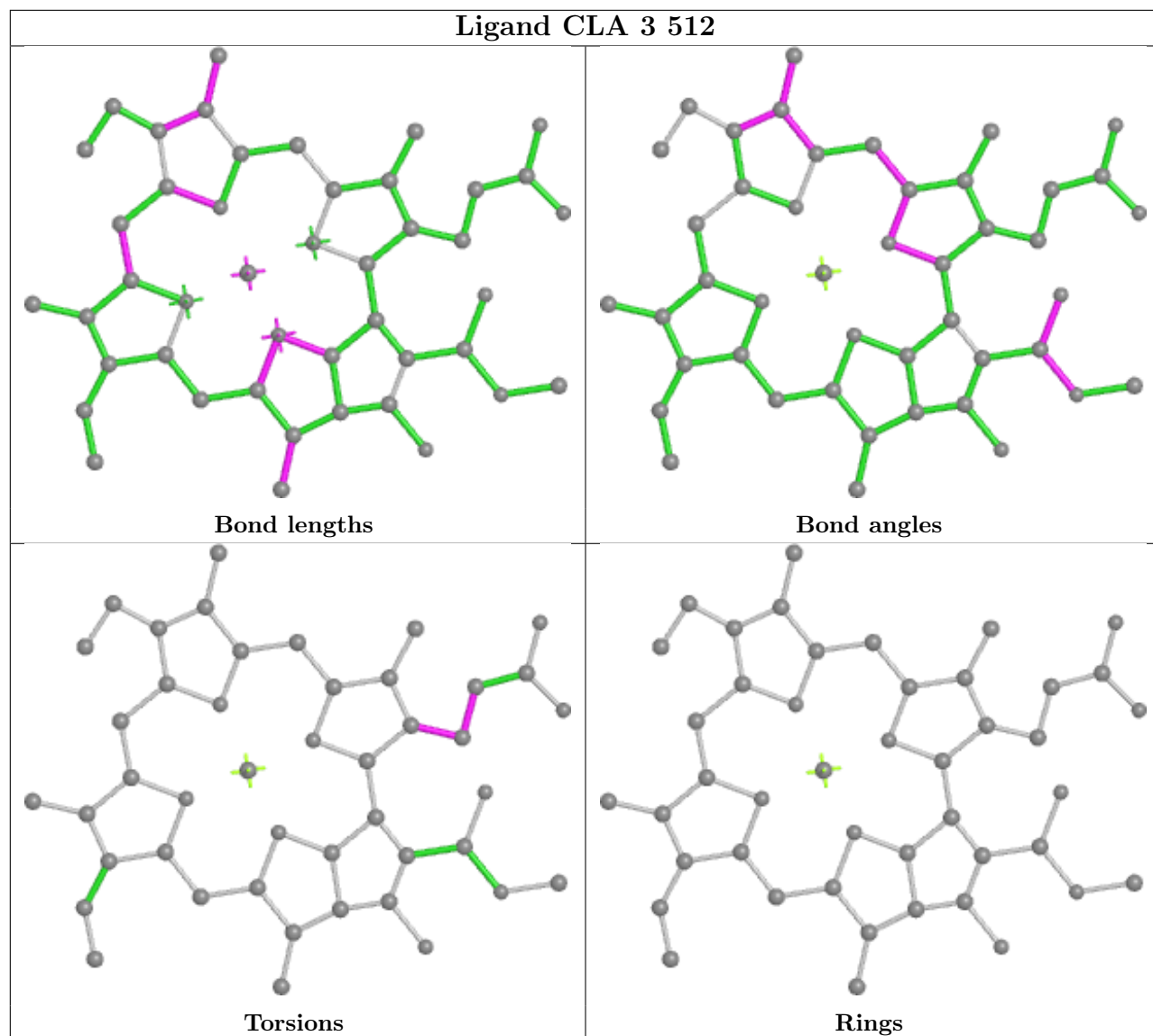




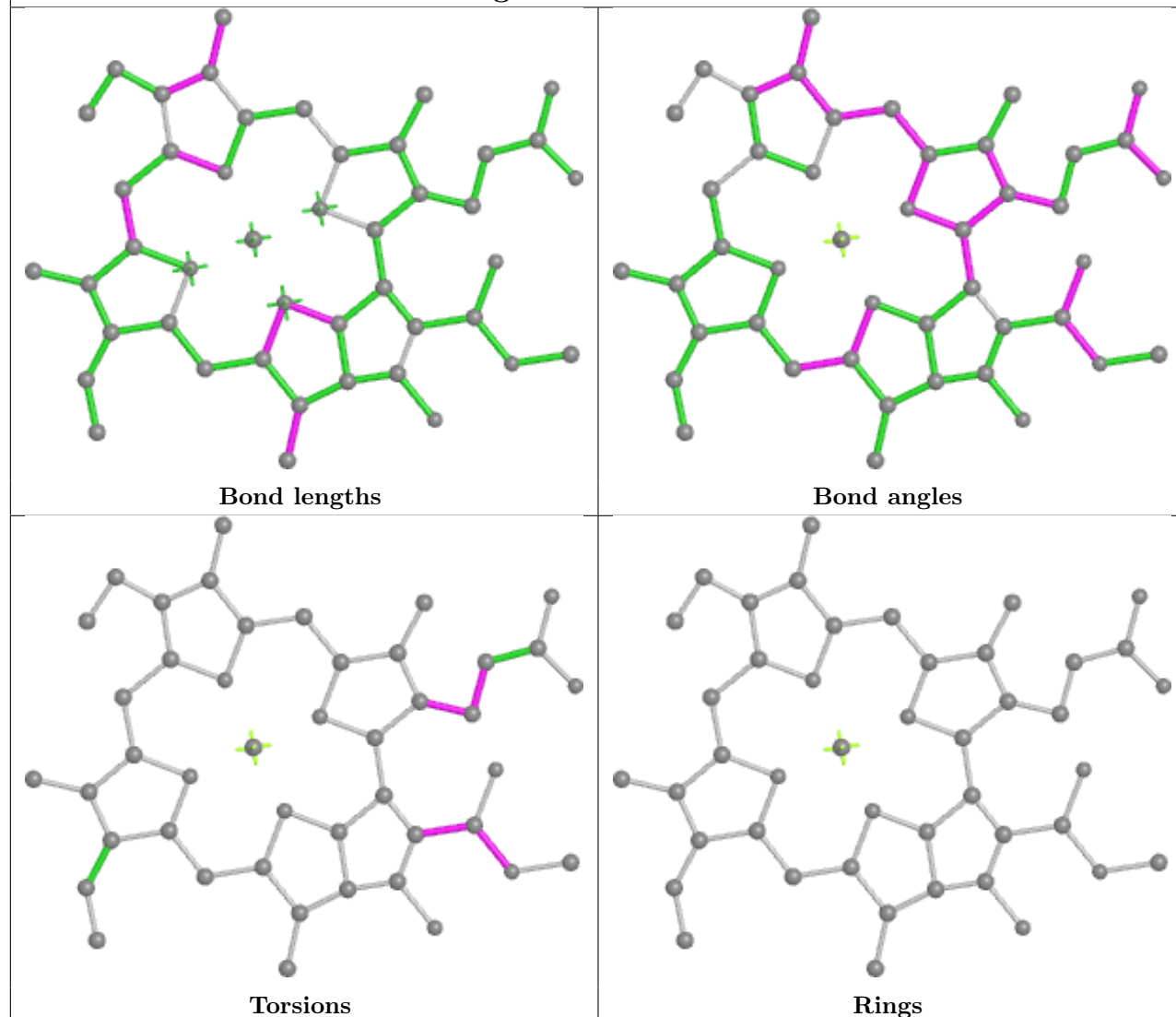
Ligand CLA b 519



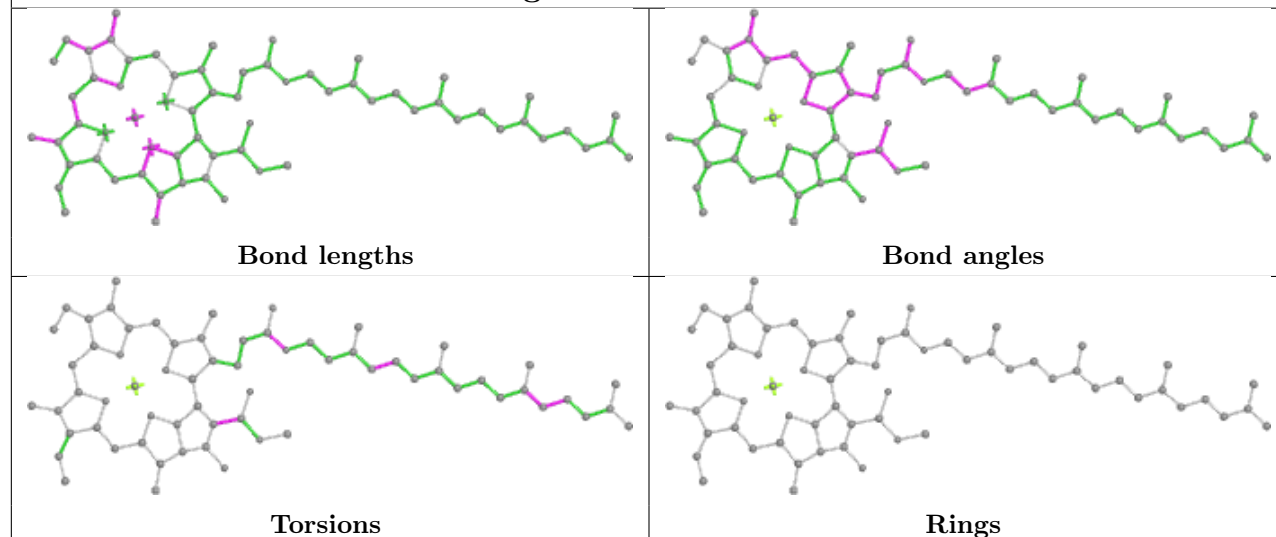
Ligand CLA 3 512



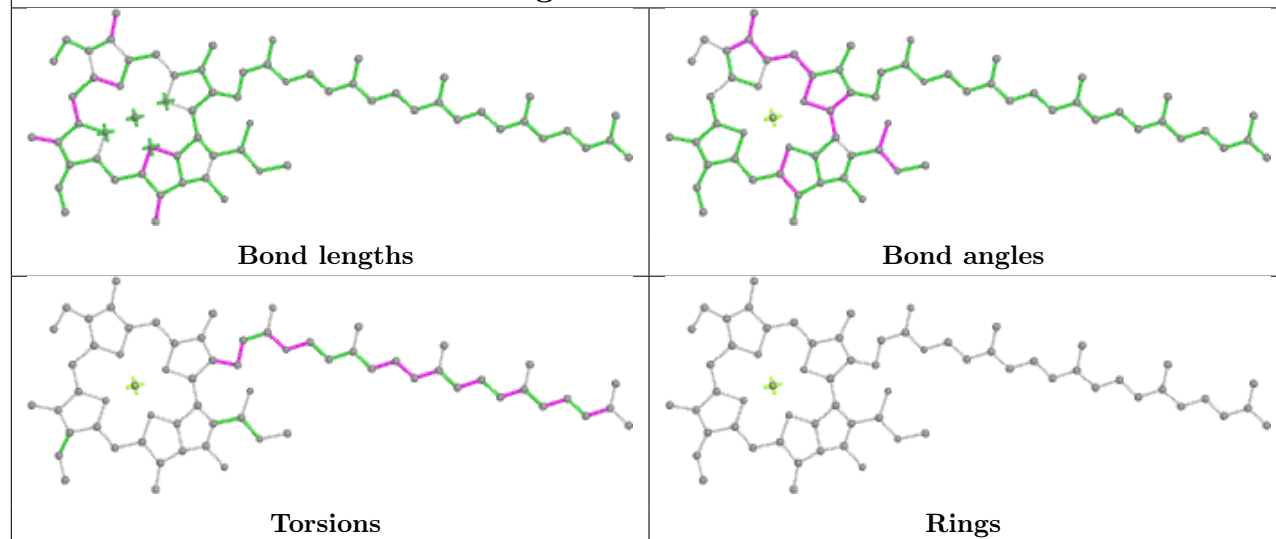
Ligand CLA u 503



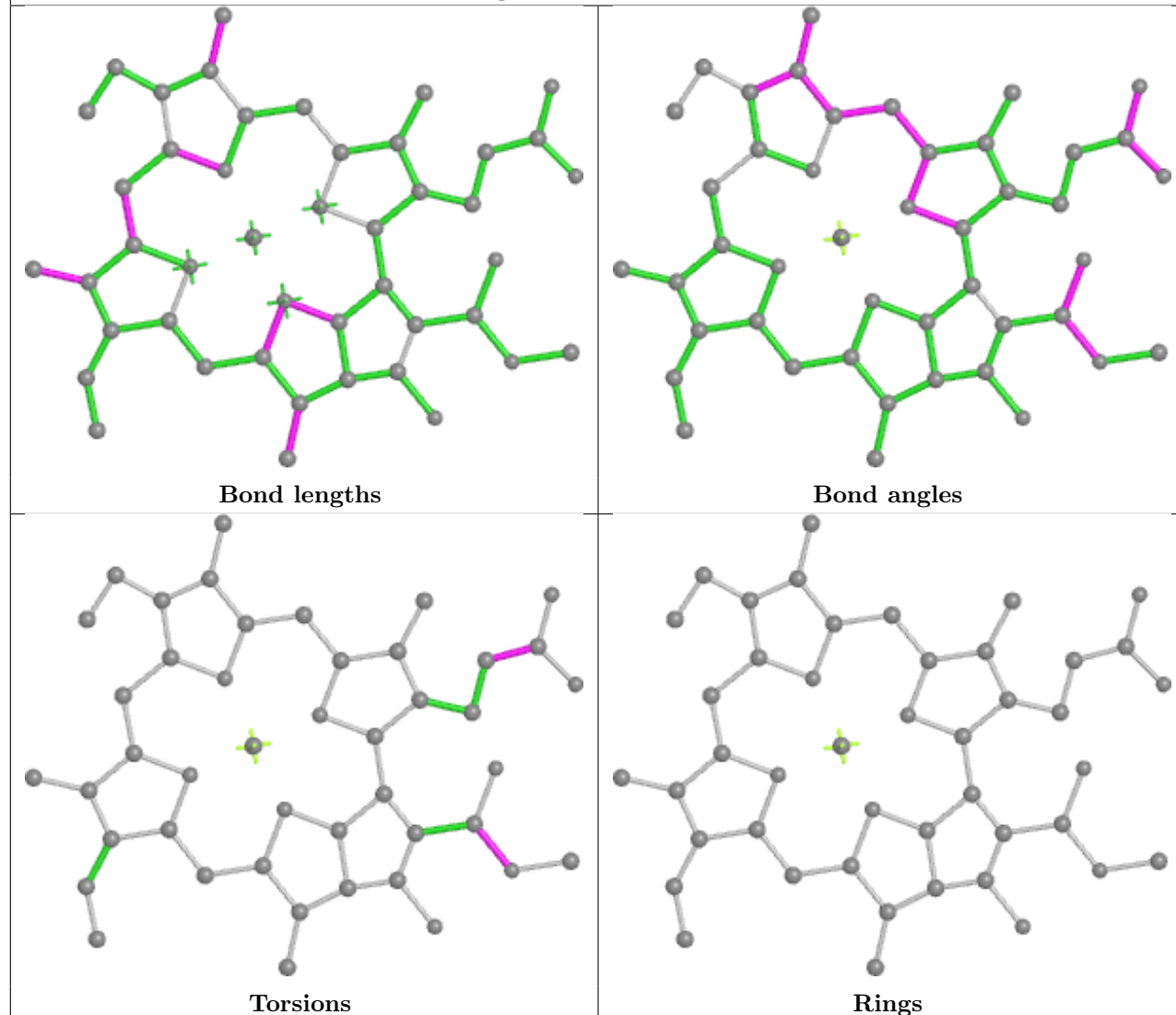
Ligand CLA B 1205



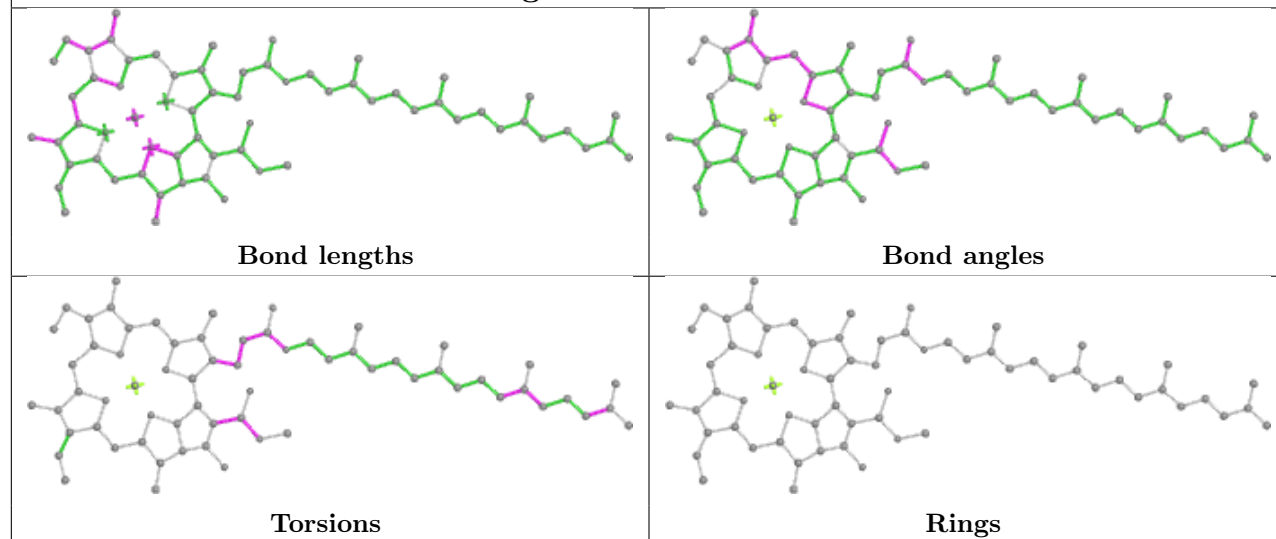
Ligand CLA v 505



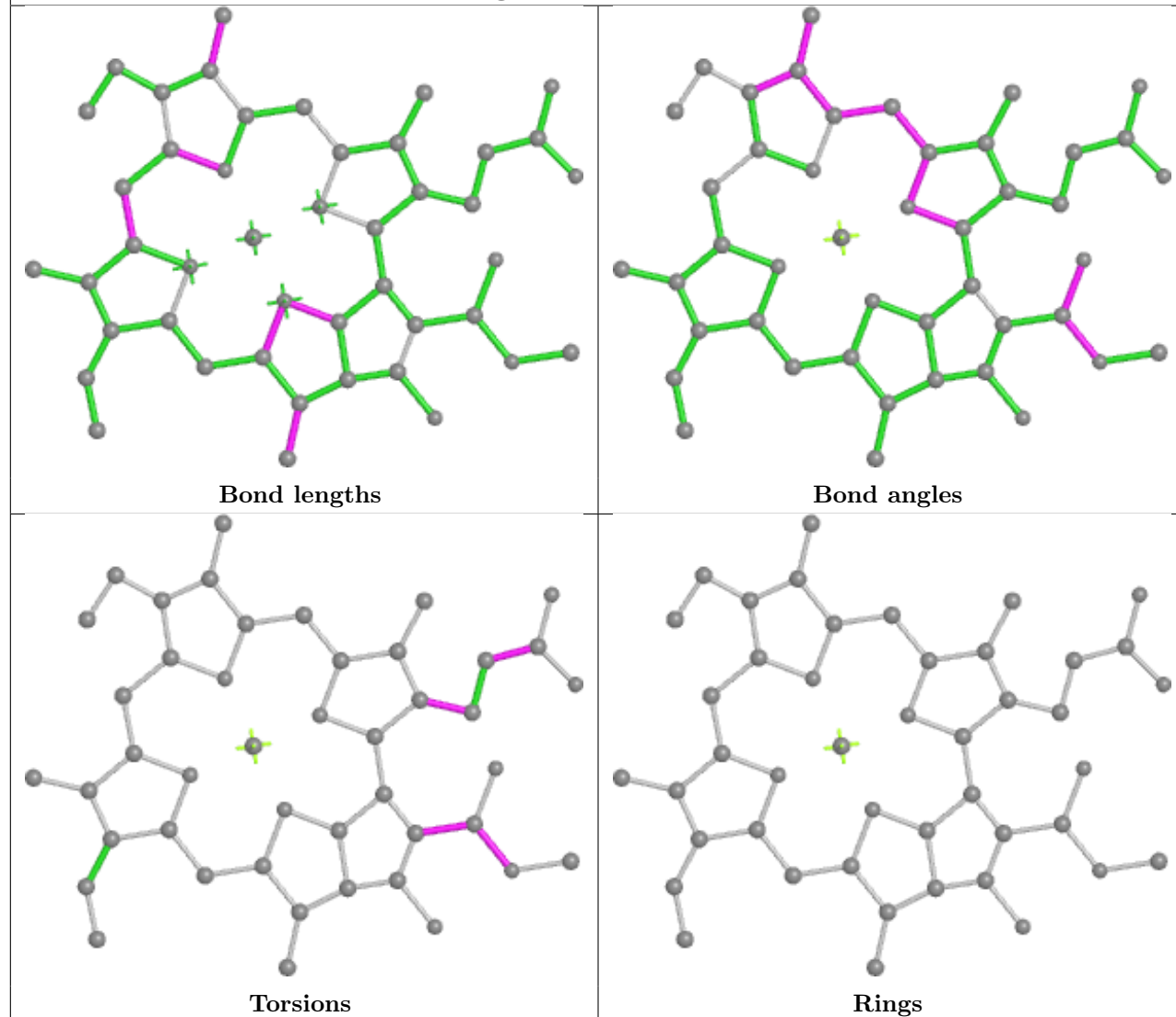
Ligand CLA v 509



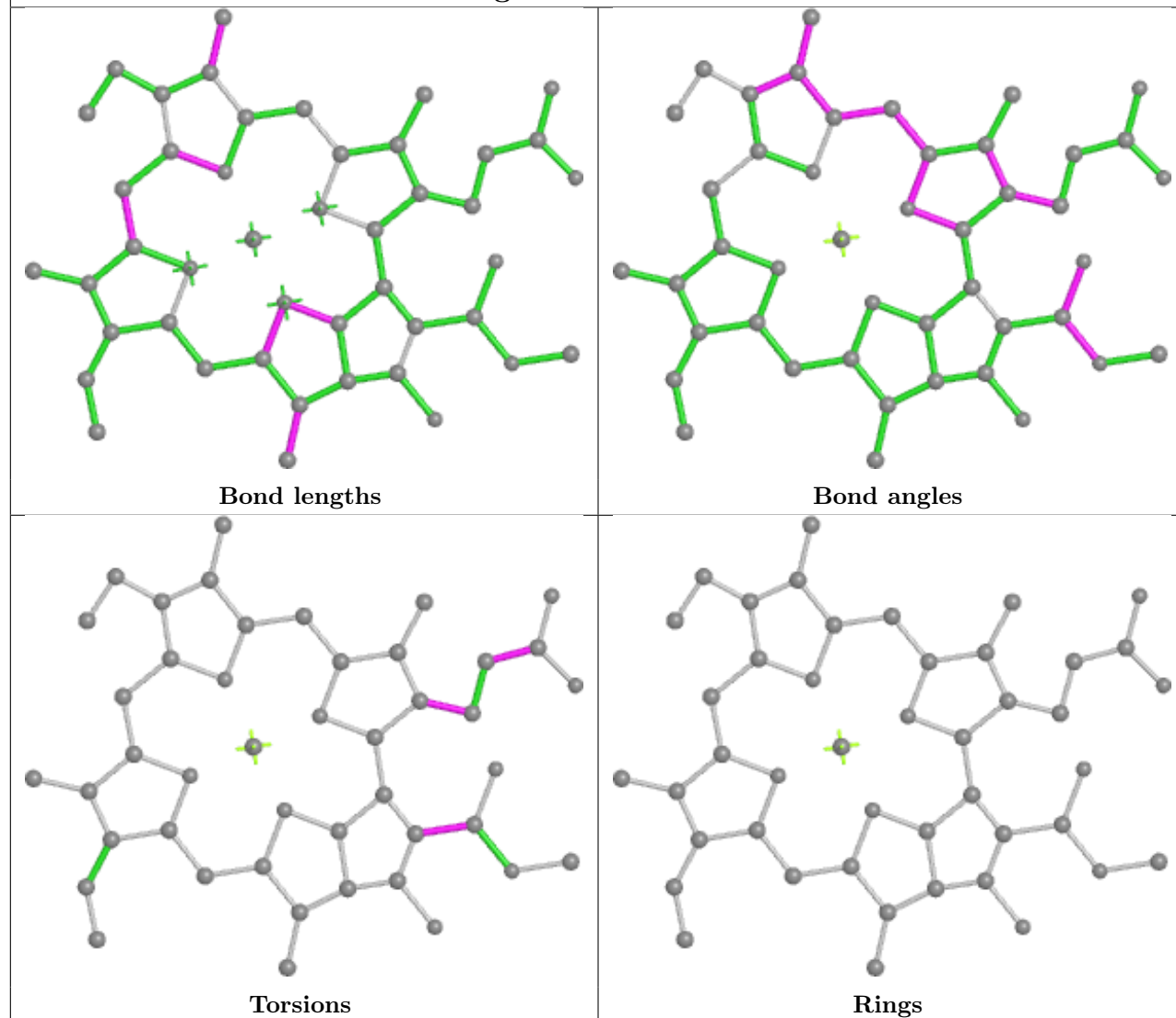
Ligand CLA G 1111



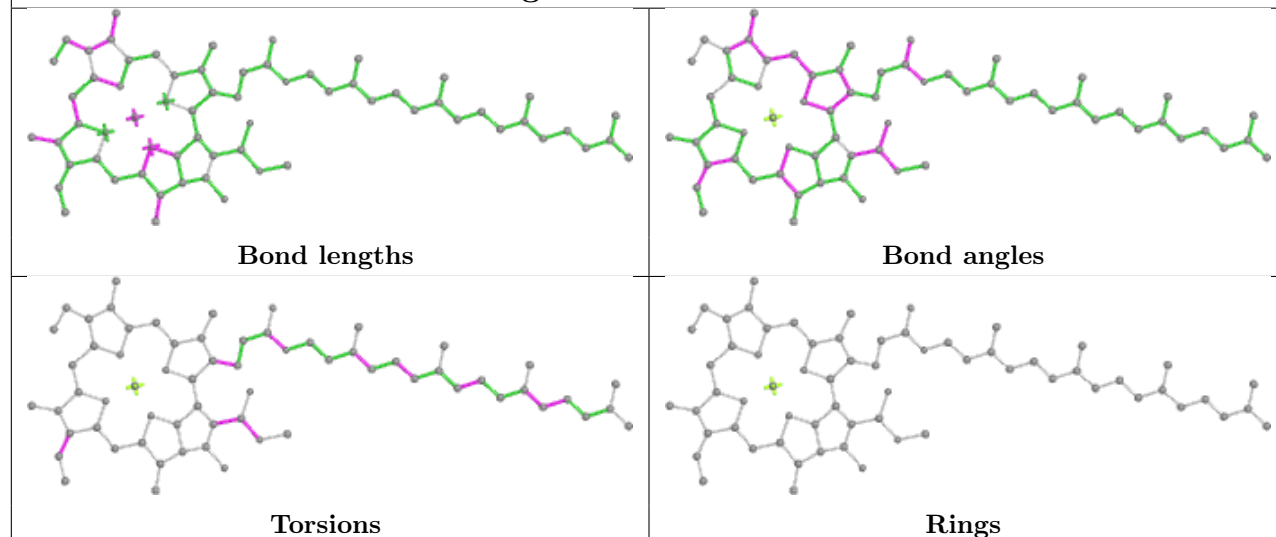
Ligand CLA d 518



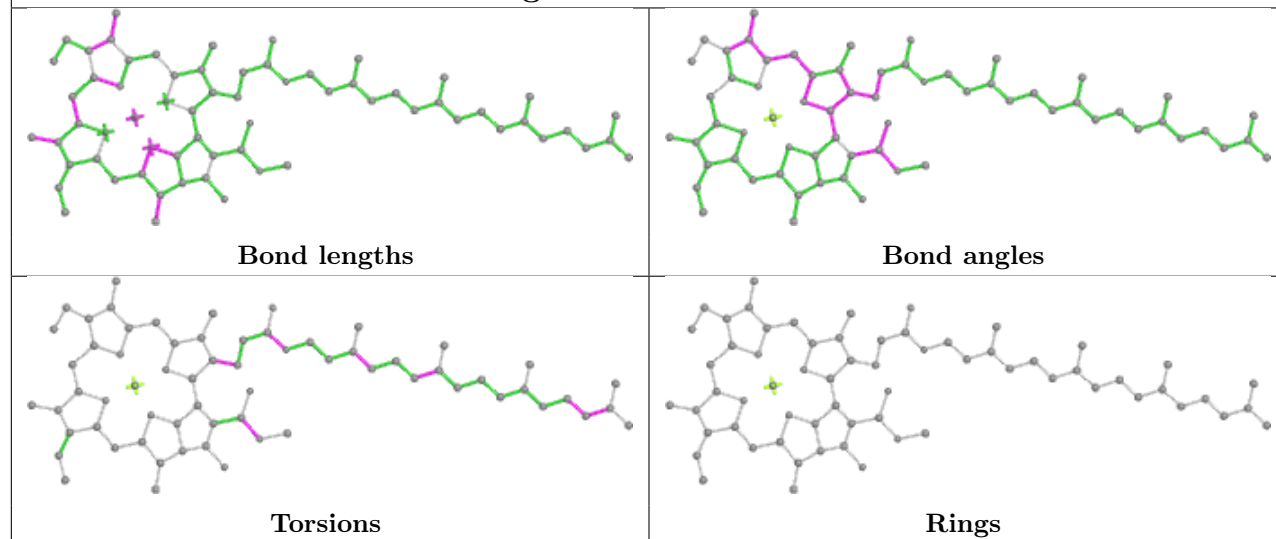
Ligand CLA 4 516



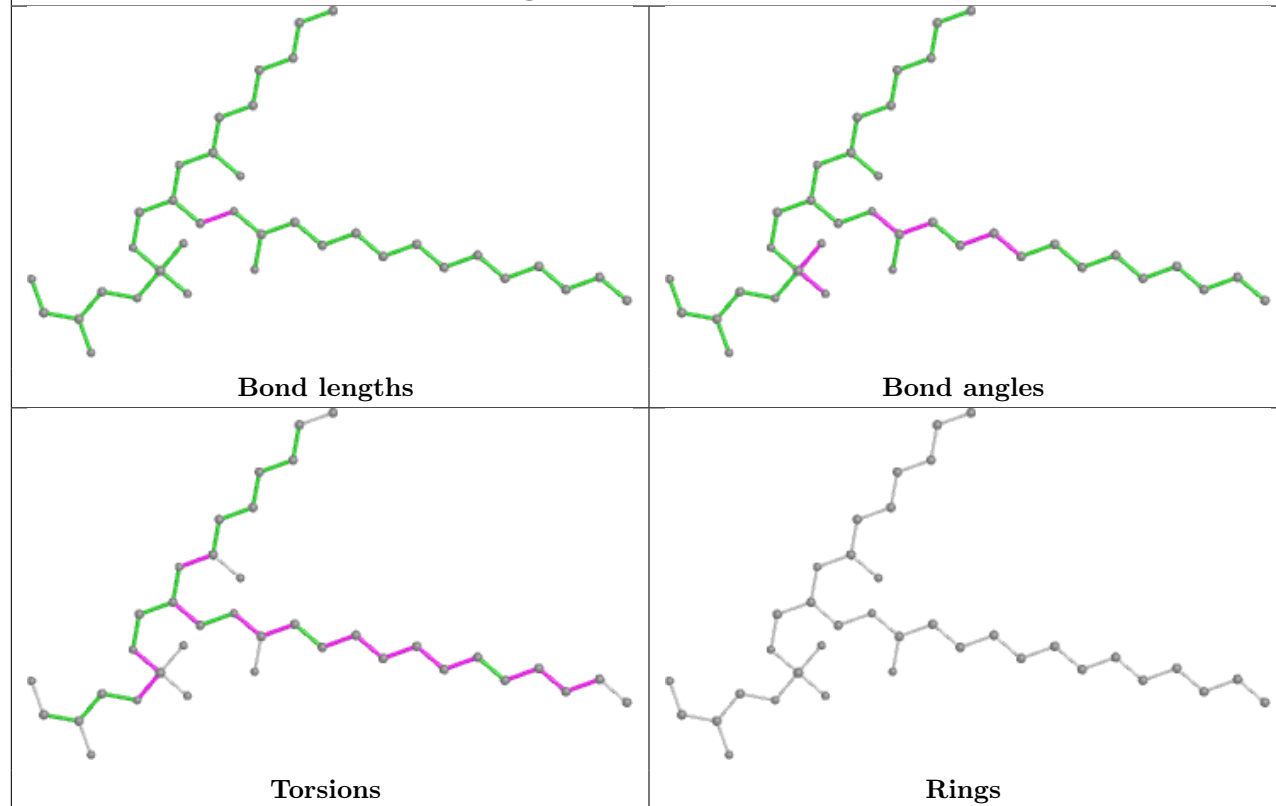
Ligand CLA G 1132



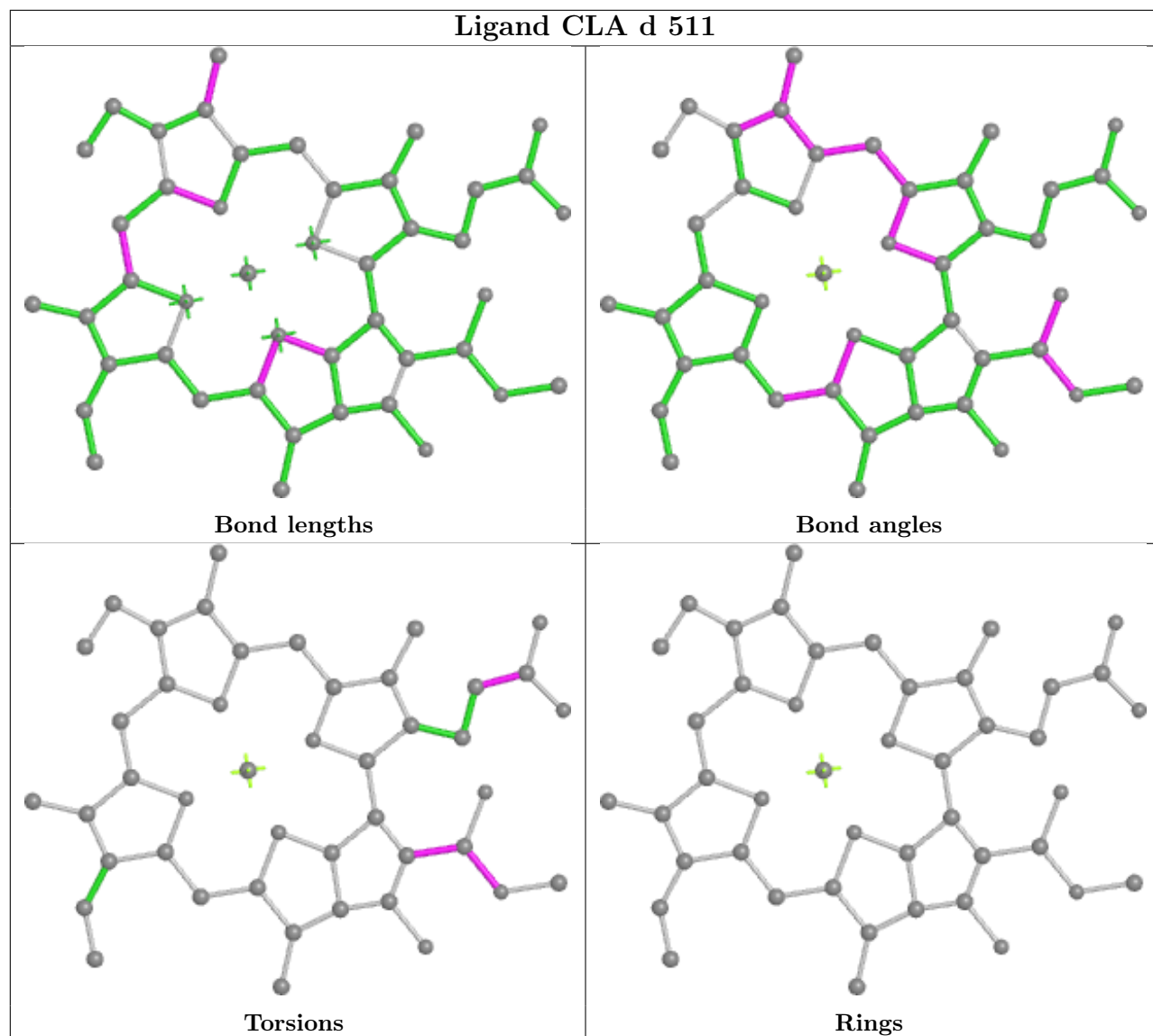
Ligand CLA A 1140



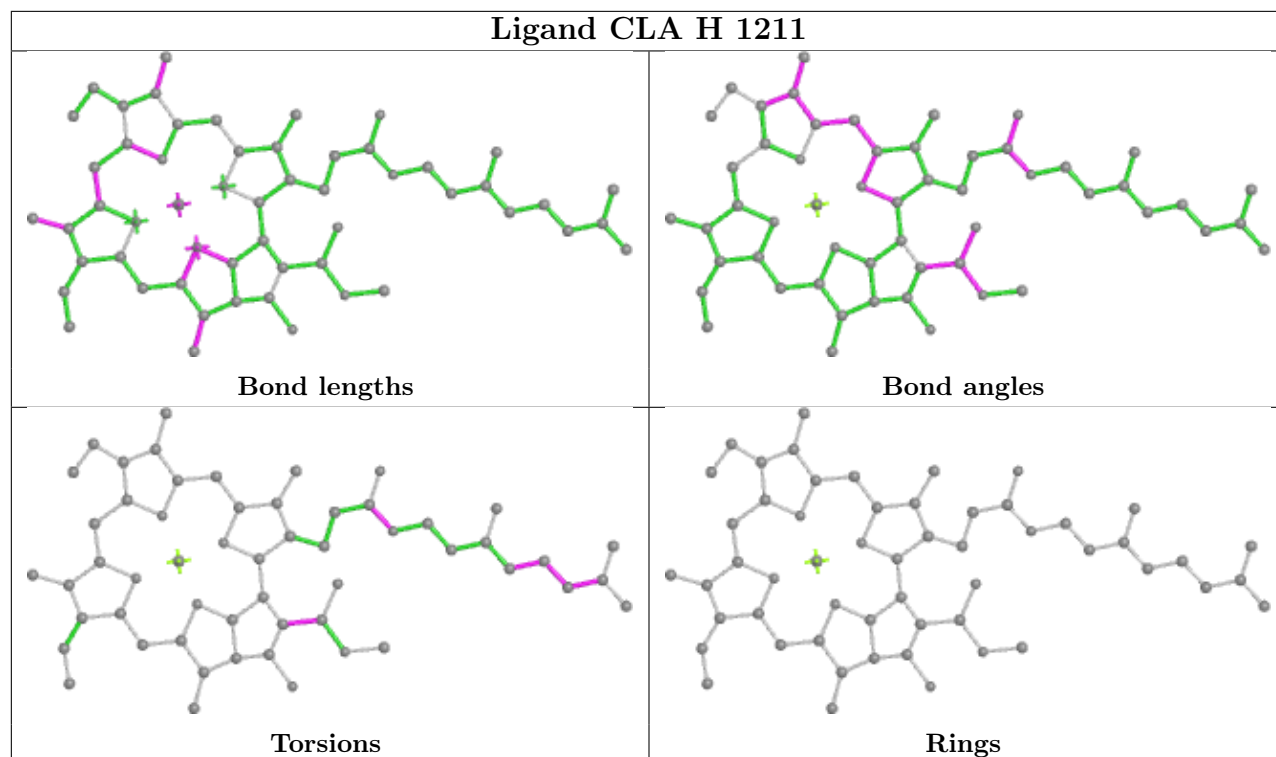
Ligand LHG H 1842



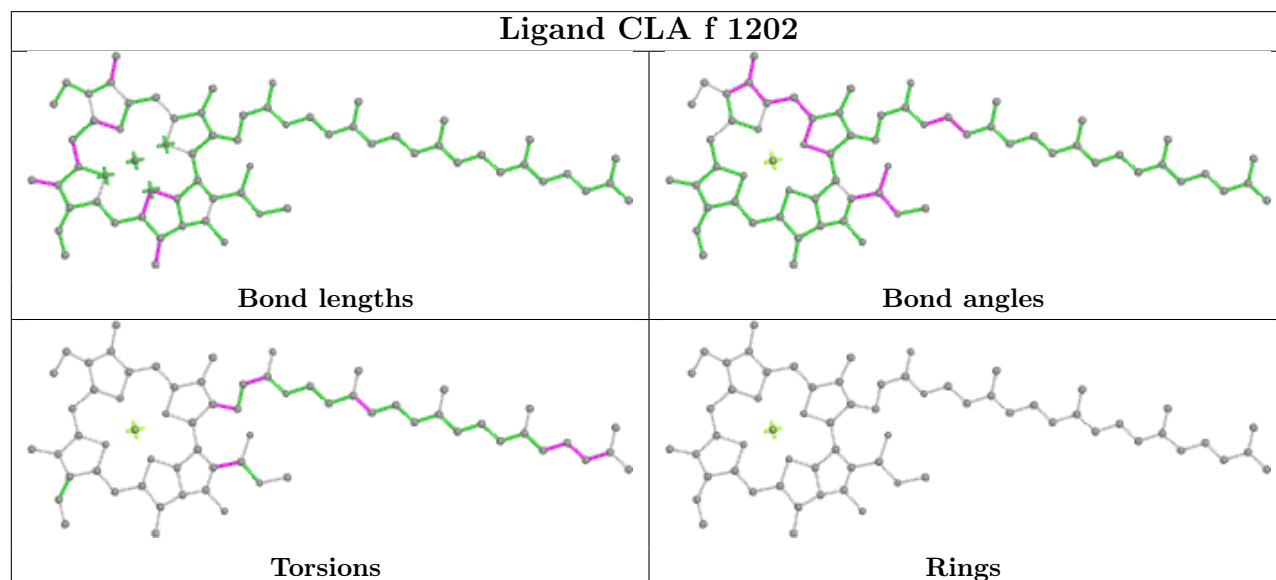
Ligand CLA d 511



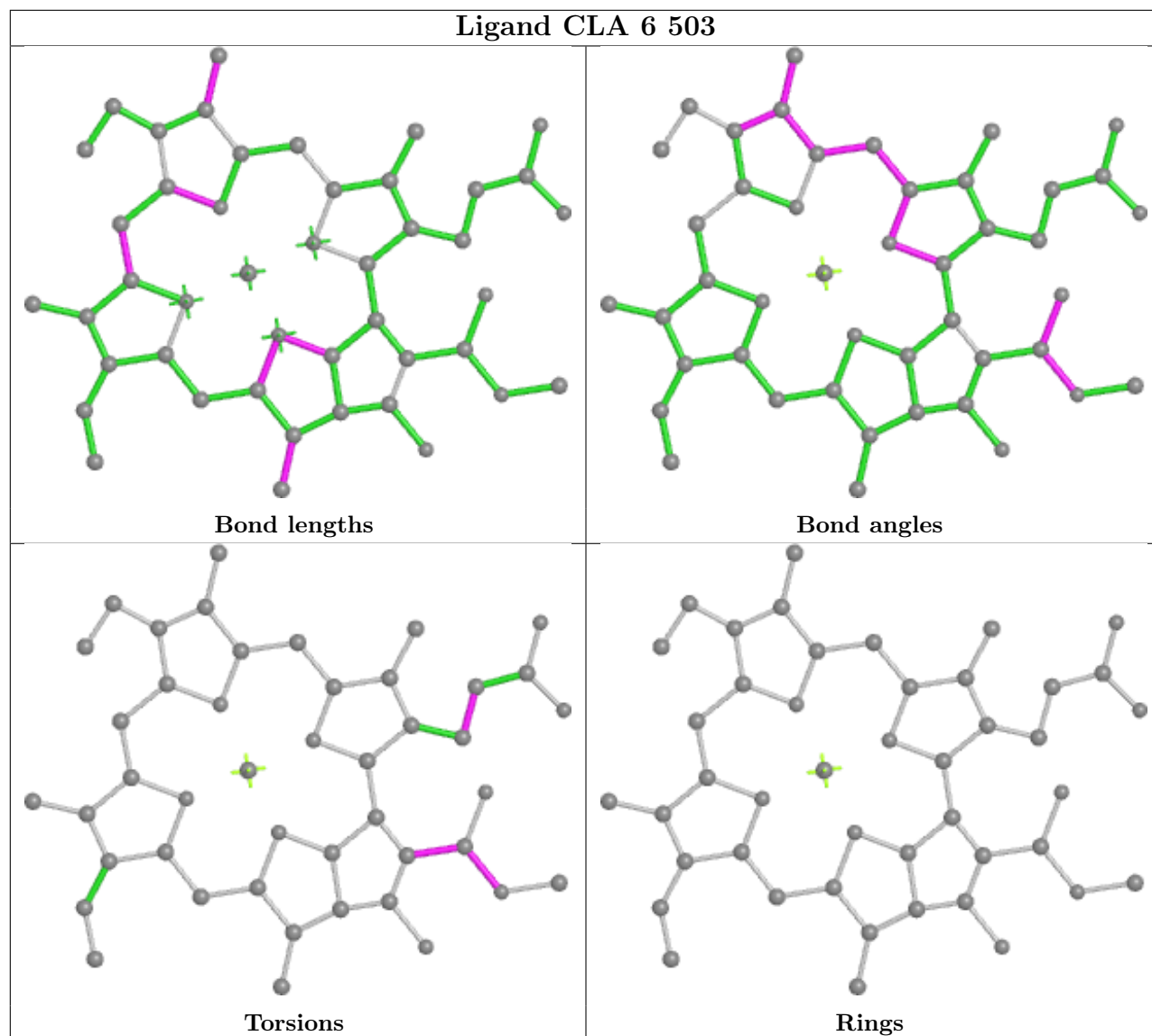
Ligand CLA H 1211



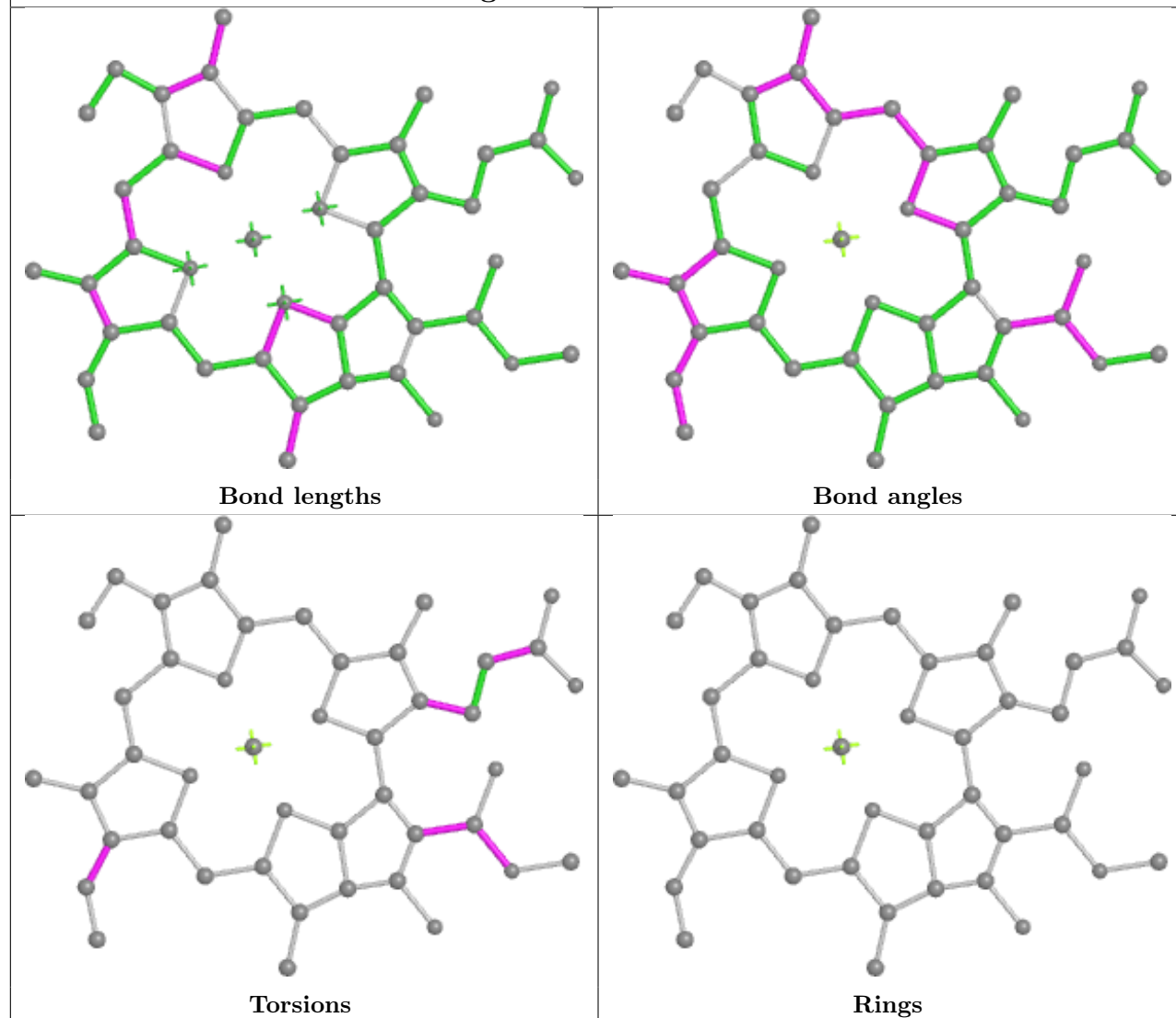
Ligand CLA f 1202



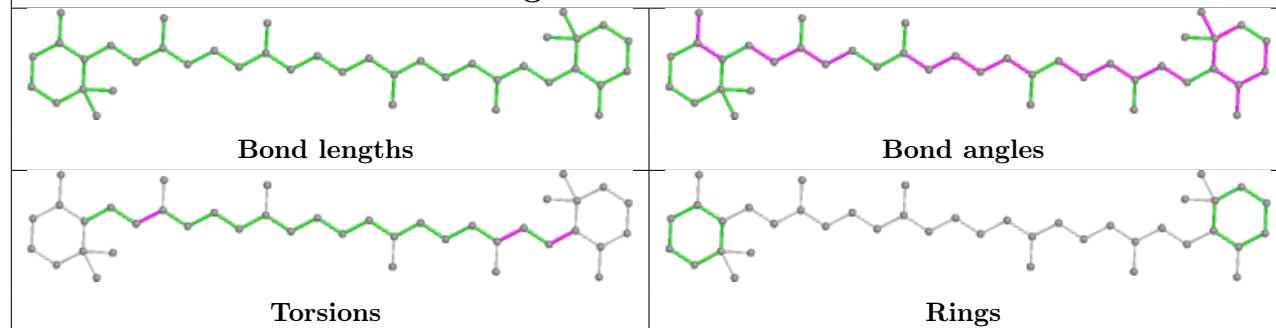
Ligand CLA 6 503



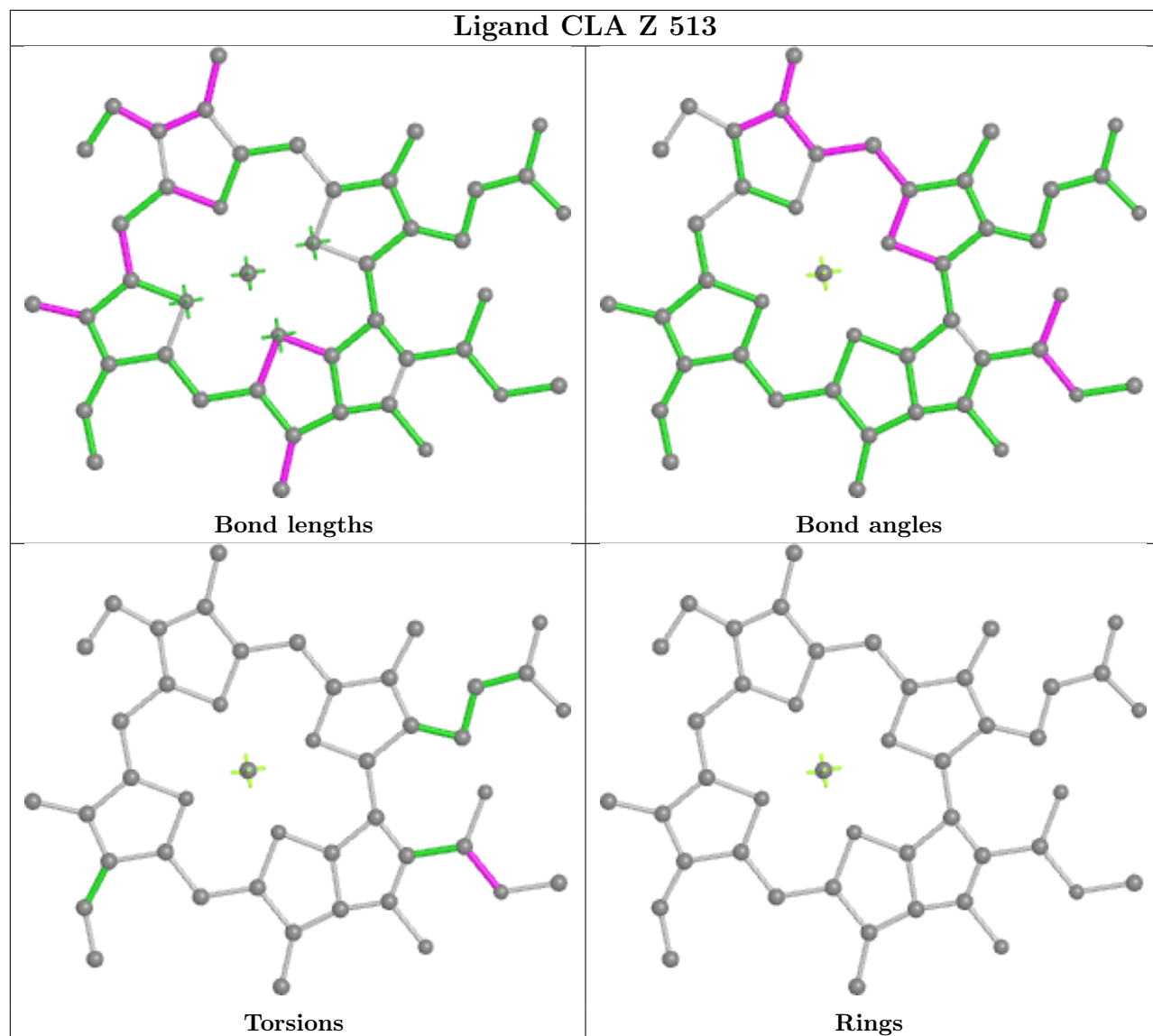
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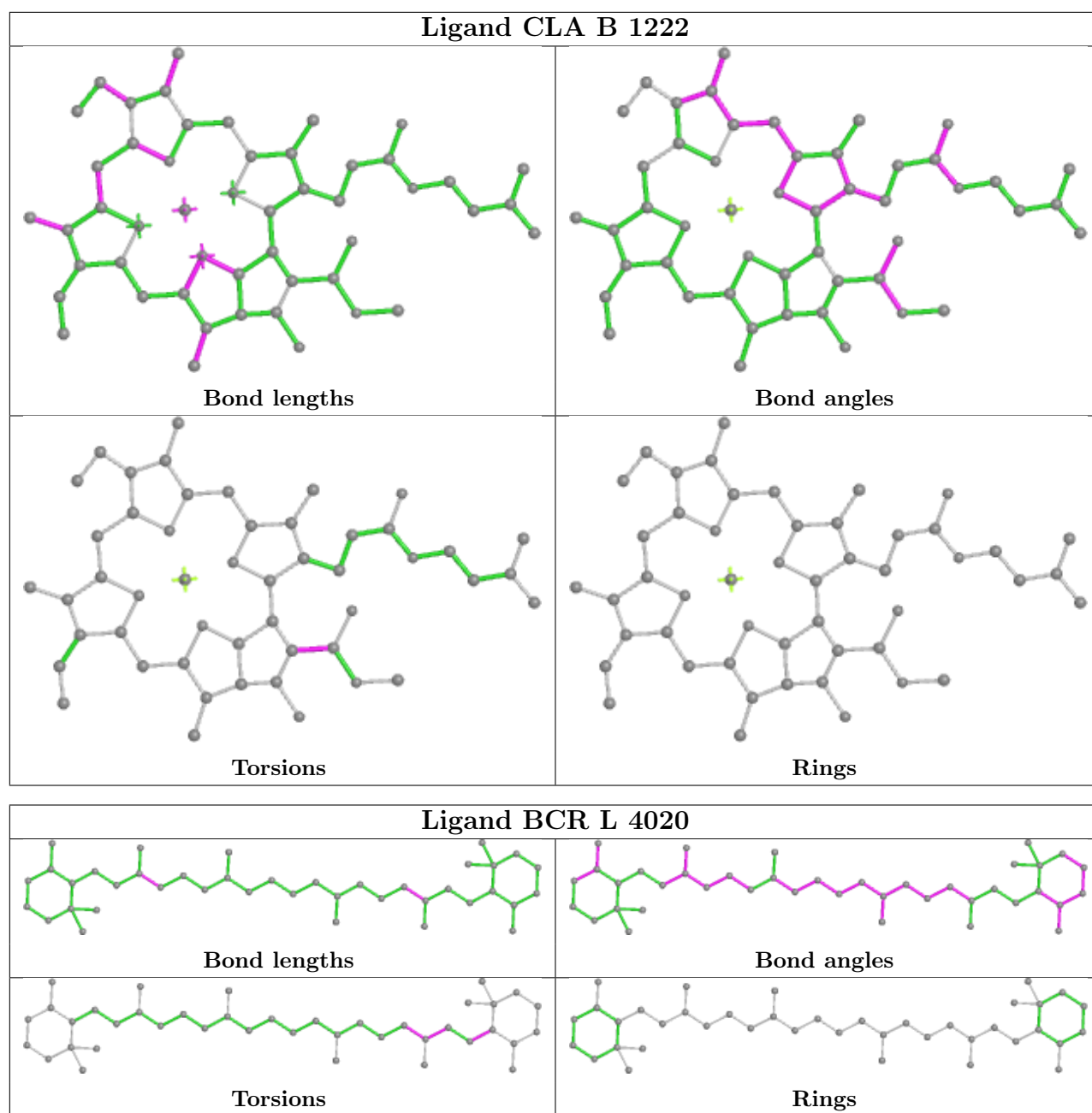


Ligand BCR L 4019

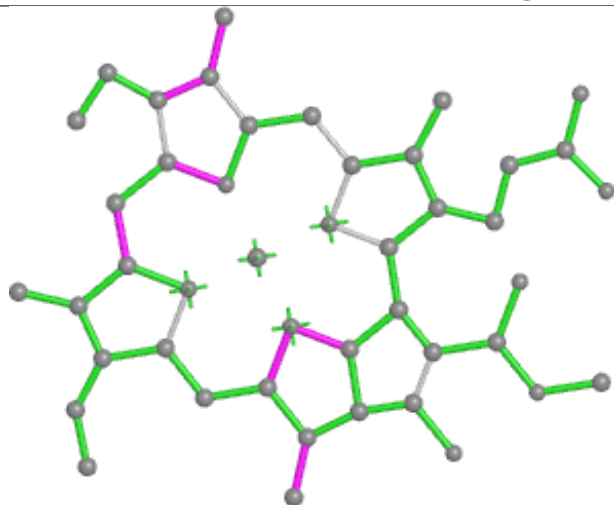


Ligand CLA Z 513

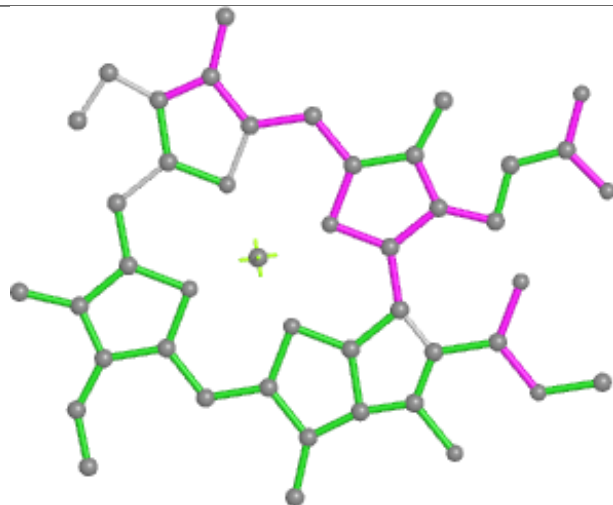




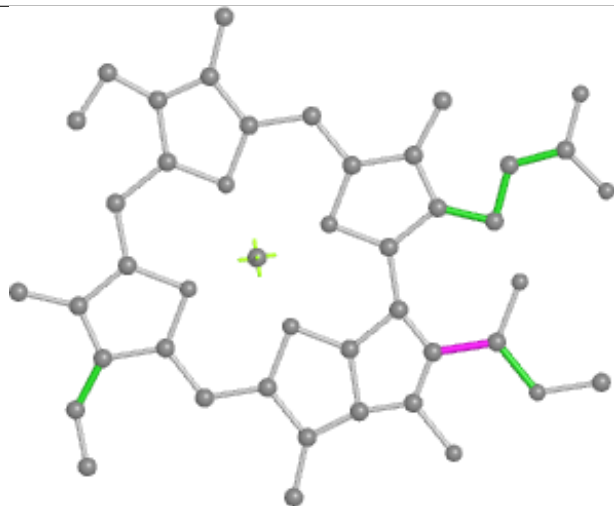
Ligand CLA 3 502



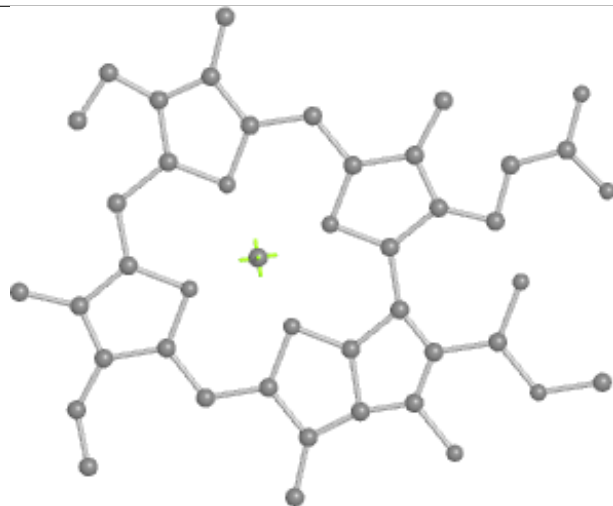
Bond lengths



Bond angles

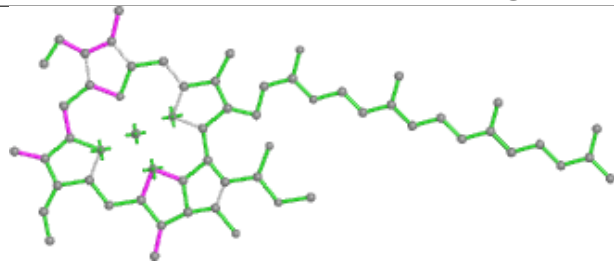


Torsions

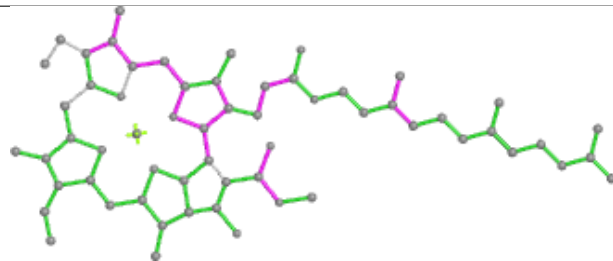


Rings

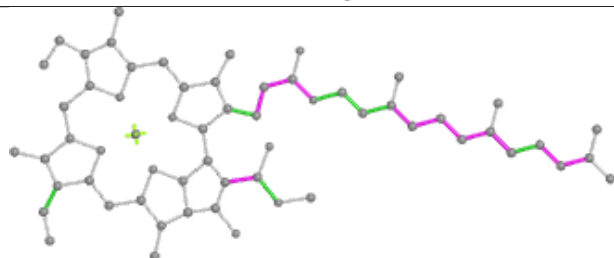
Ligand CLA A 1137



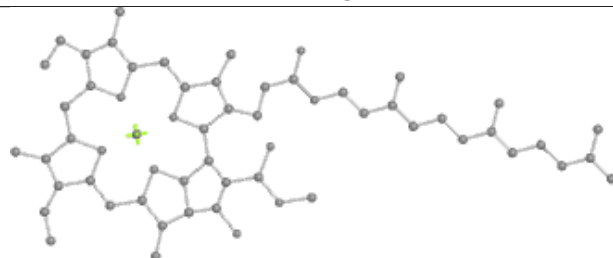
Bond lengths



Bond angles

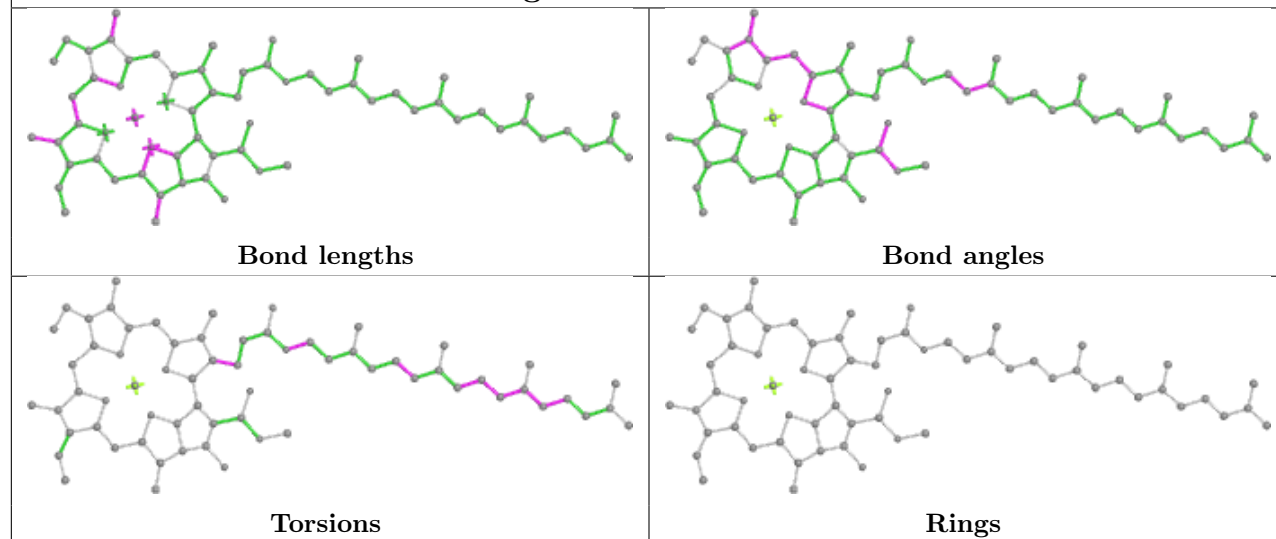


Torsions

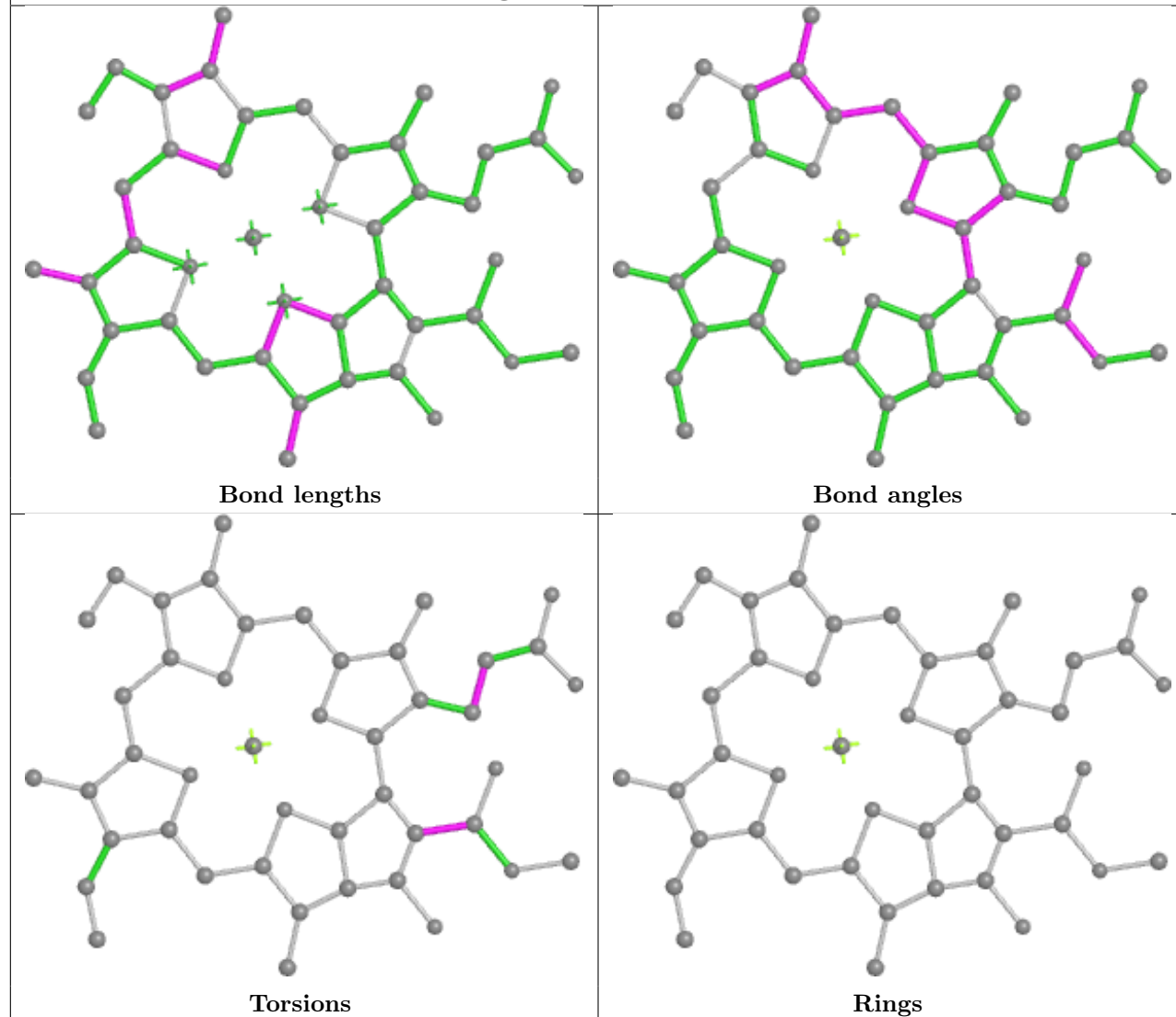


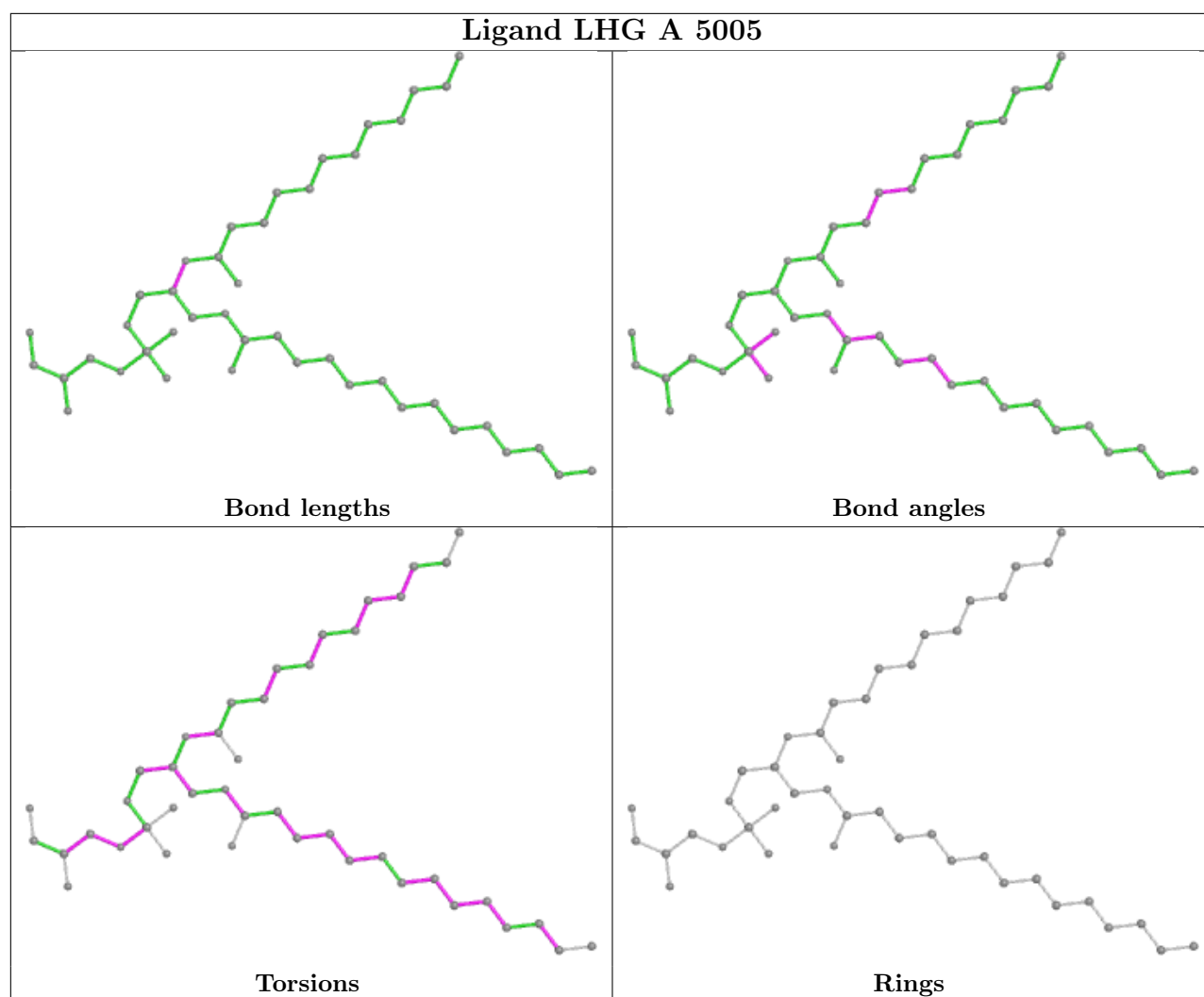
Rings

Ligand CLA B 1223

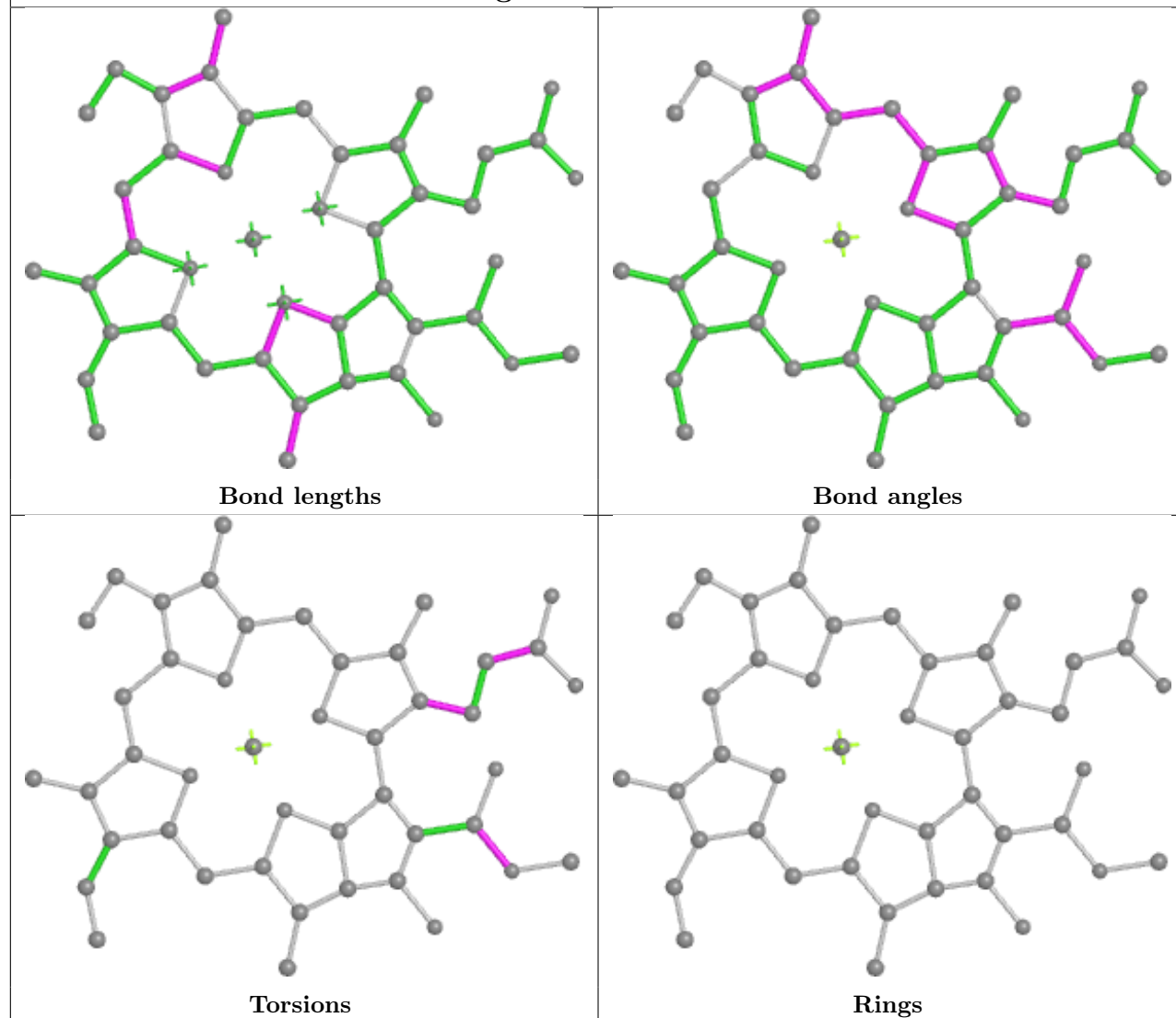


Ligand CLA t 502

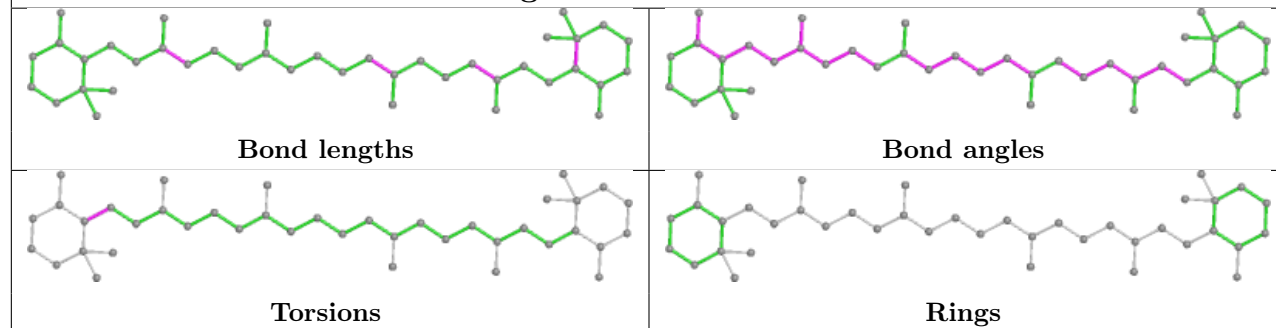




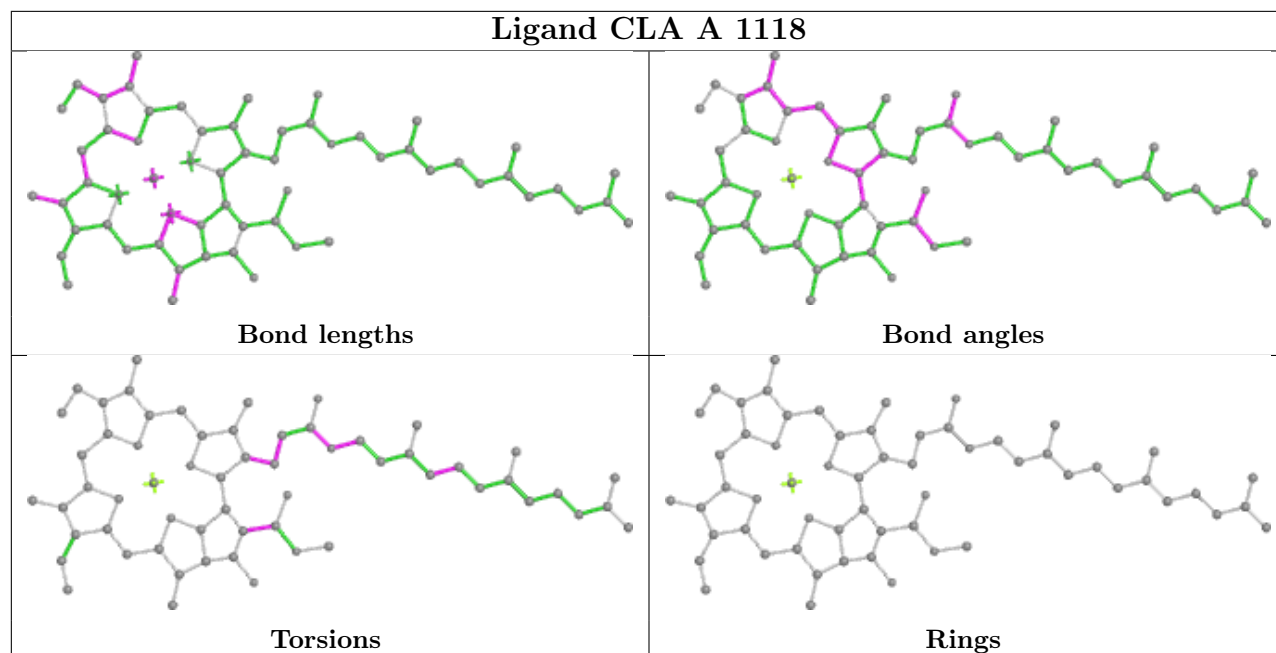
Ligand CLA r 516



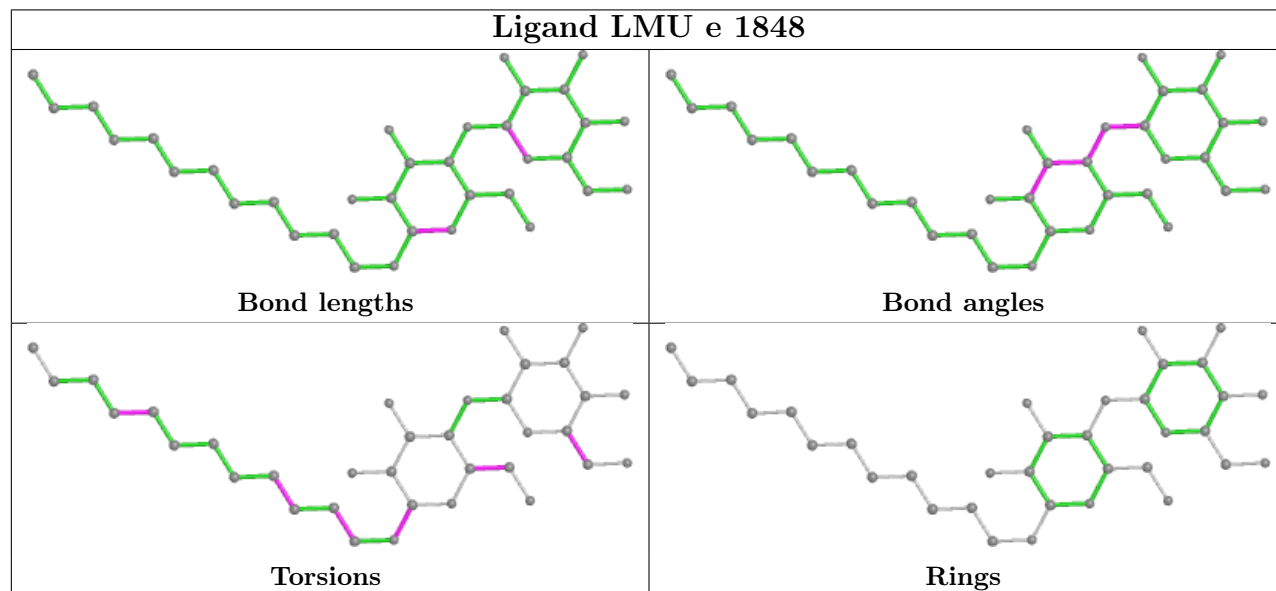
Ligand BCR H 4017



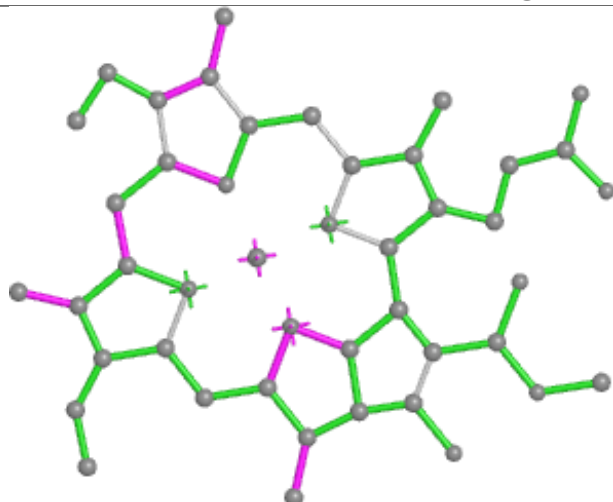
Ligand CLA A 1118



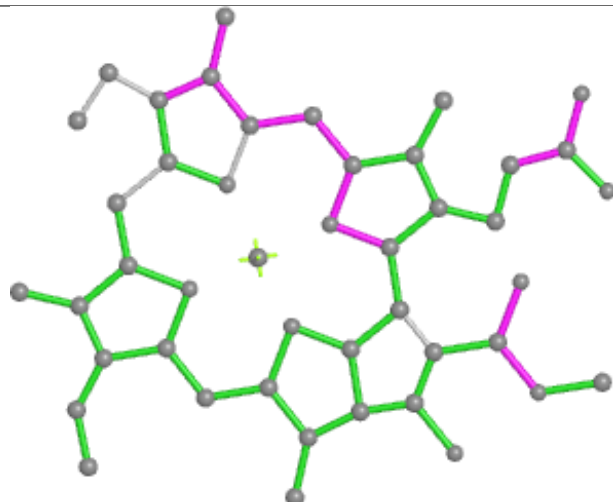
Ligand LMU e 1848



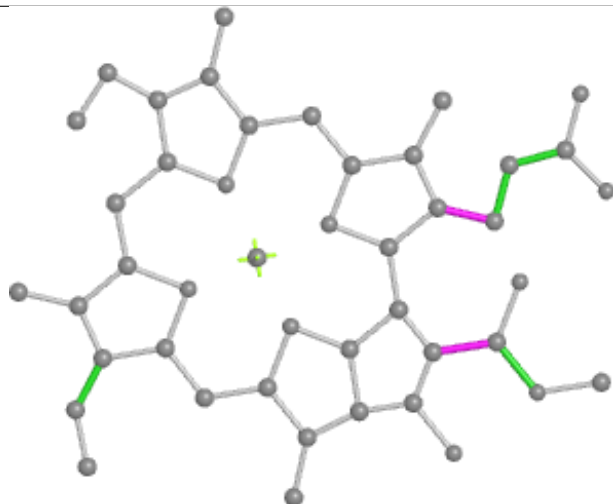
Ligand CLA 3 508



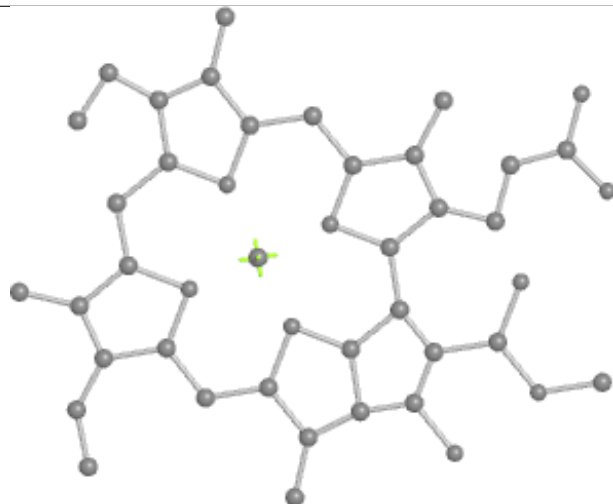
Bond lengths



Bond angles

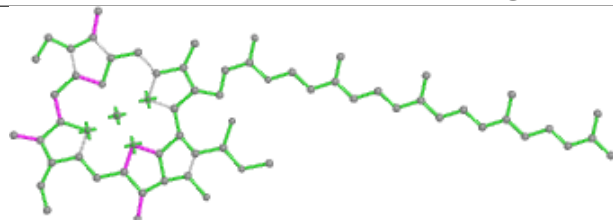


Torsions

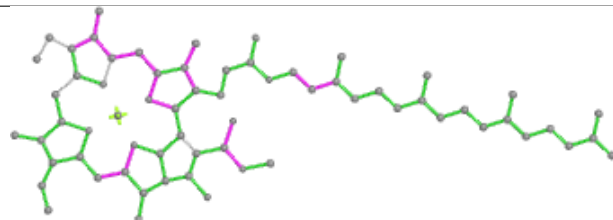


Rings

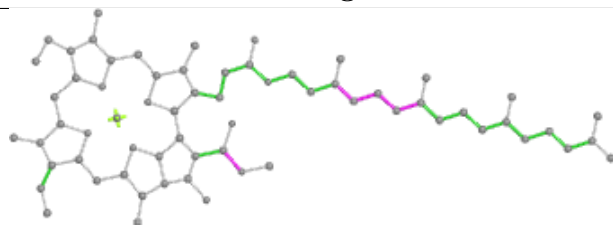
Ligand CLA H 1231



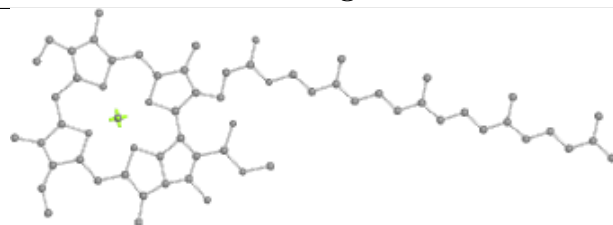
Bond lengths



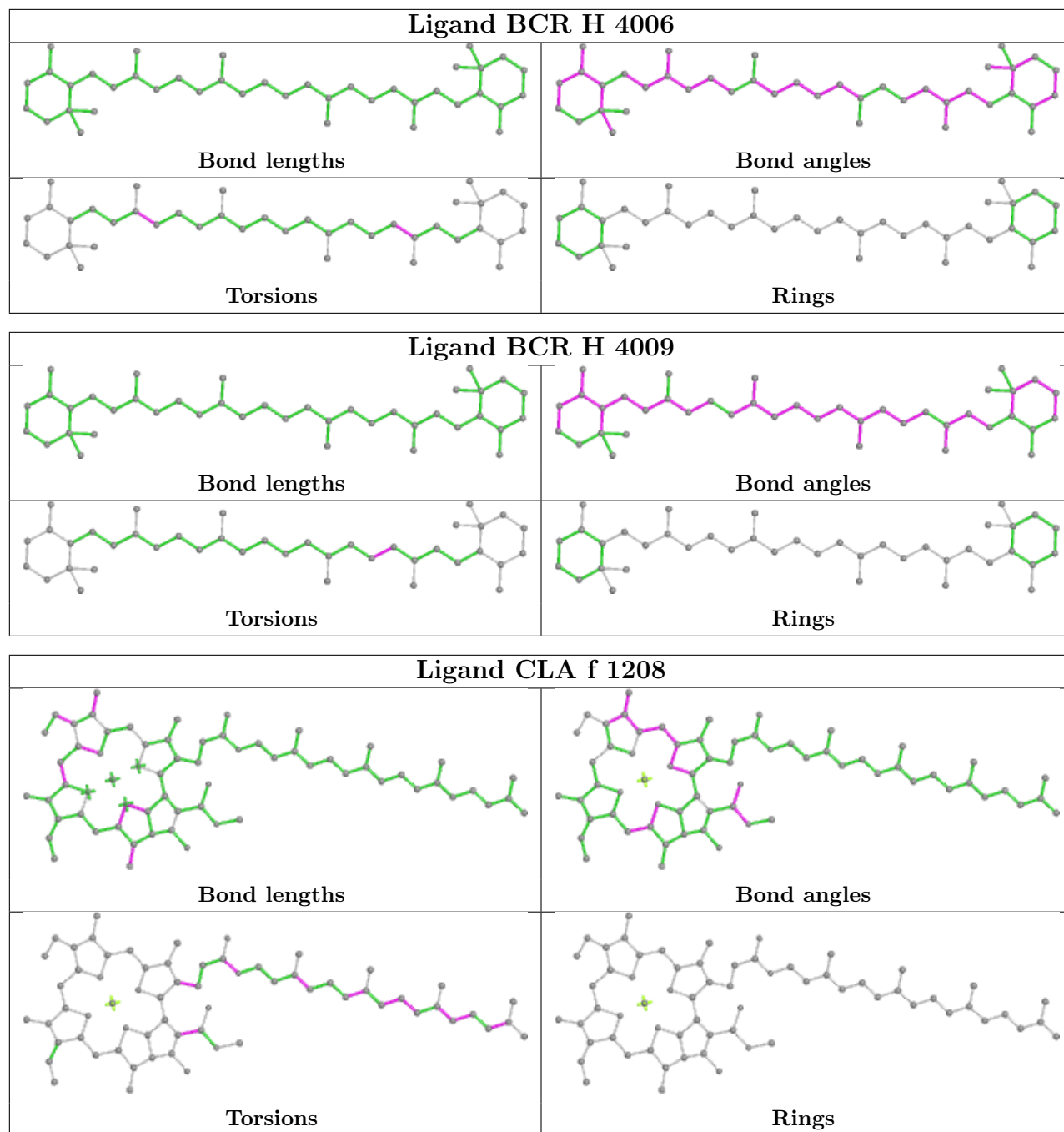
Bond angles



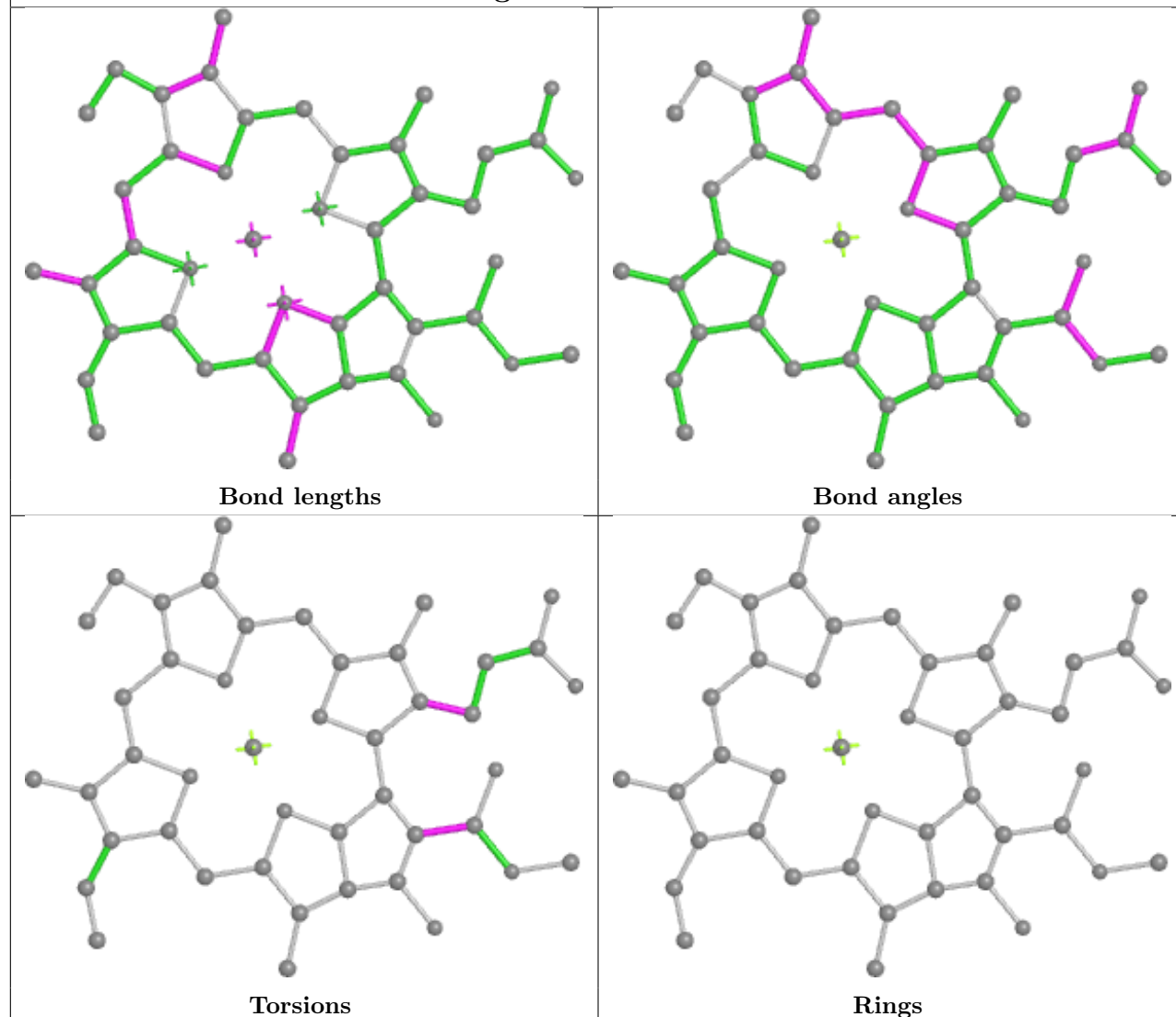
Torsions



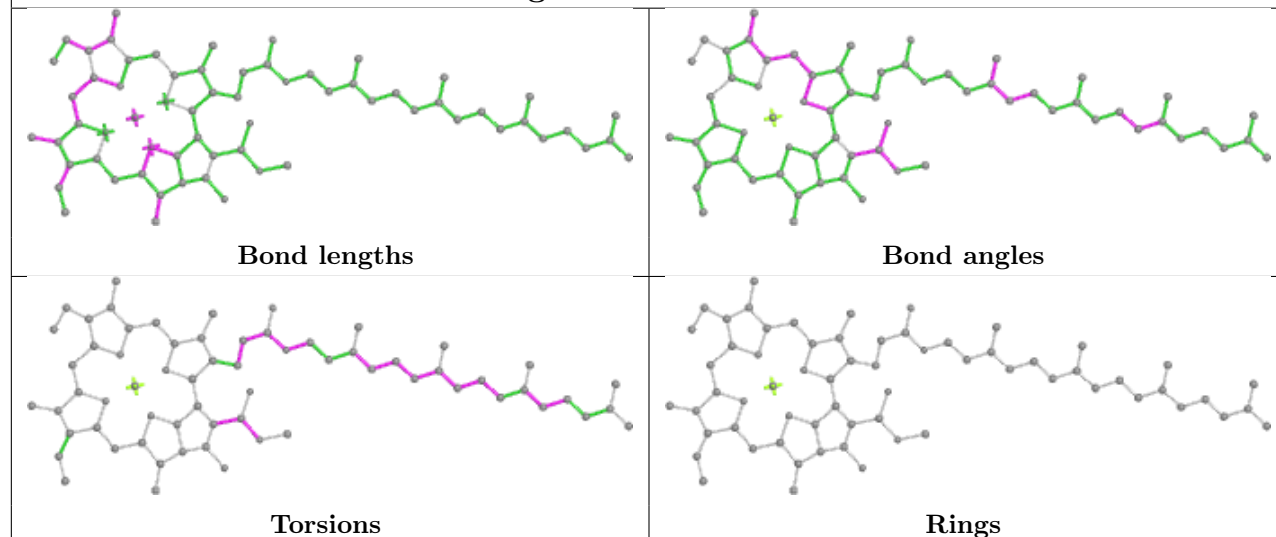
Rings

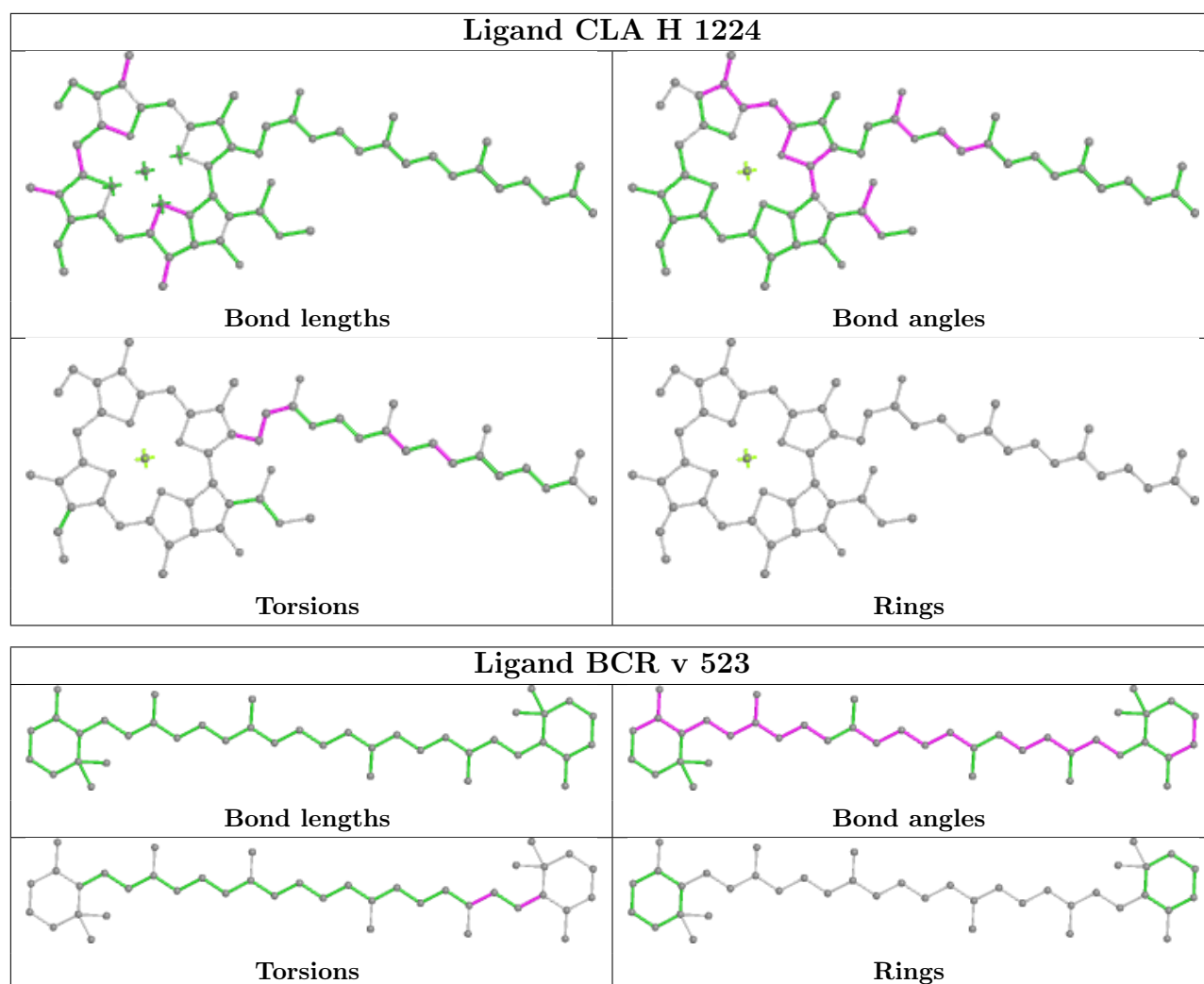


Ligand CLA a 508

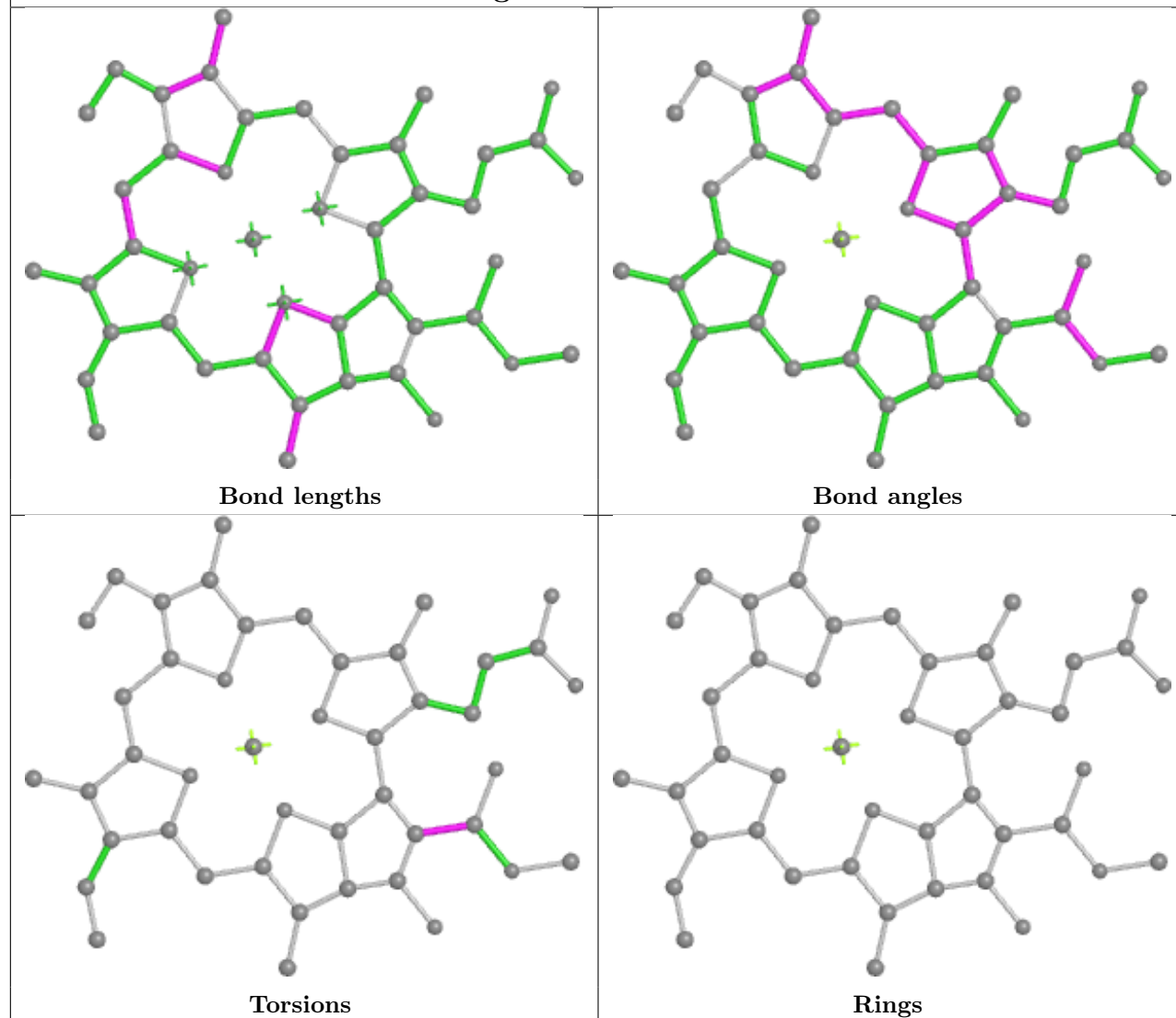


Ligand CLA e 1237

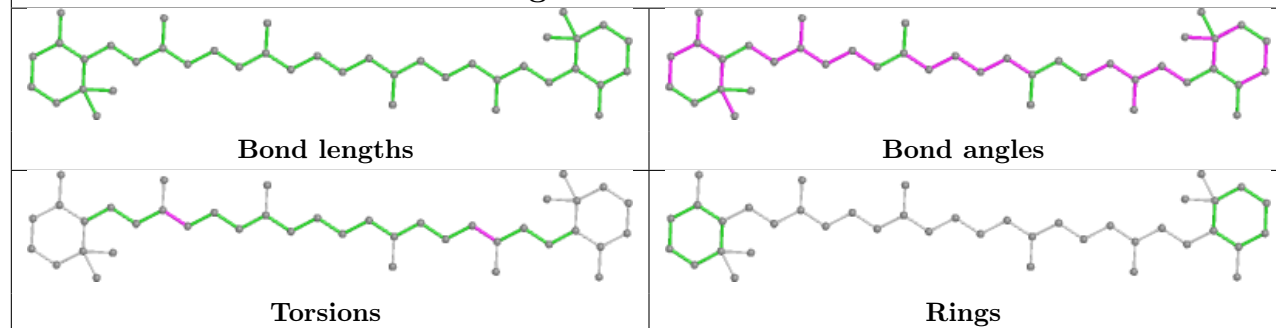


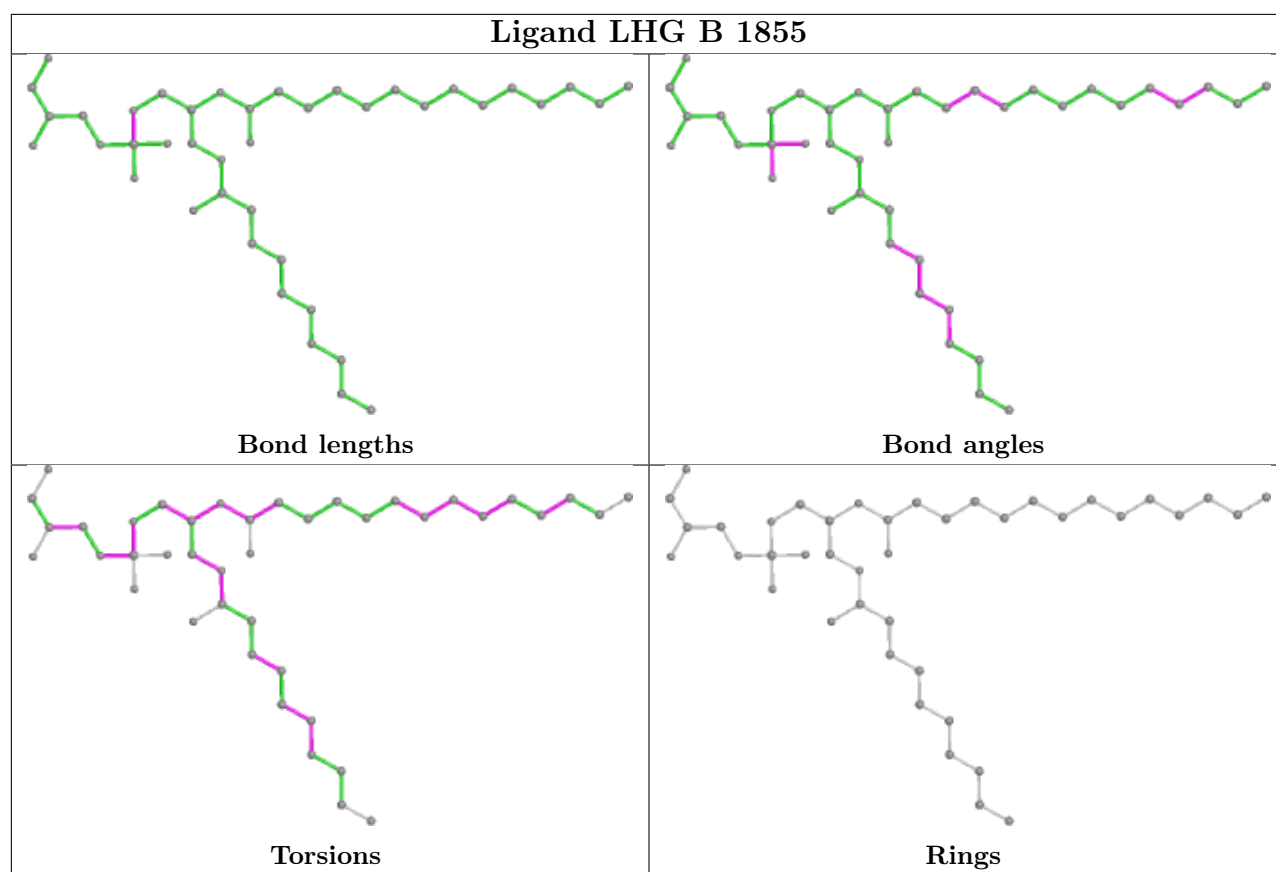


Ligand CLA v 502

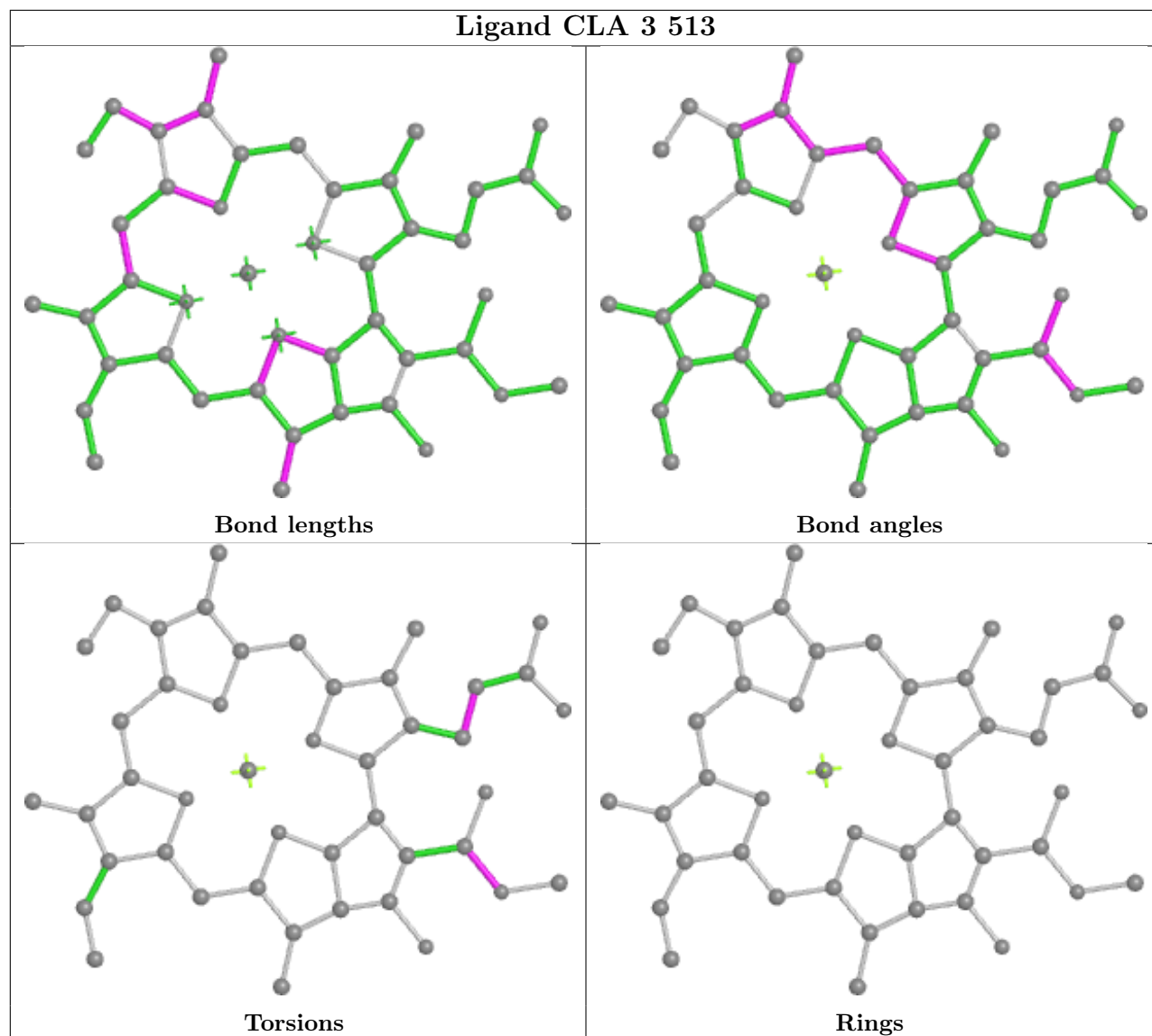


Ligand BCR f 4006

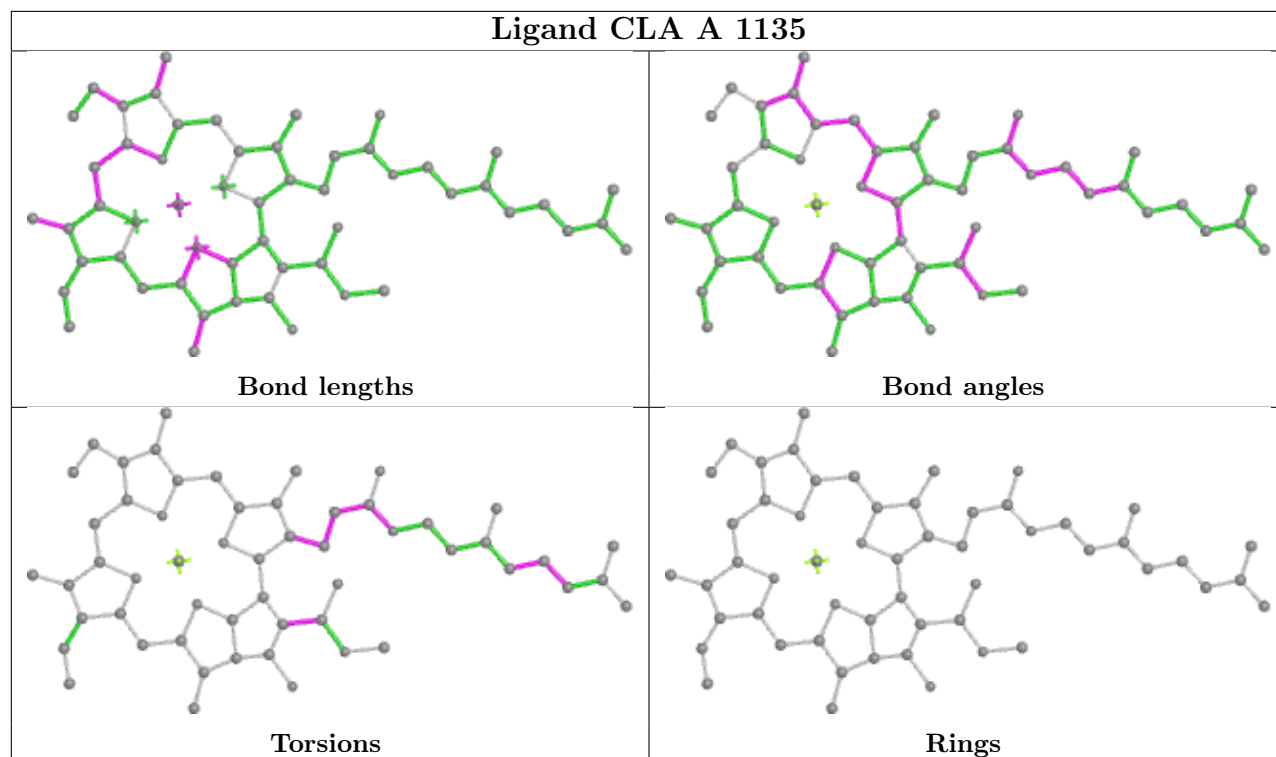




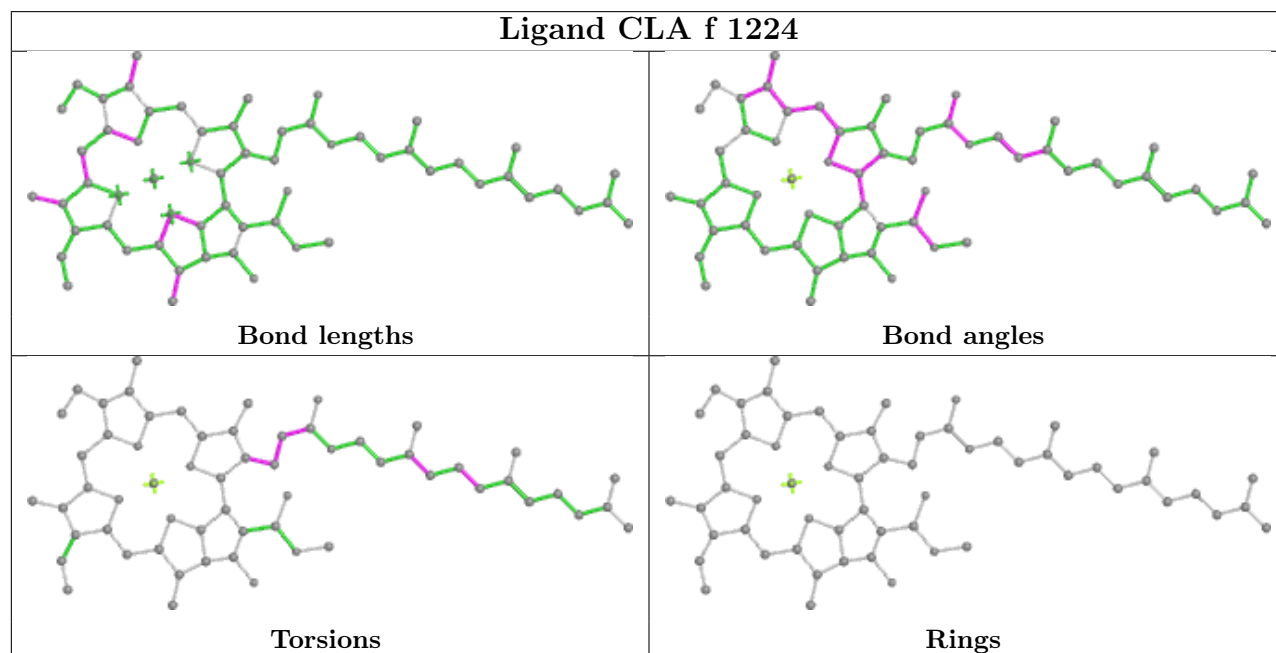
Ligand CLA 3 513

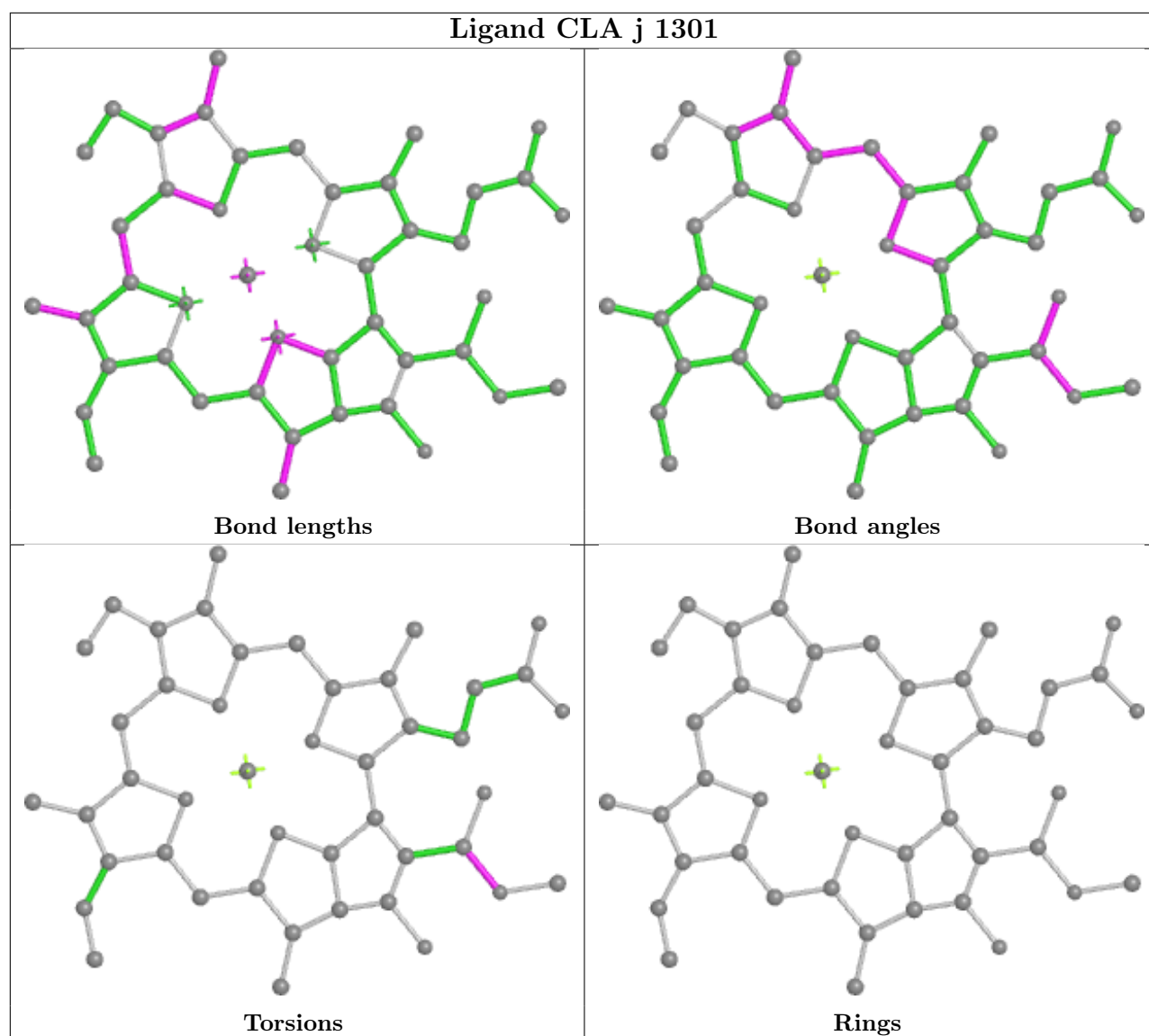


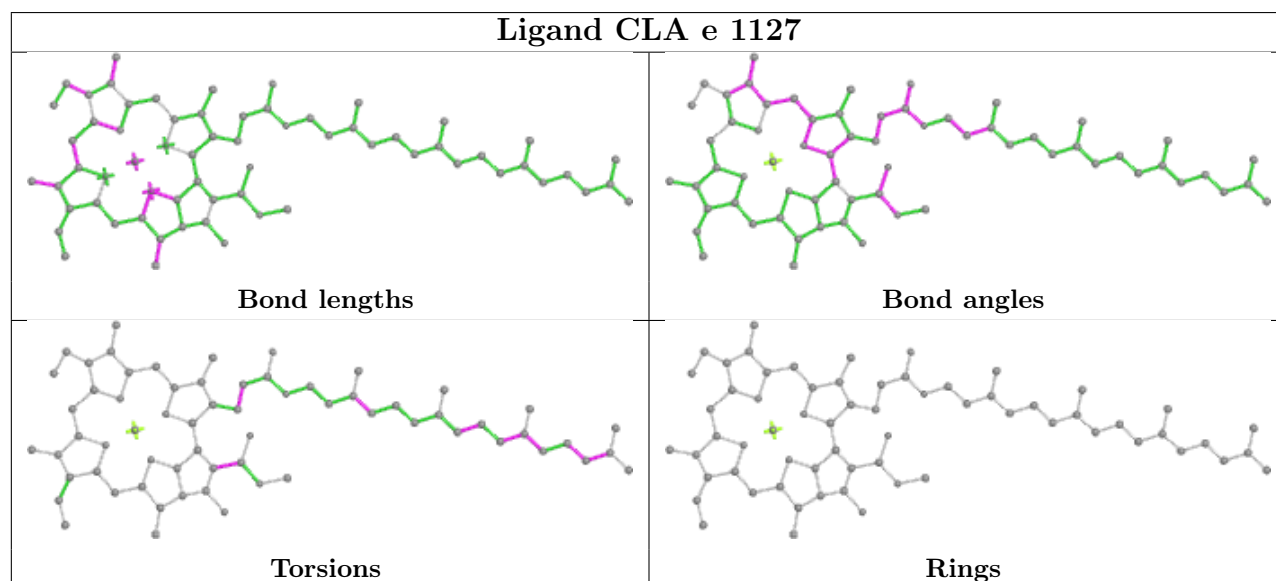
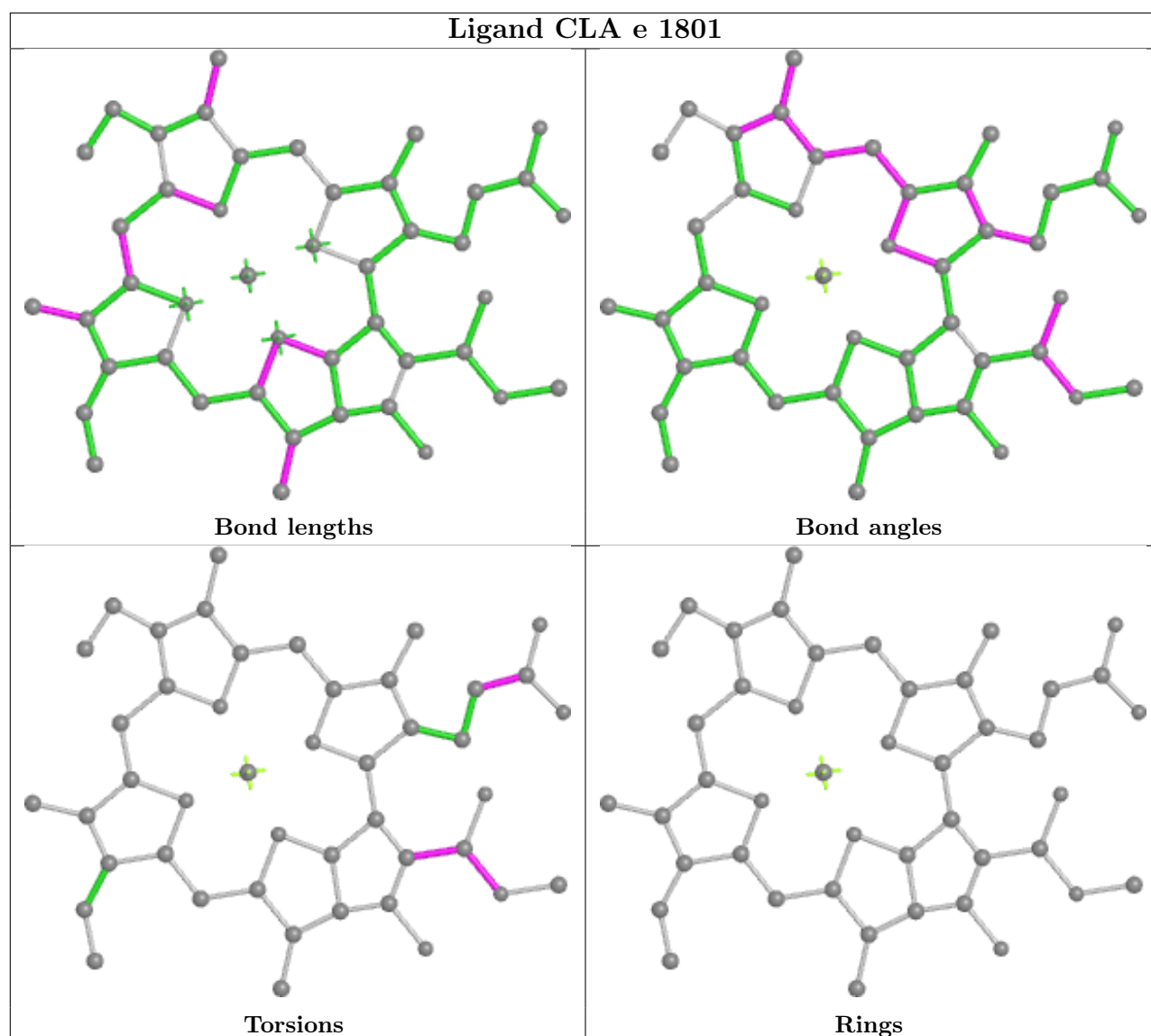
Ligand CLA A 1135



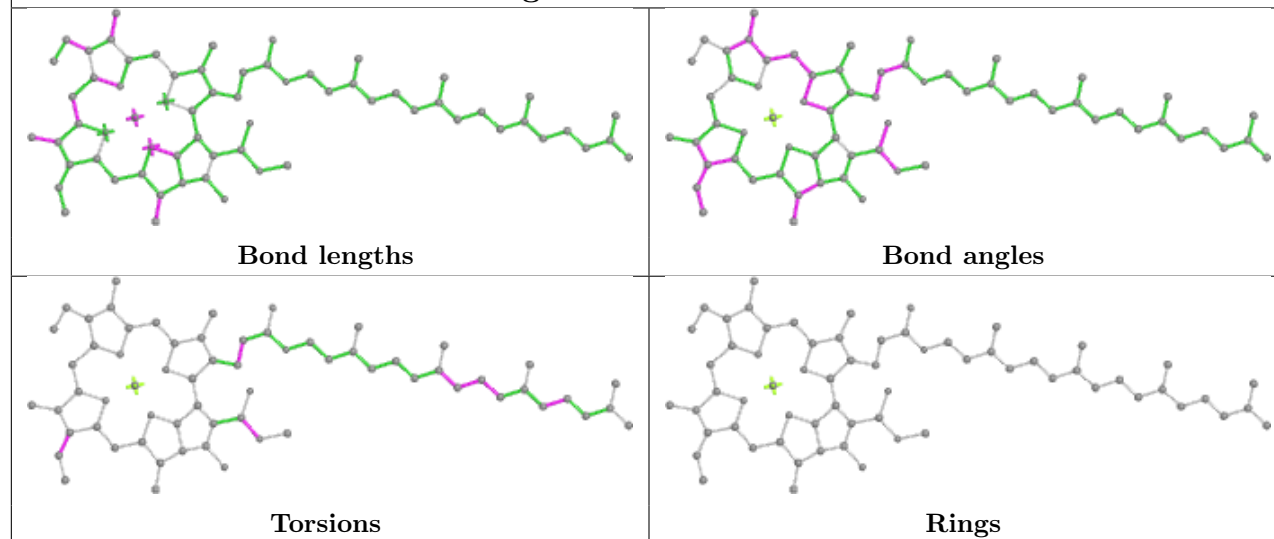
Ligand CLA f 1224



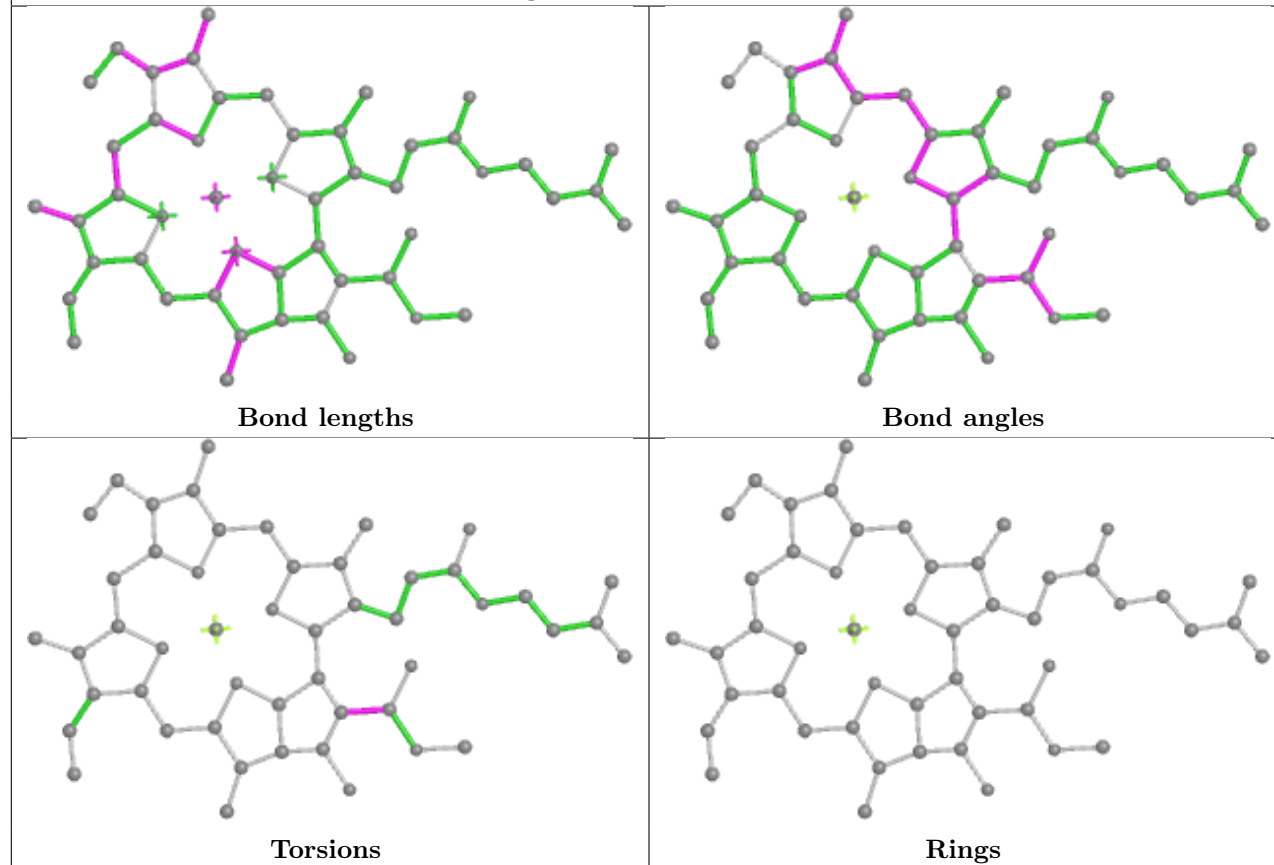


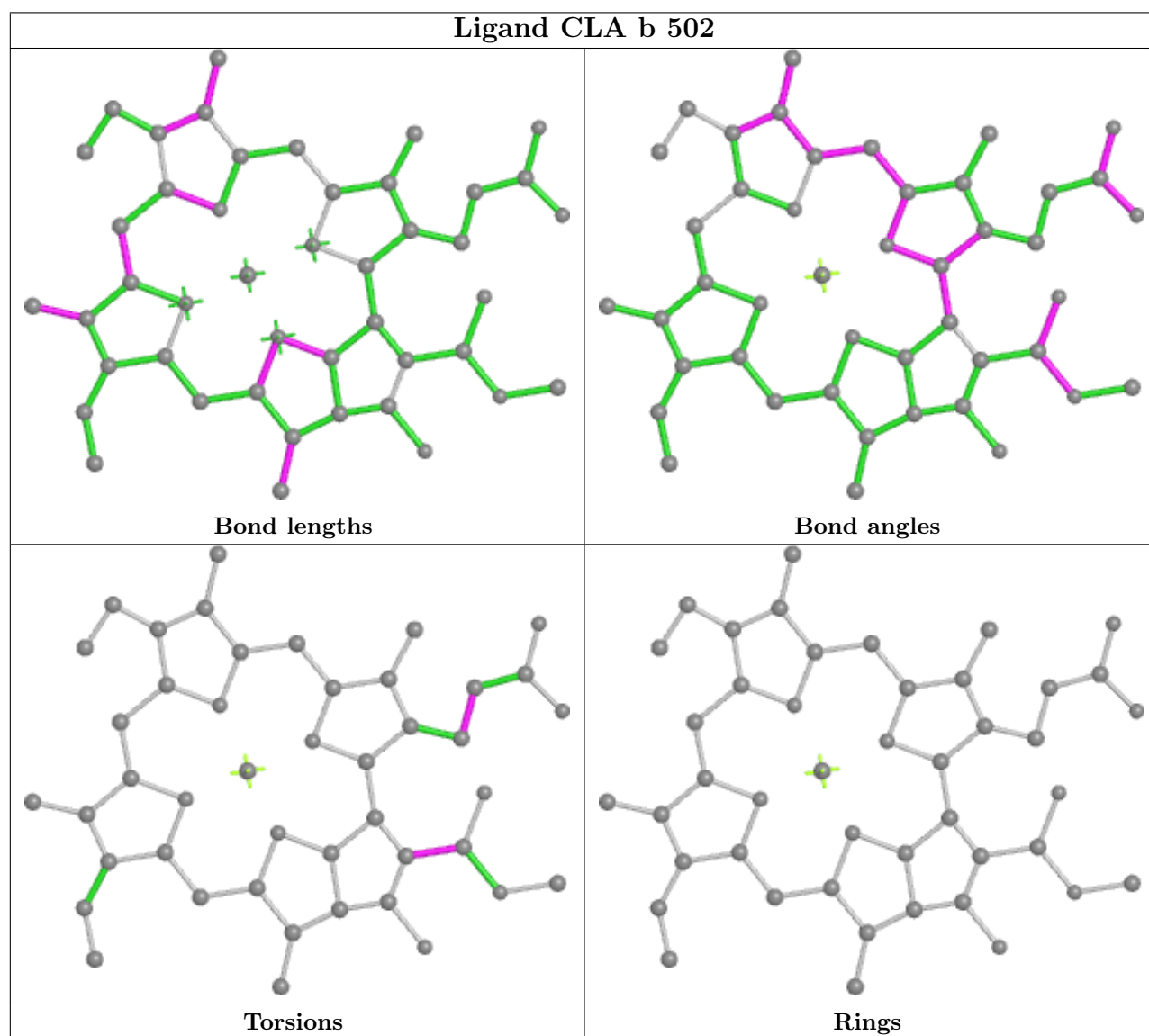
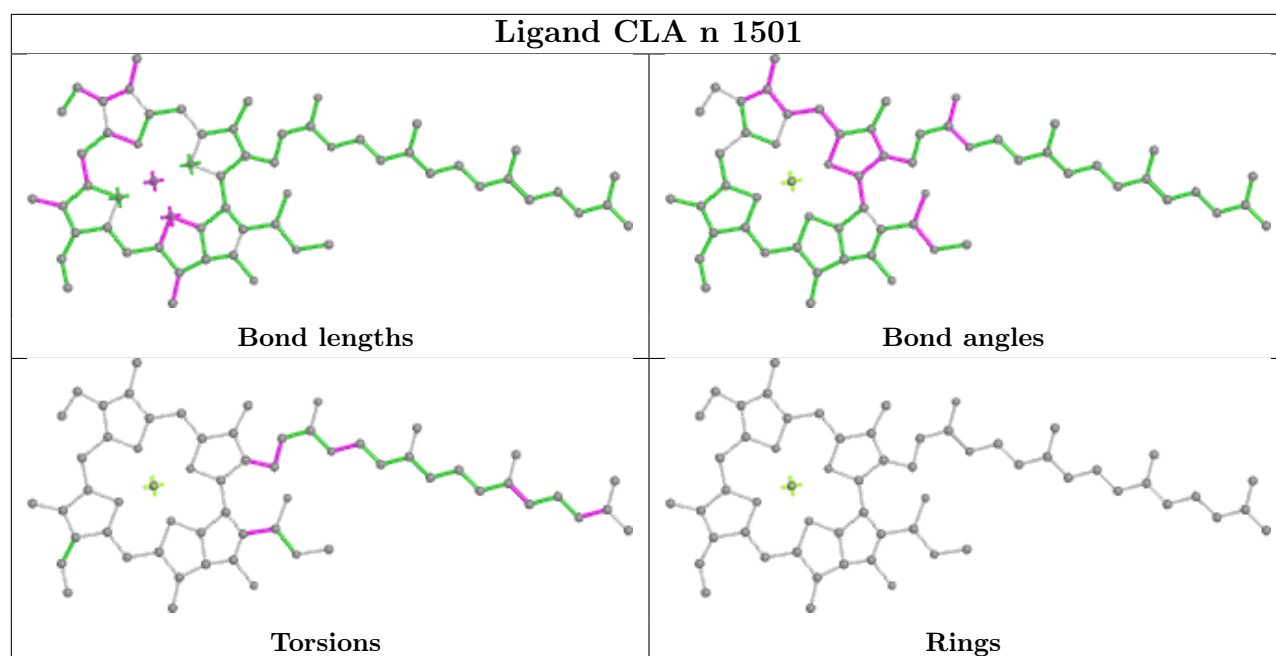


Ligand CLA H 1023

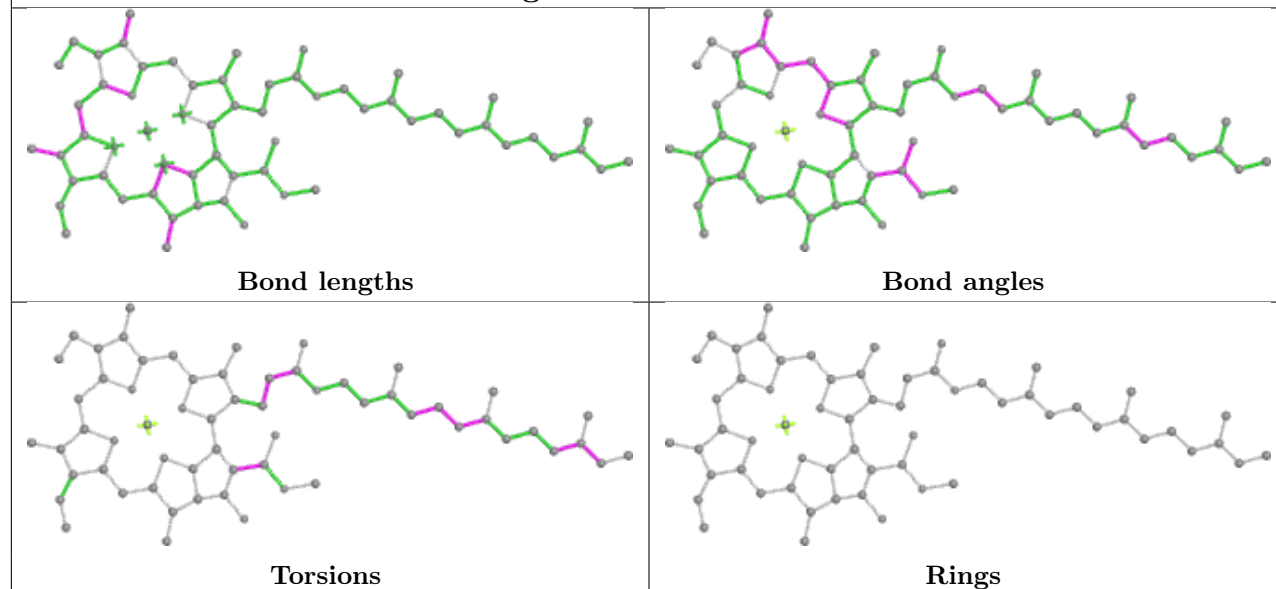


Ligand CLA A 1112

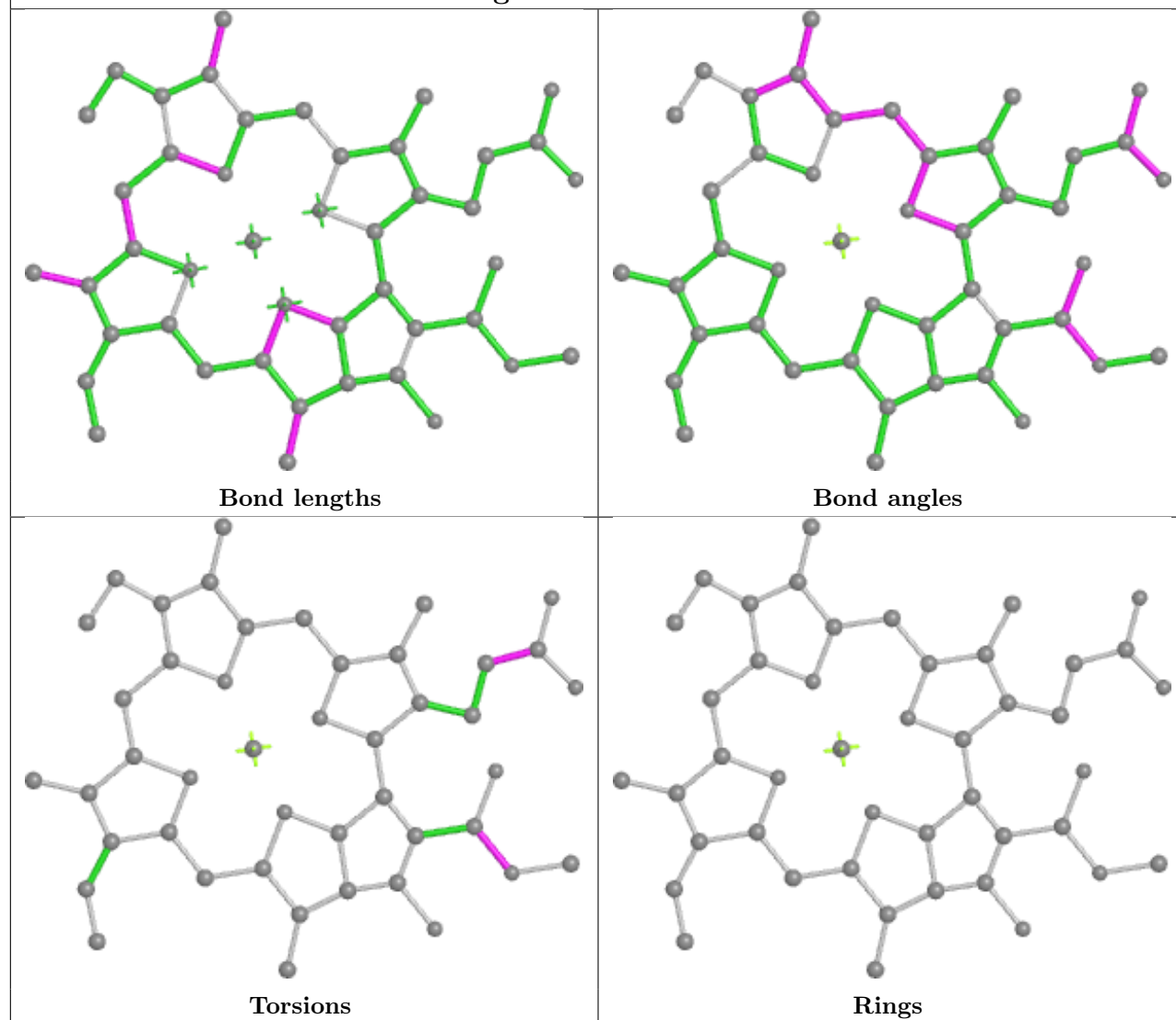


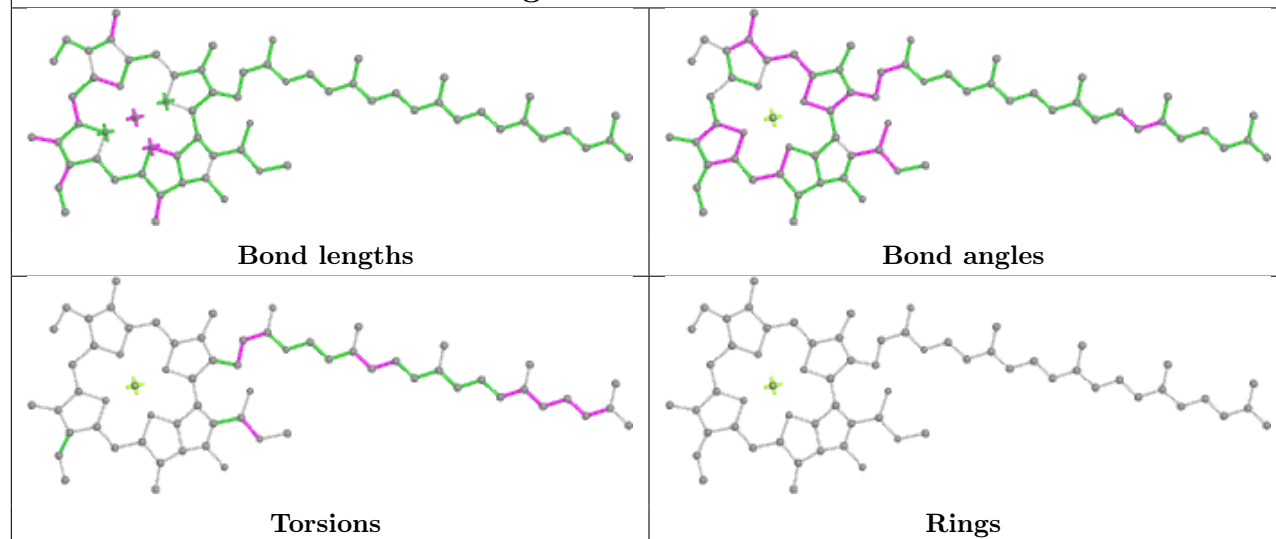
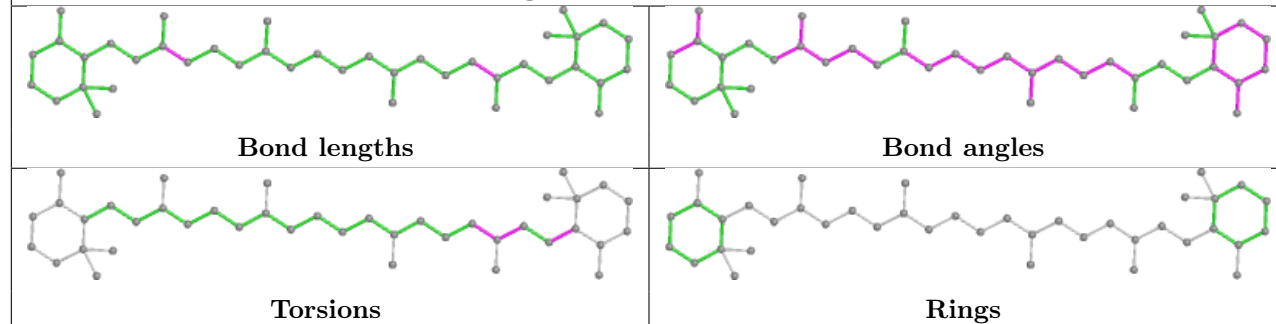


Ligand CLA H 1213

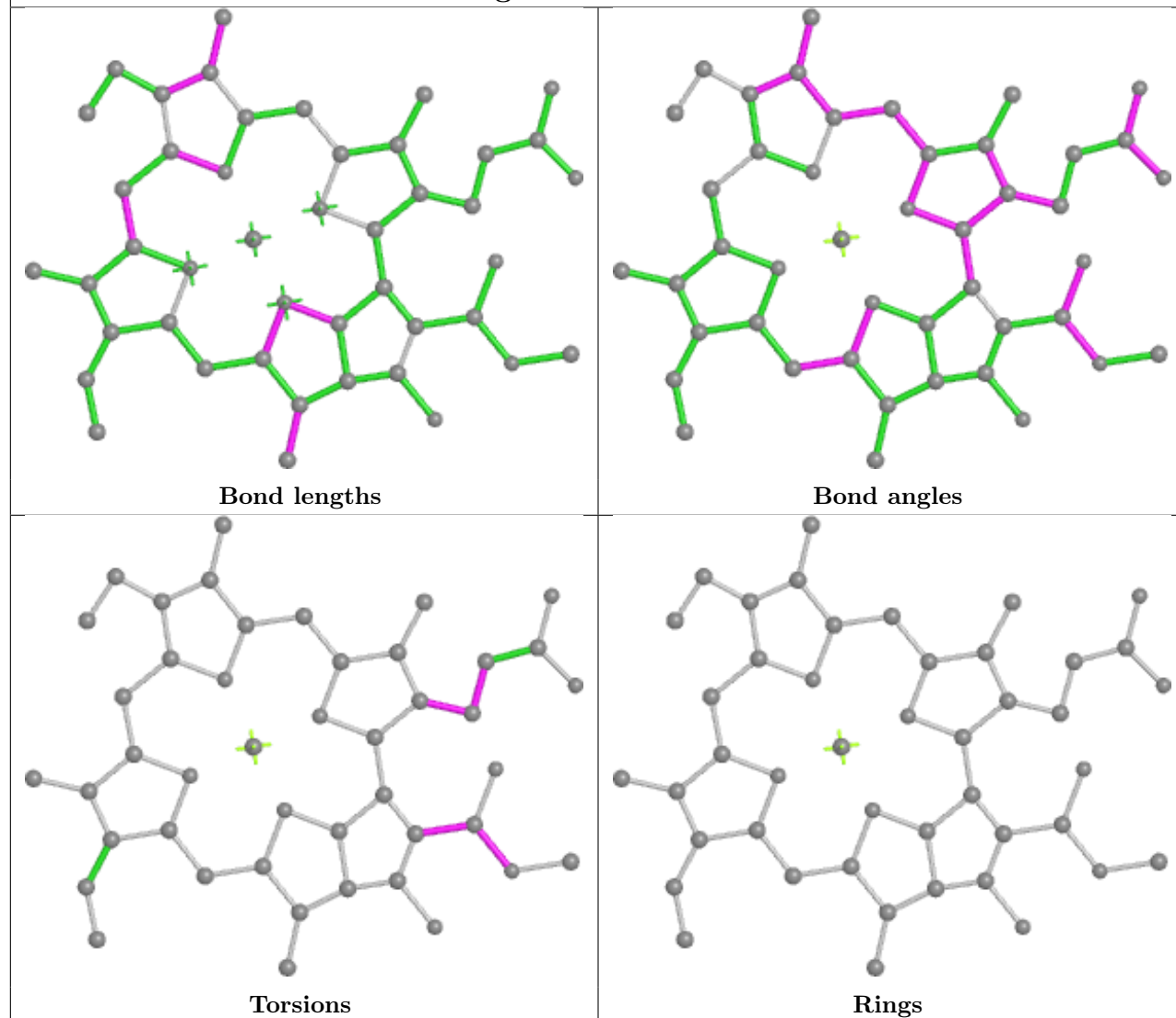


Ligand CLA d 509

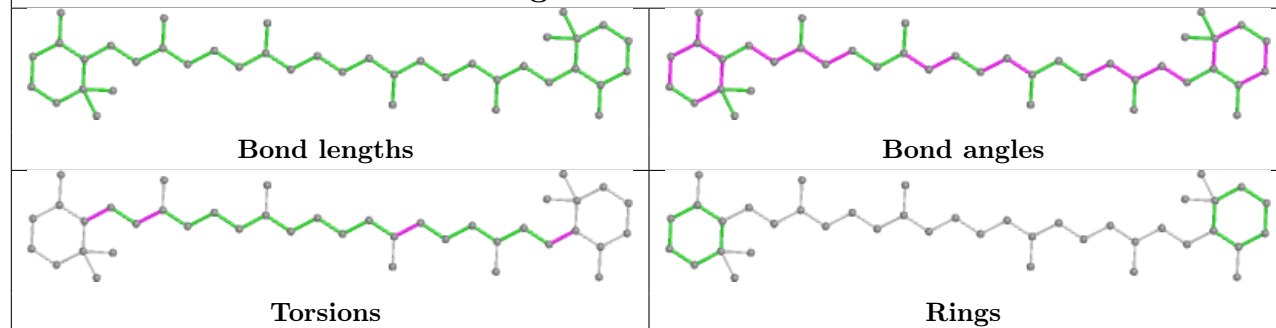


Ligand CLA A 1013**Ligand BCR V 4020**

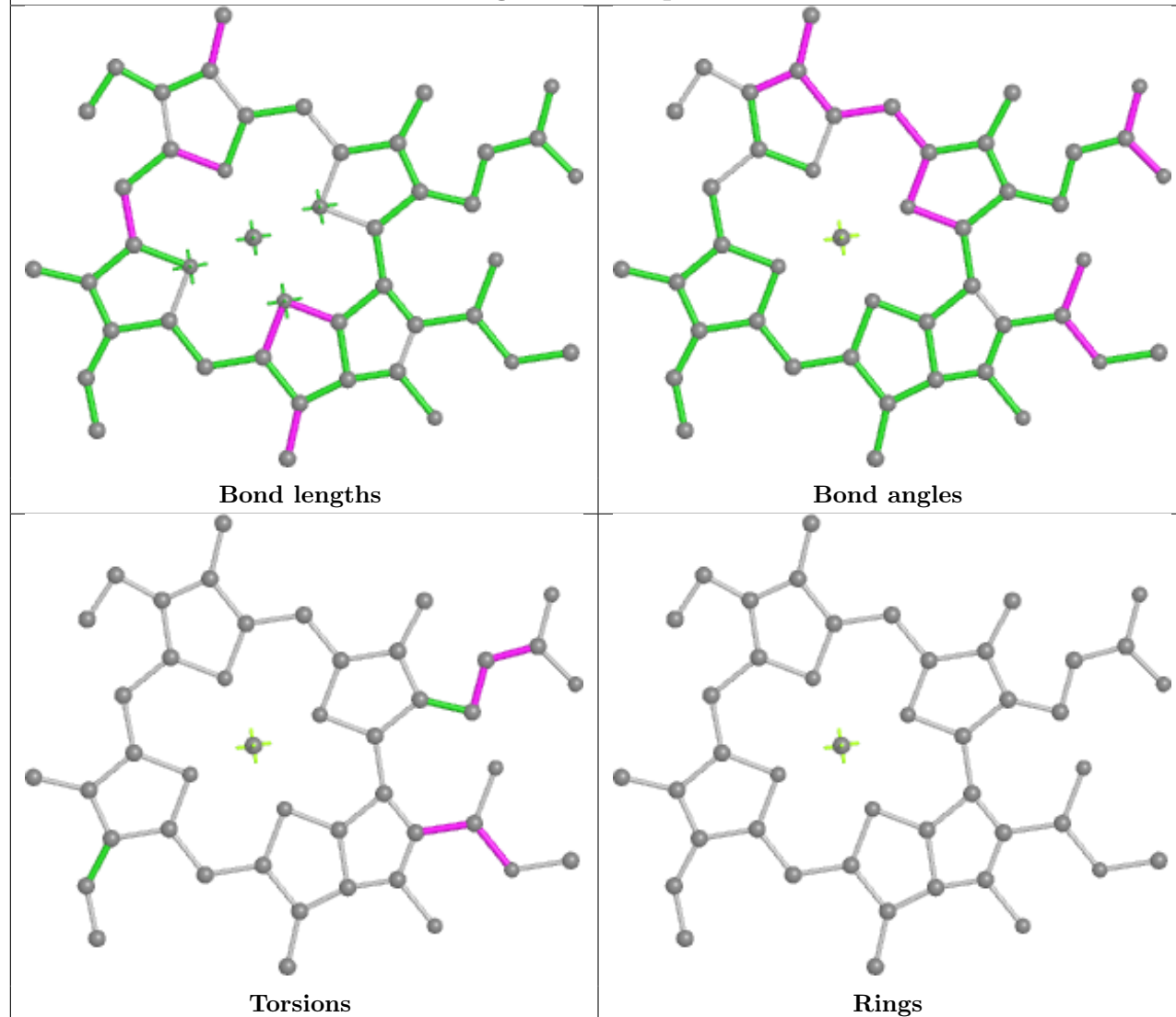
Ligand CLA c 503



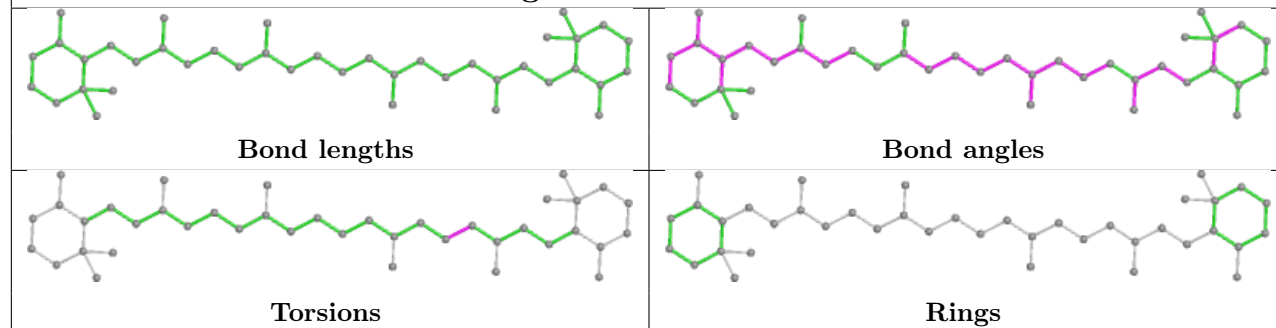
Ligand BCR Y 521



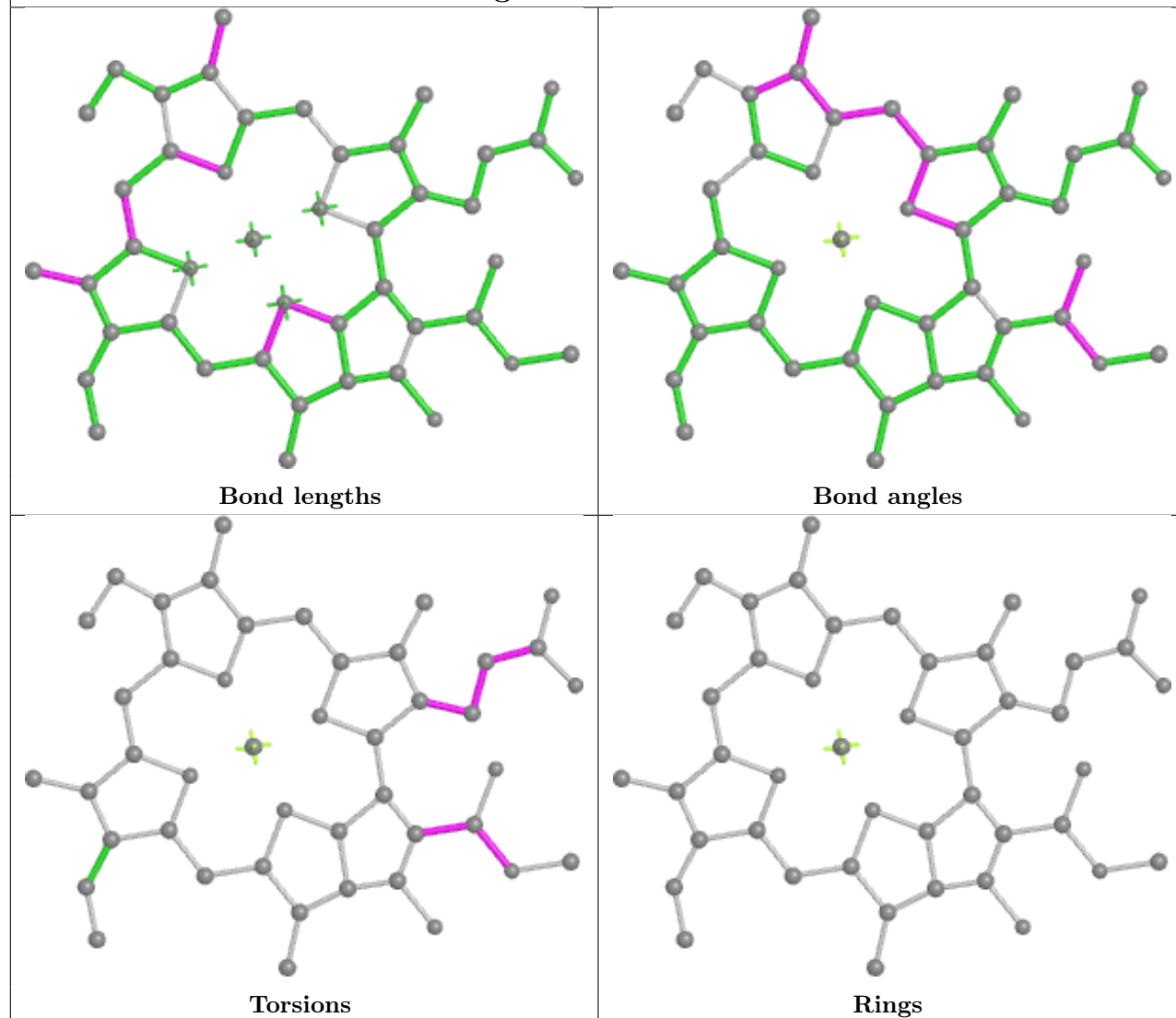
Ligand CLA q 518



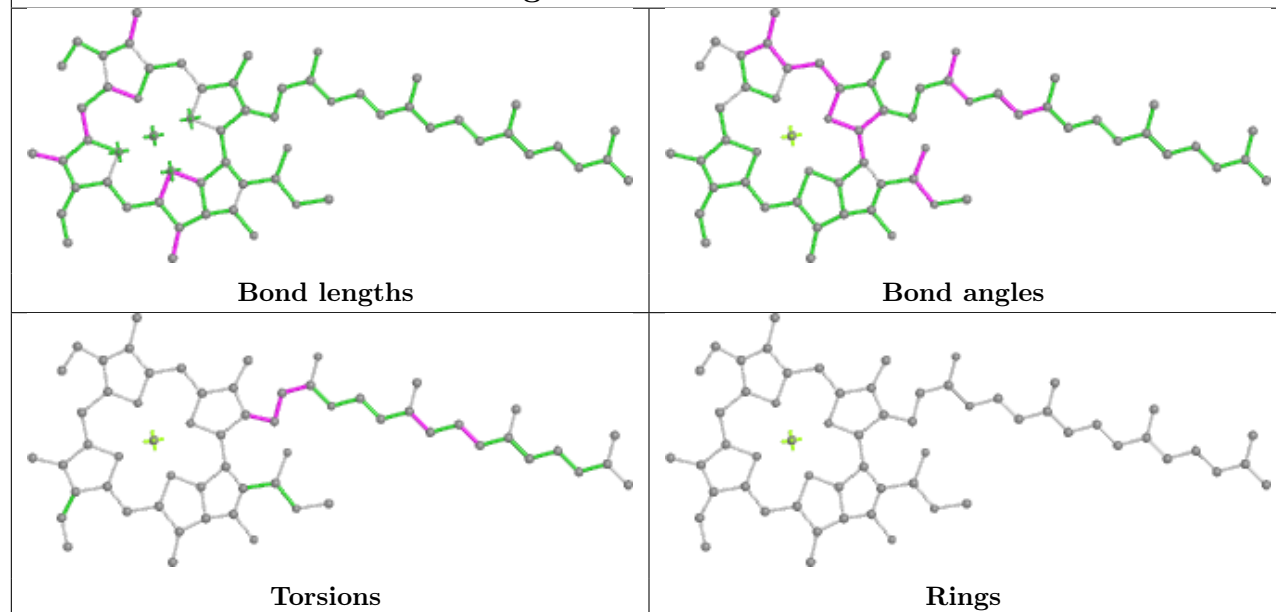
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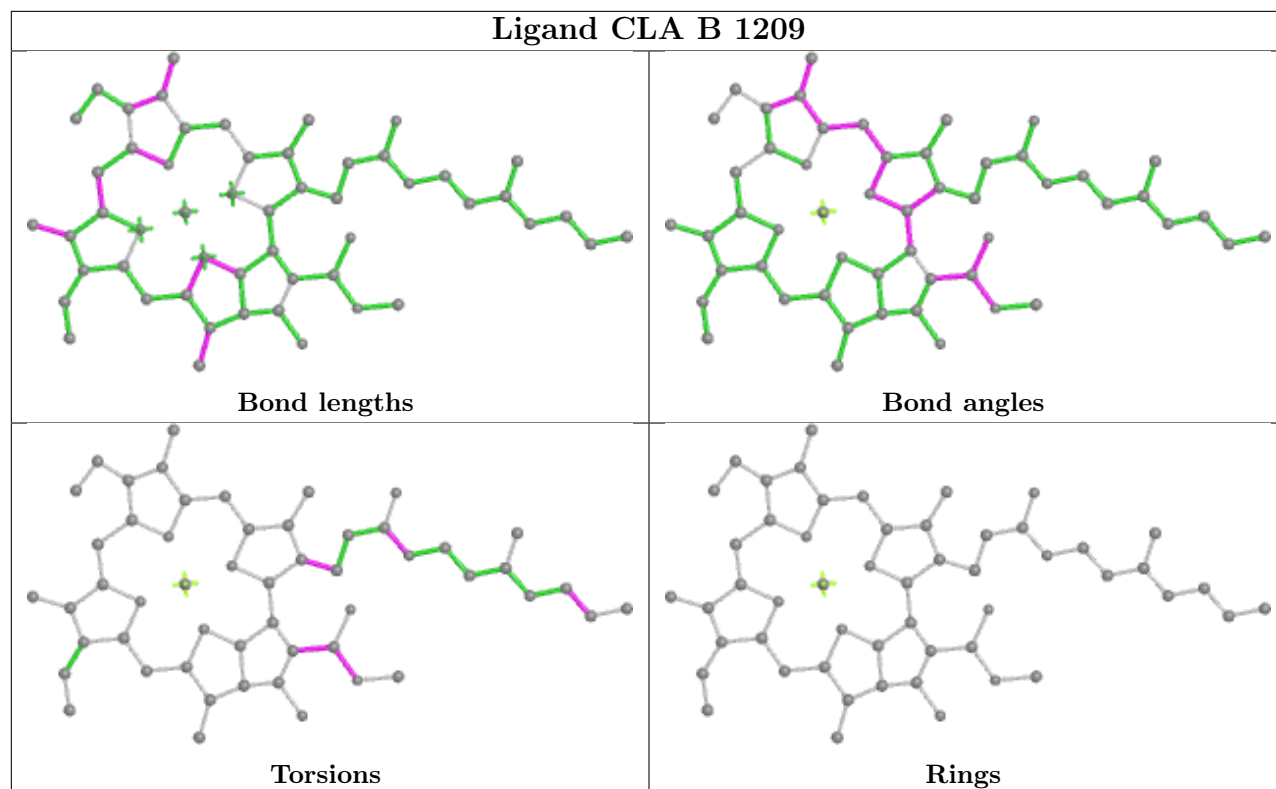


Ligand CLA 1 501

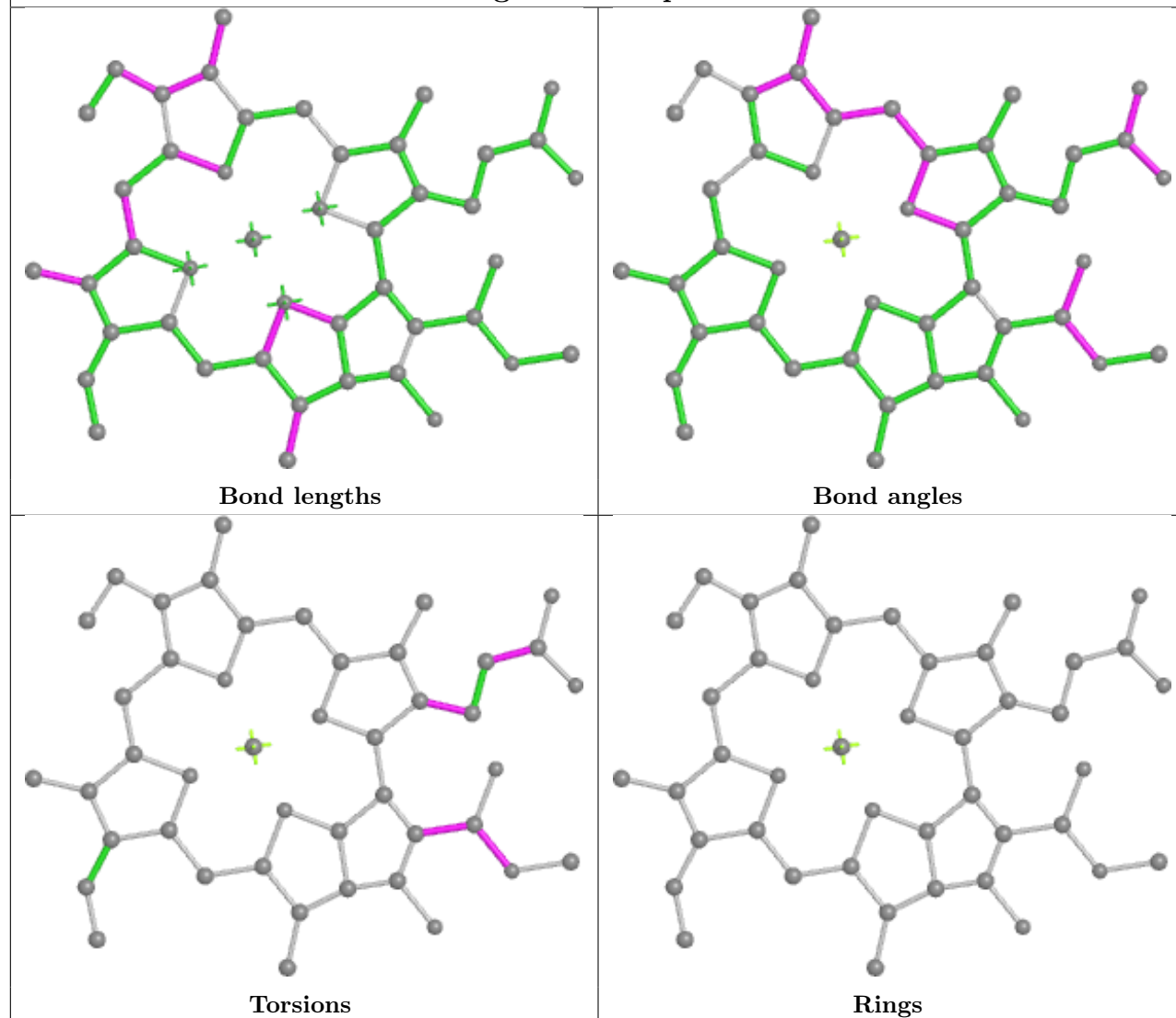


Ligand CLA B 1224

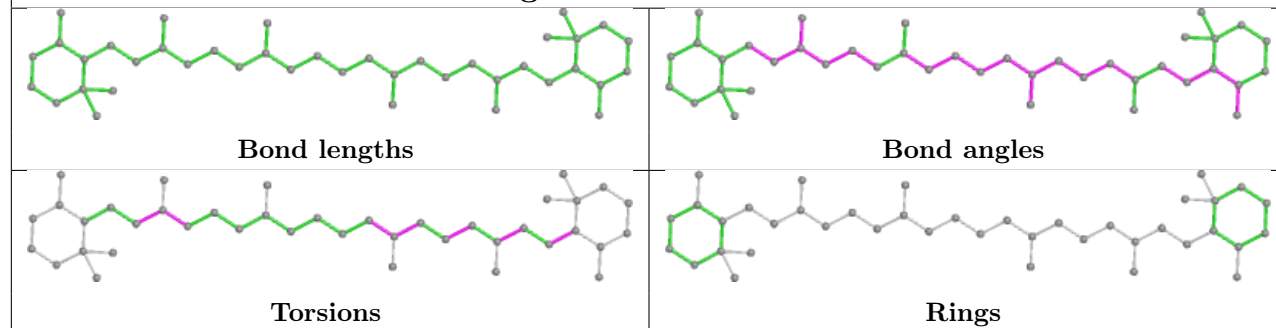




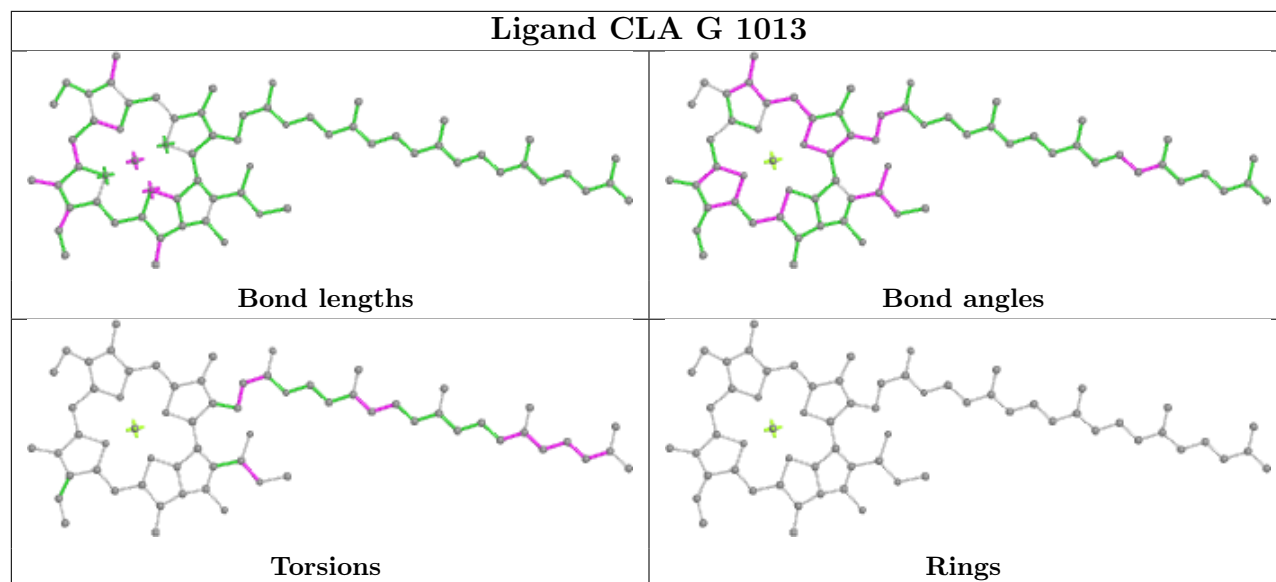
Ligand CLA q 519



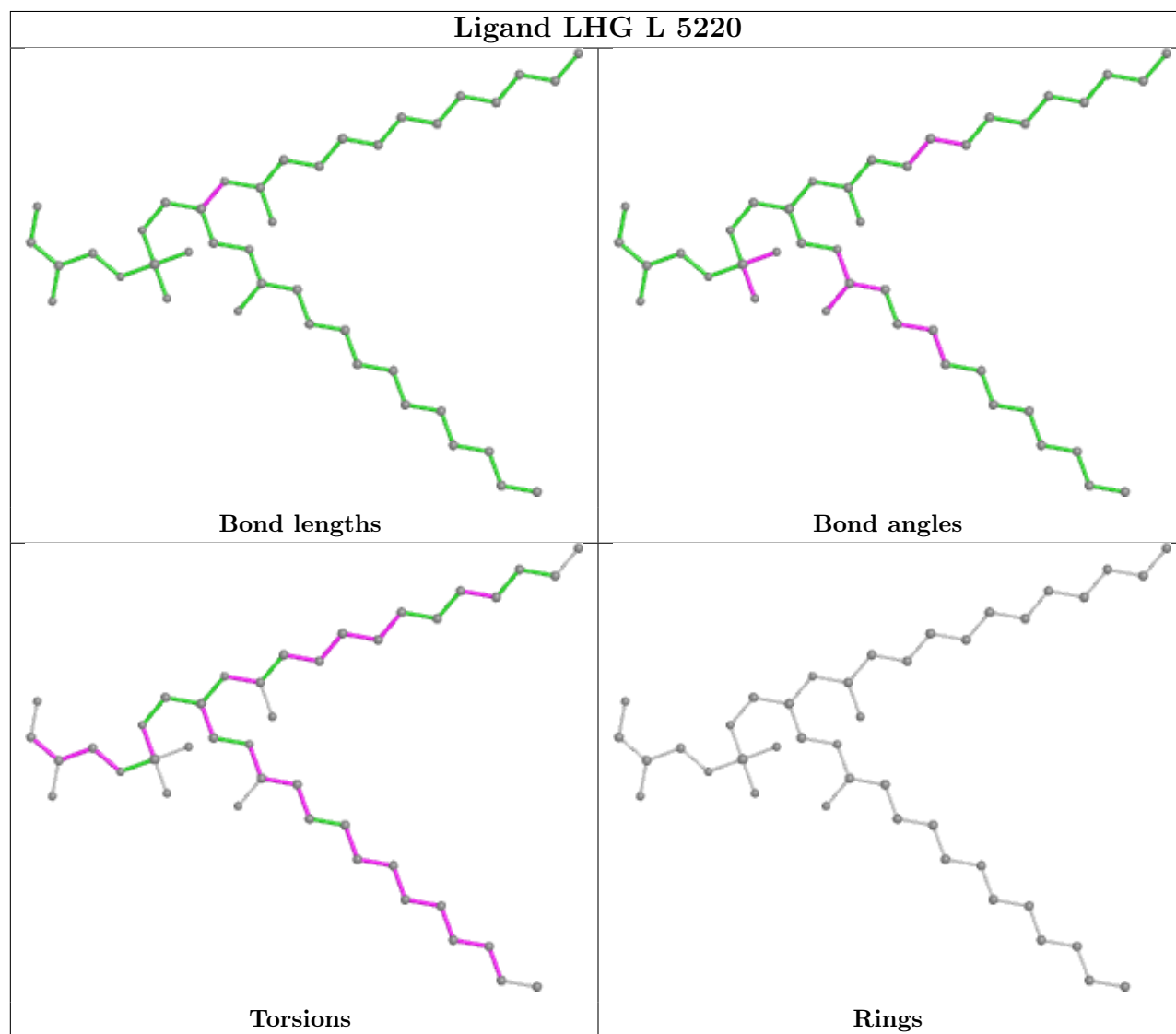
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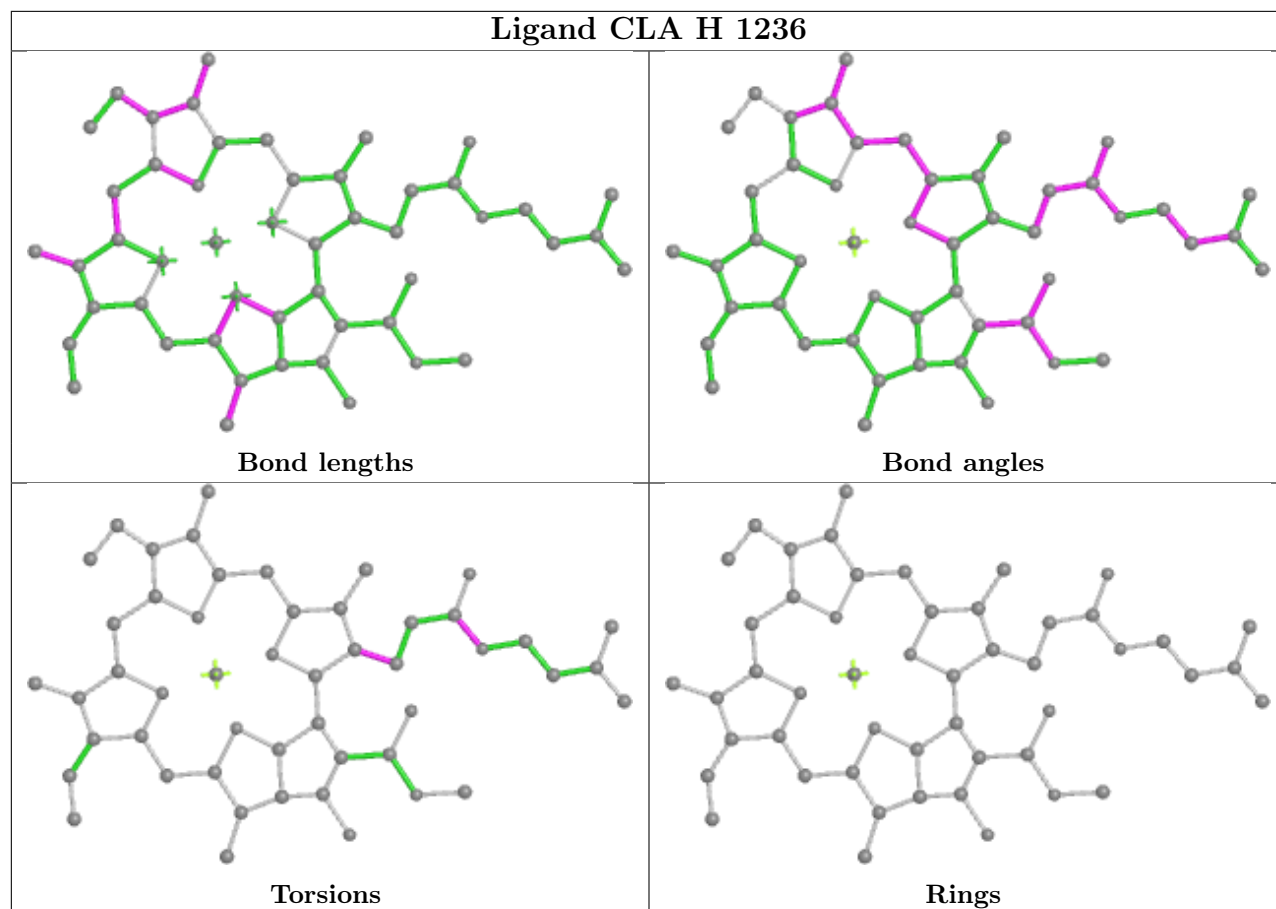


Ligand CLA G 1013

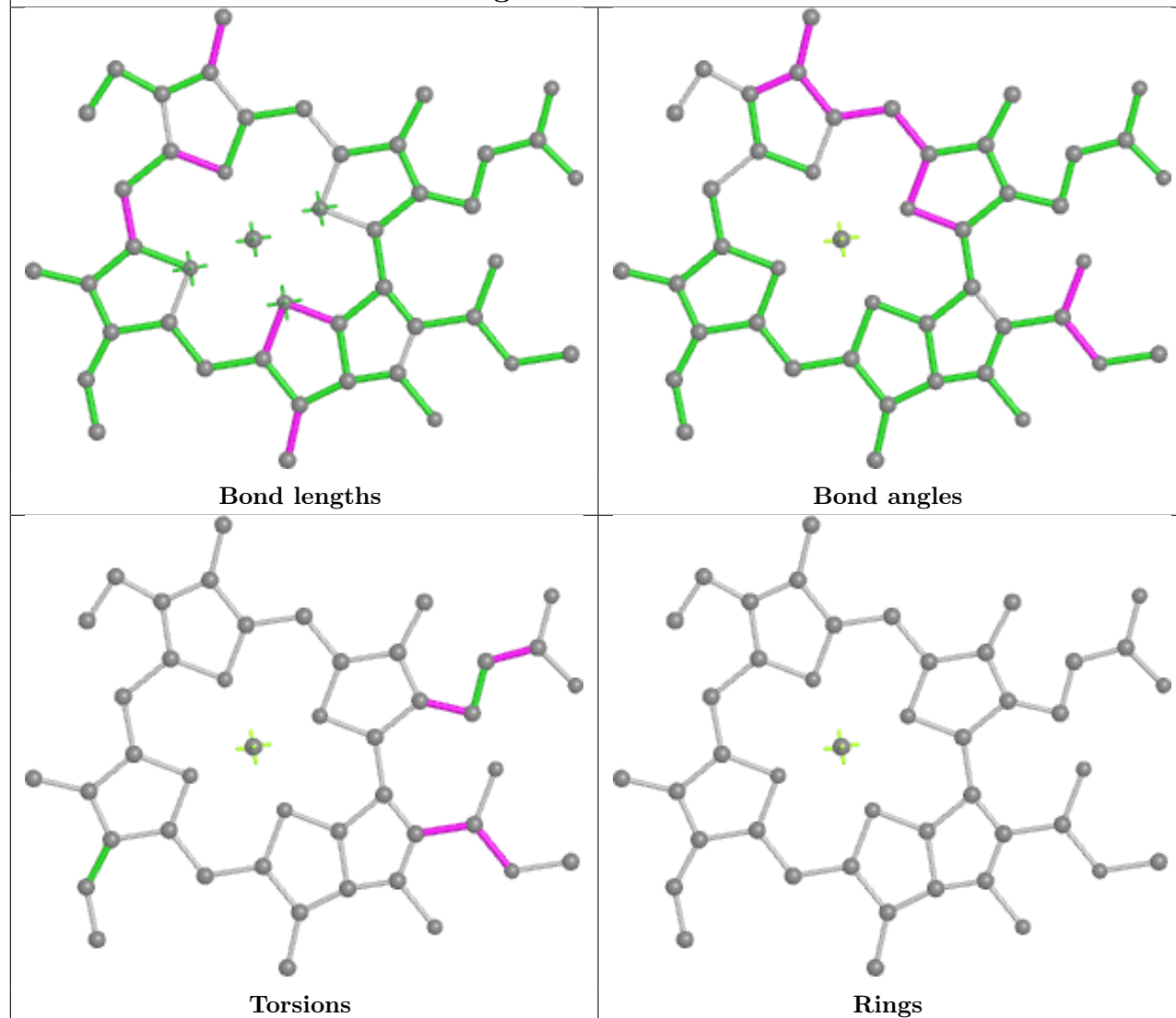


Ligand LHG L 5220

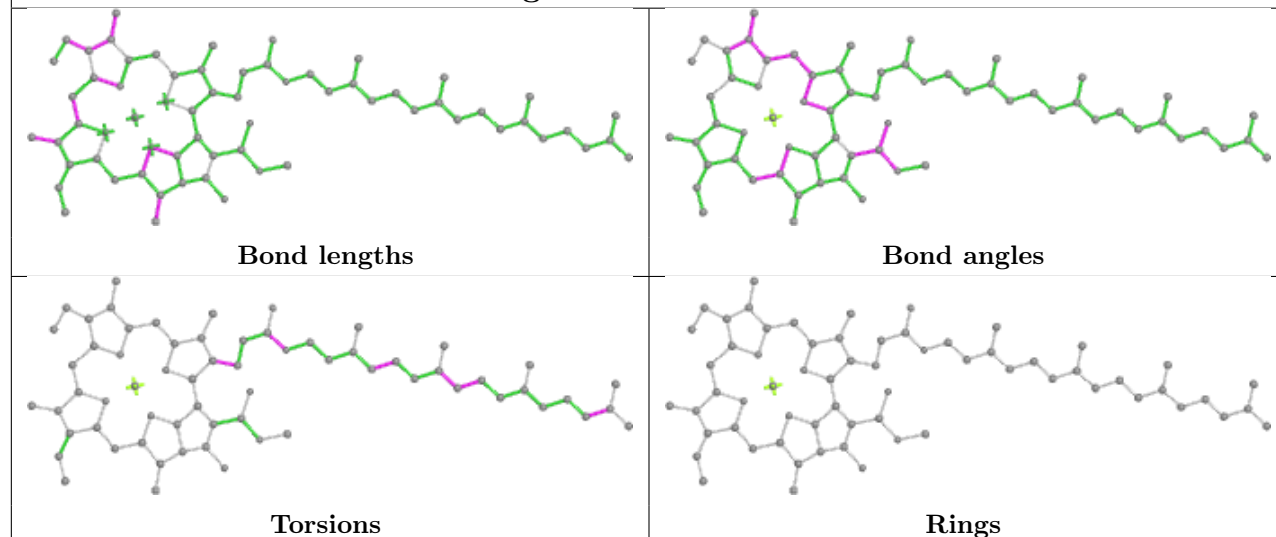


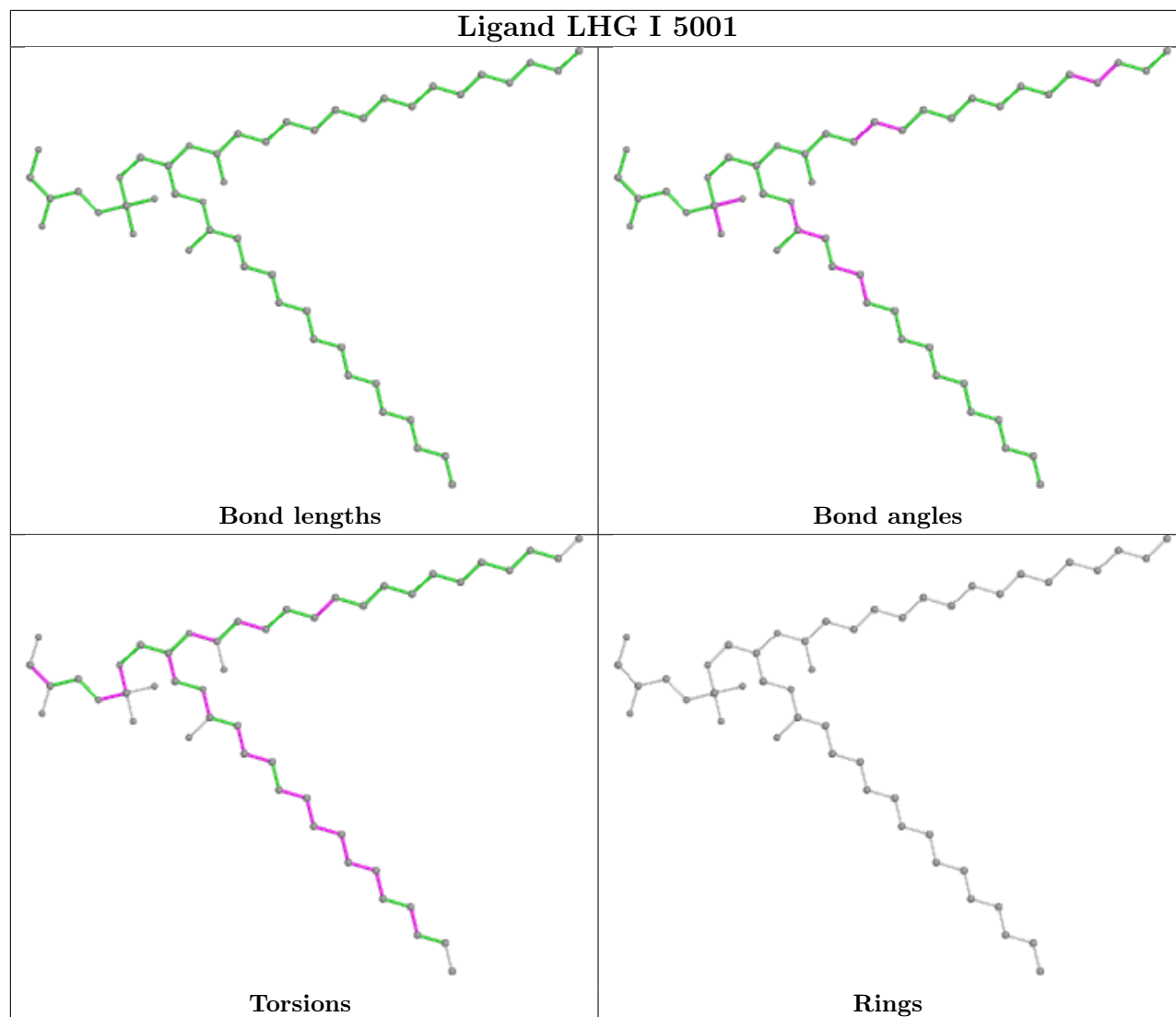
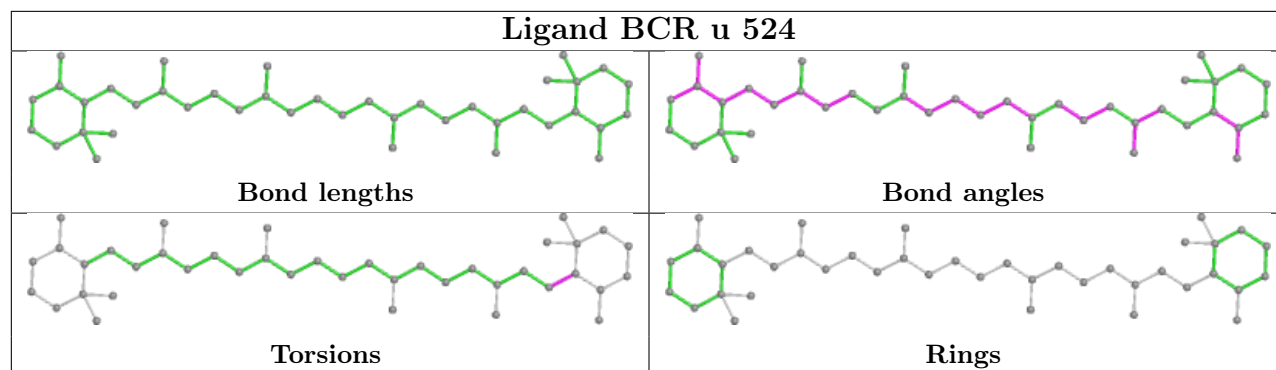


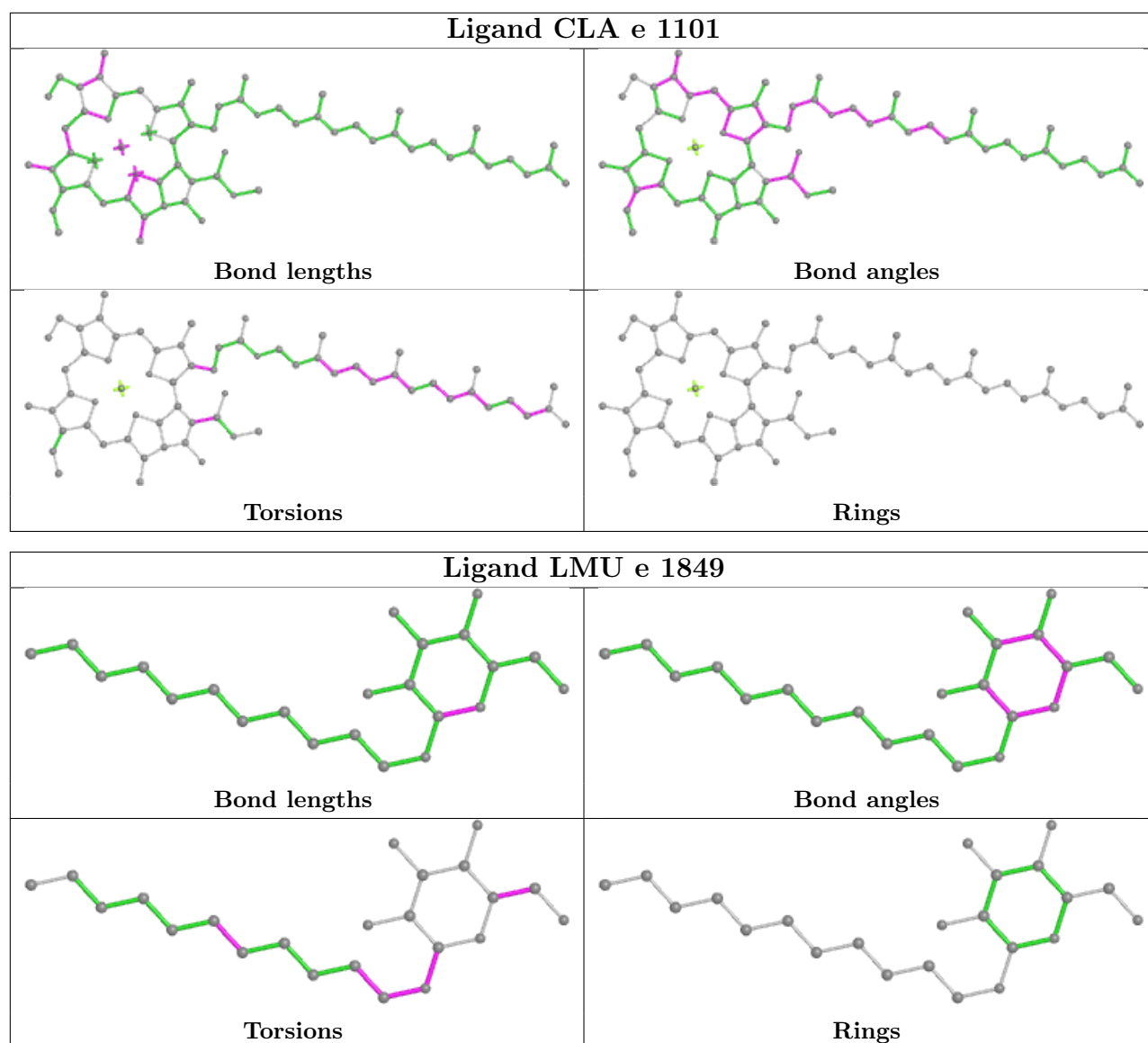
Ligand CLA v 518



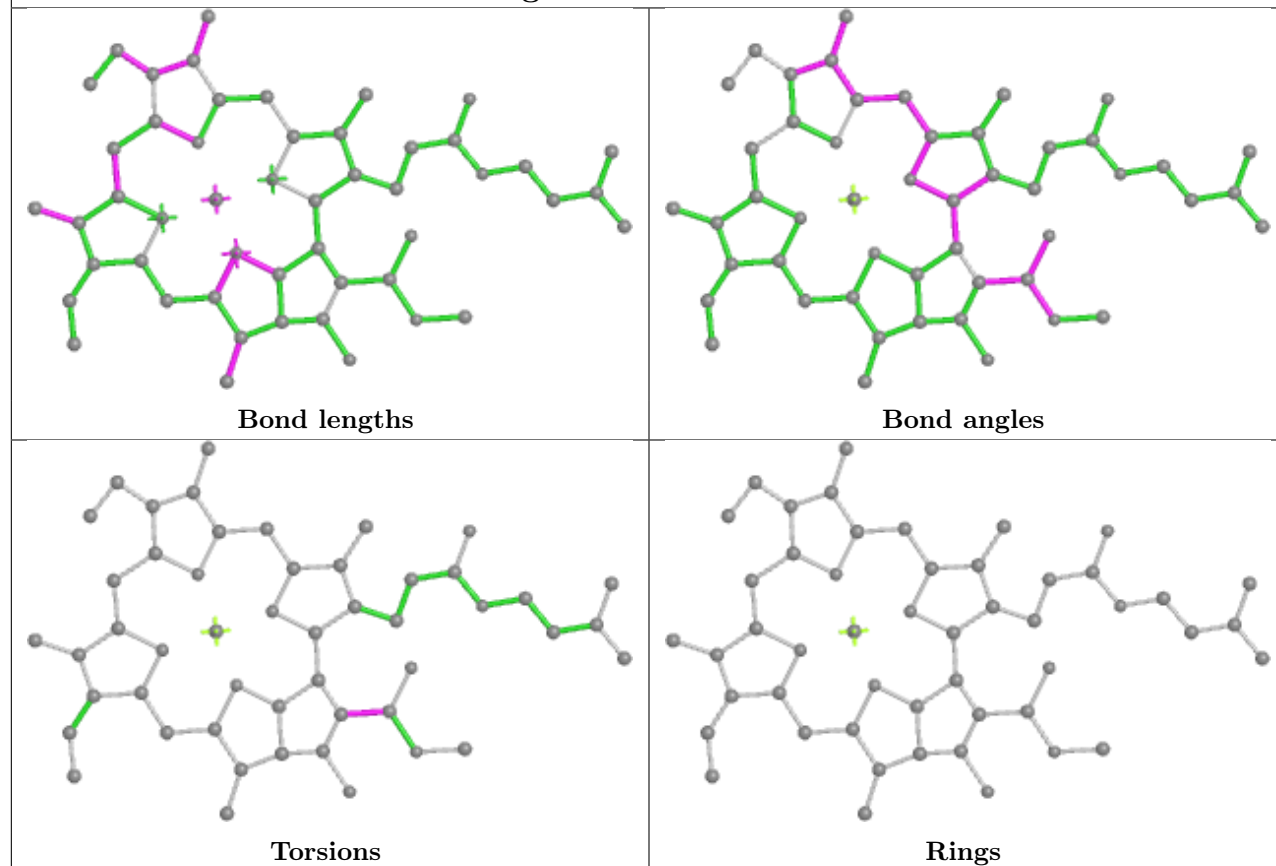
Ligand CLA V 1502



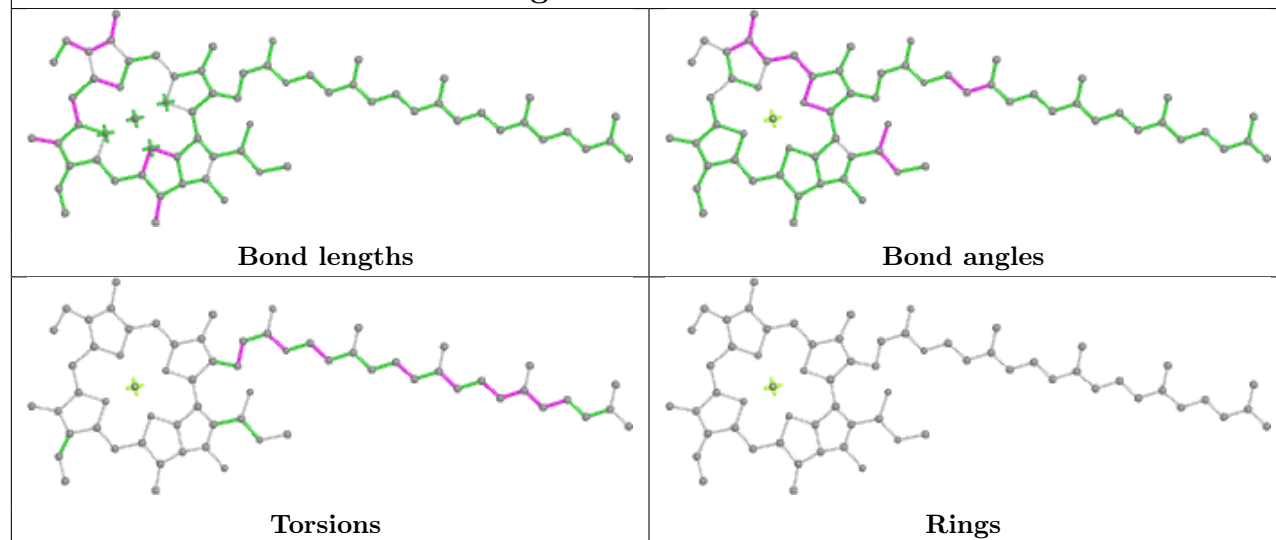




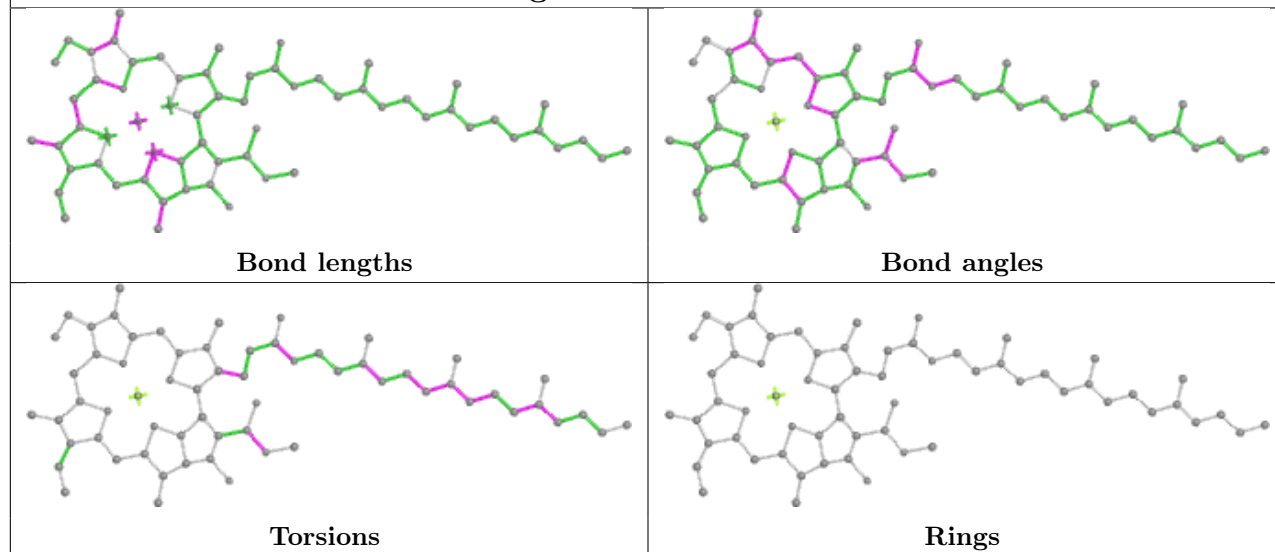
Ligand CLA G 1112



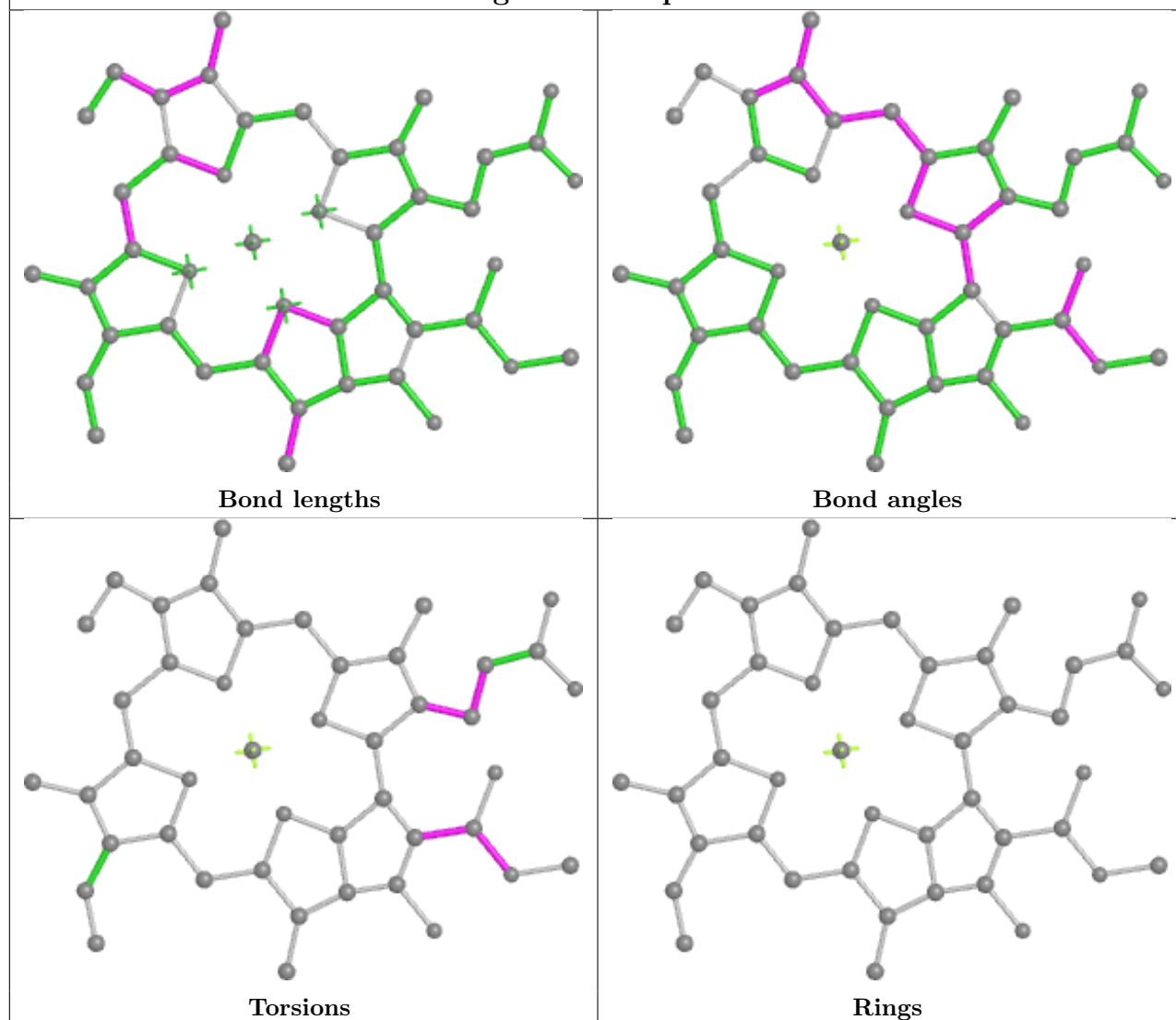
Ligand CLA f 1214



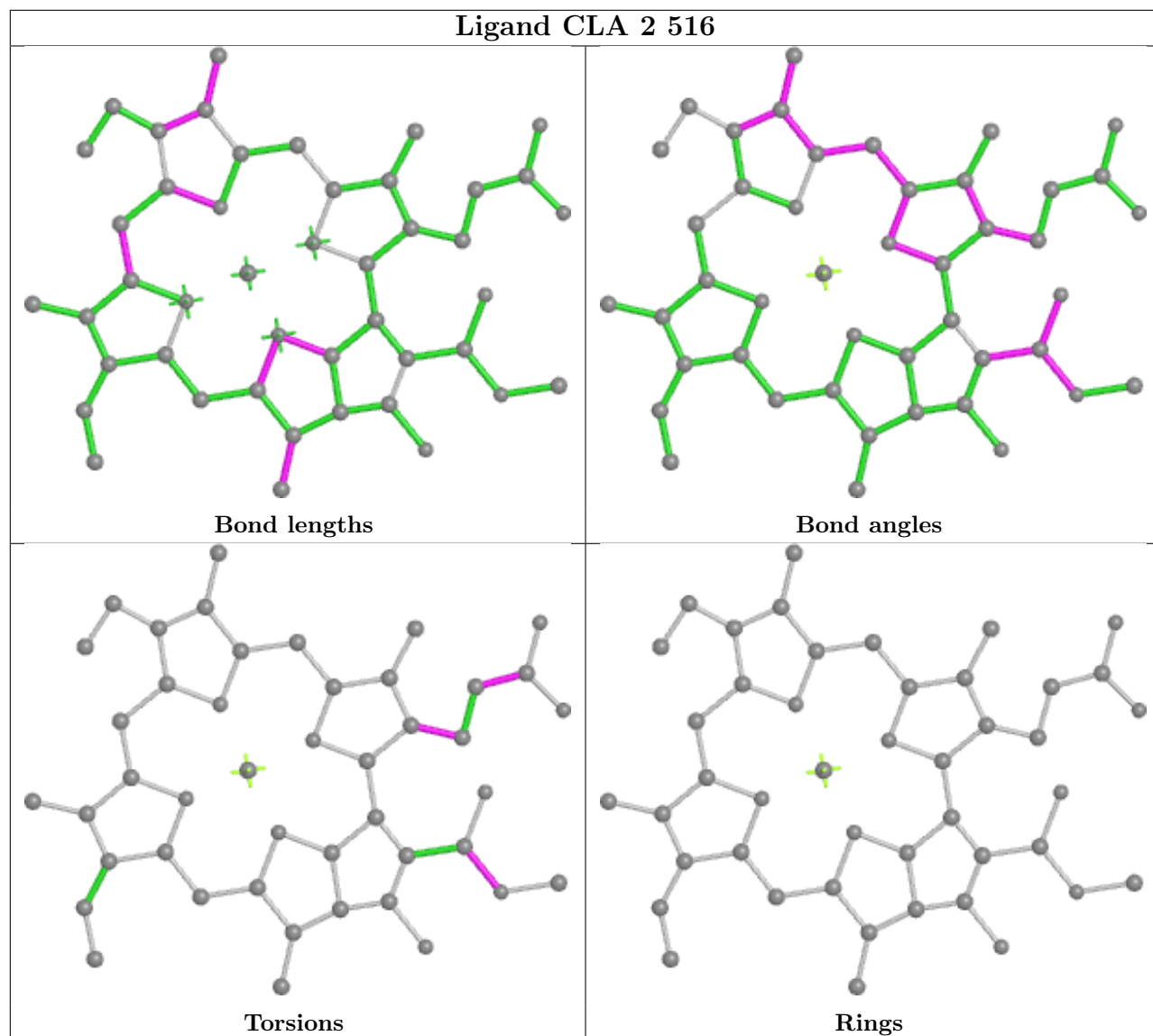
Ligand CLA f 1219



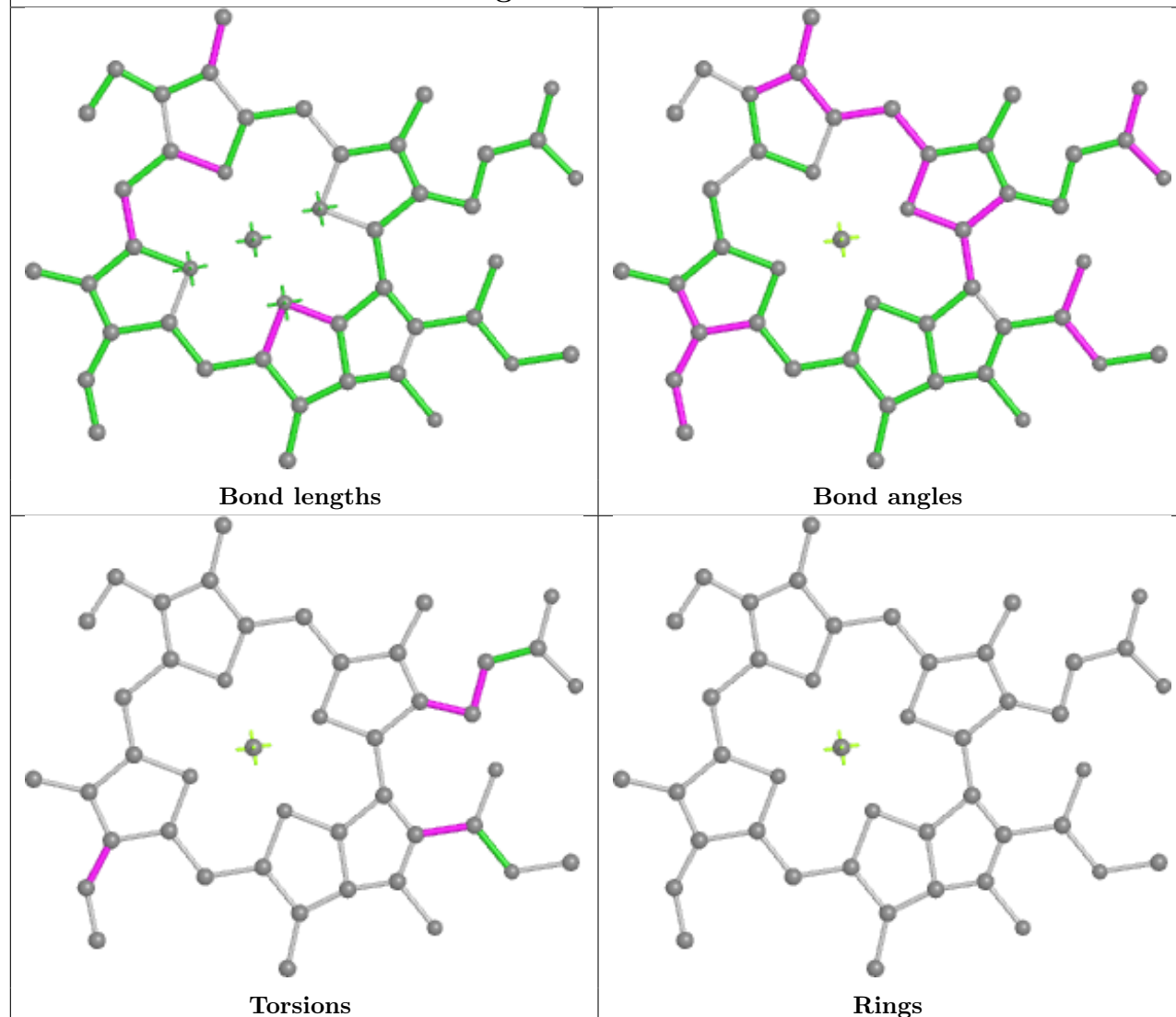
Ligand CLA q 503



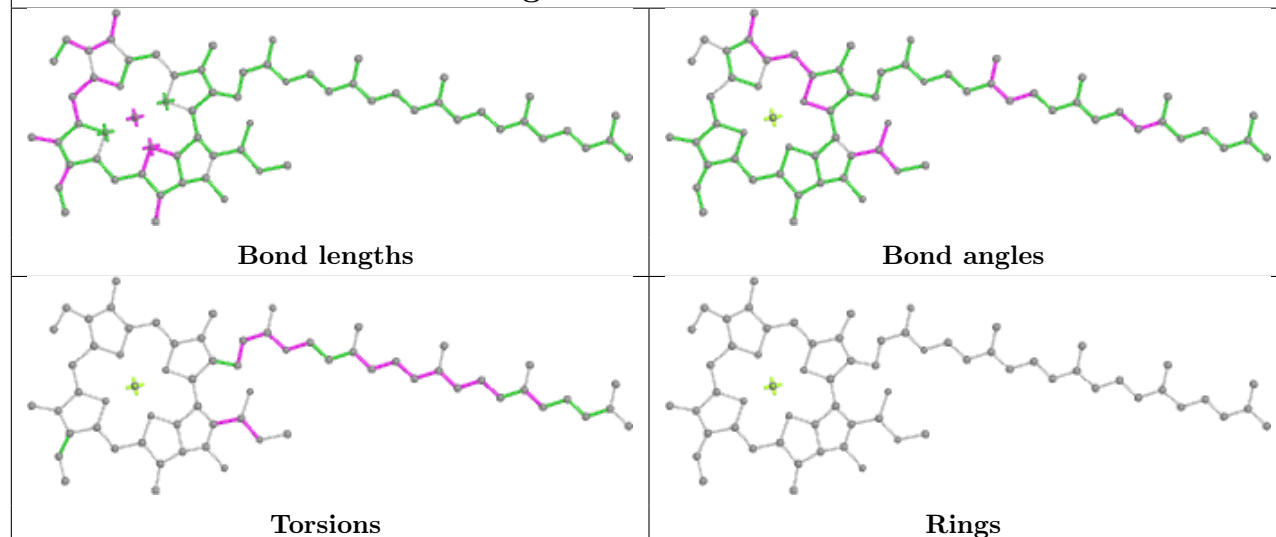
Ligand CLA 2 516

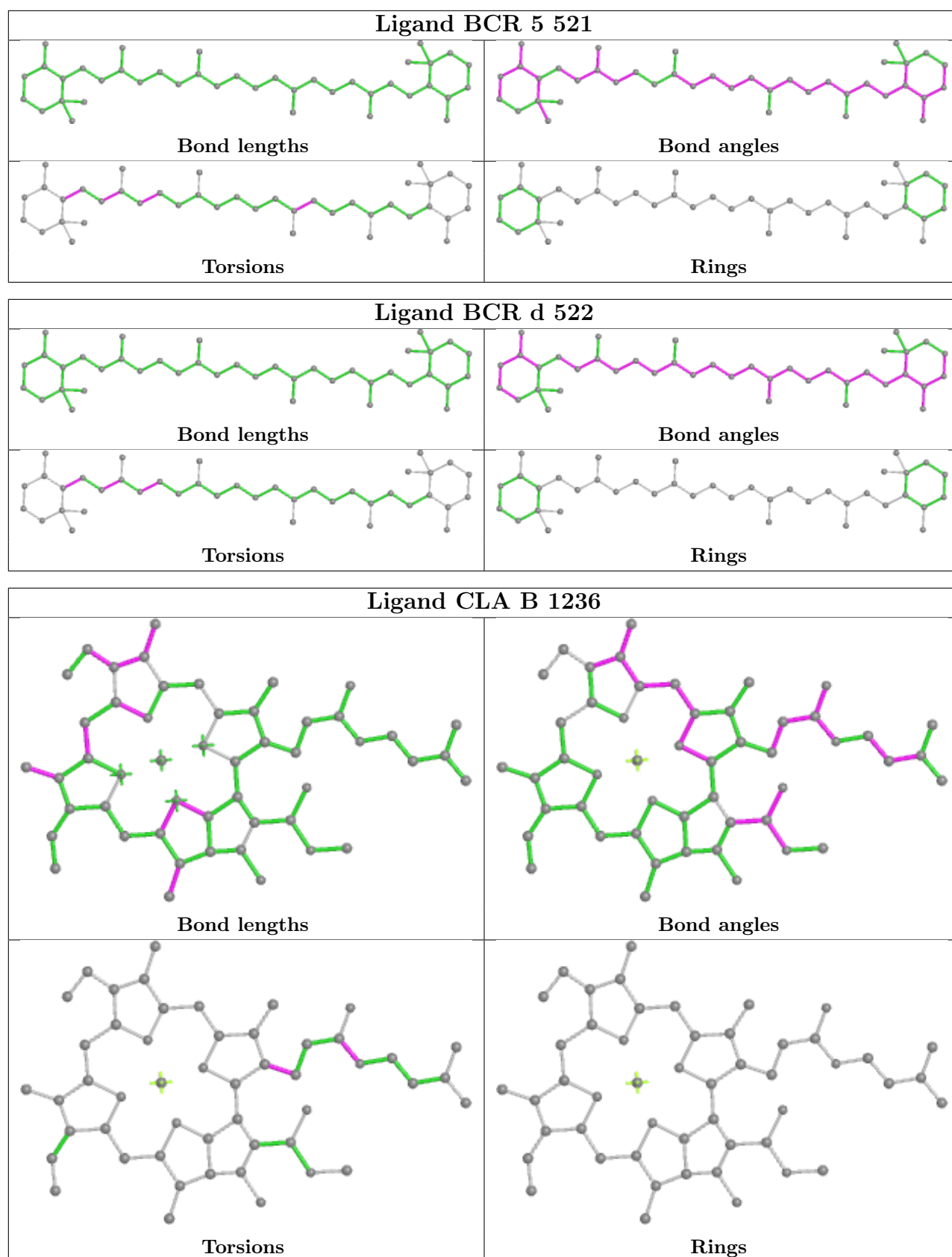


Ligand CLA s 516

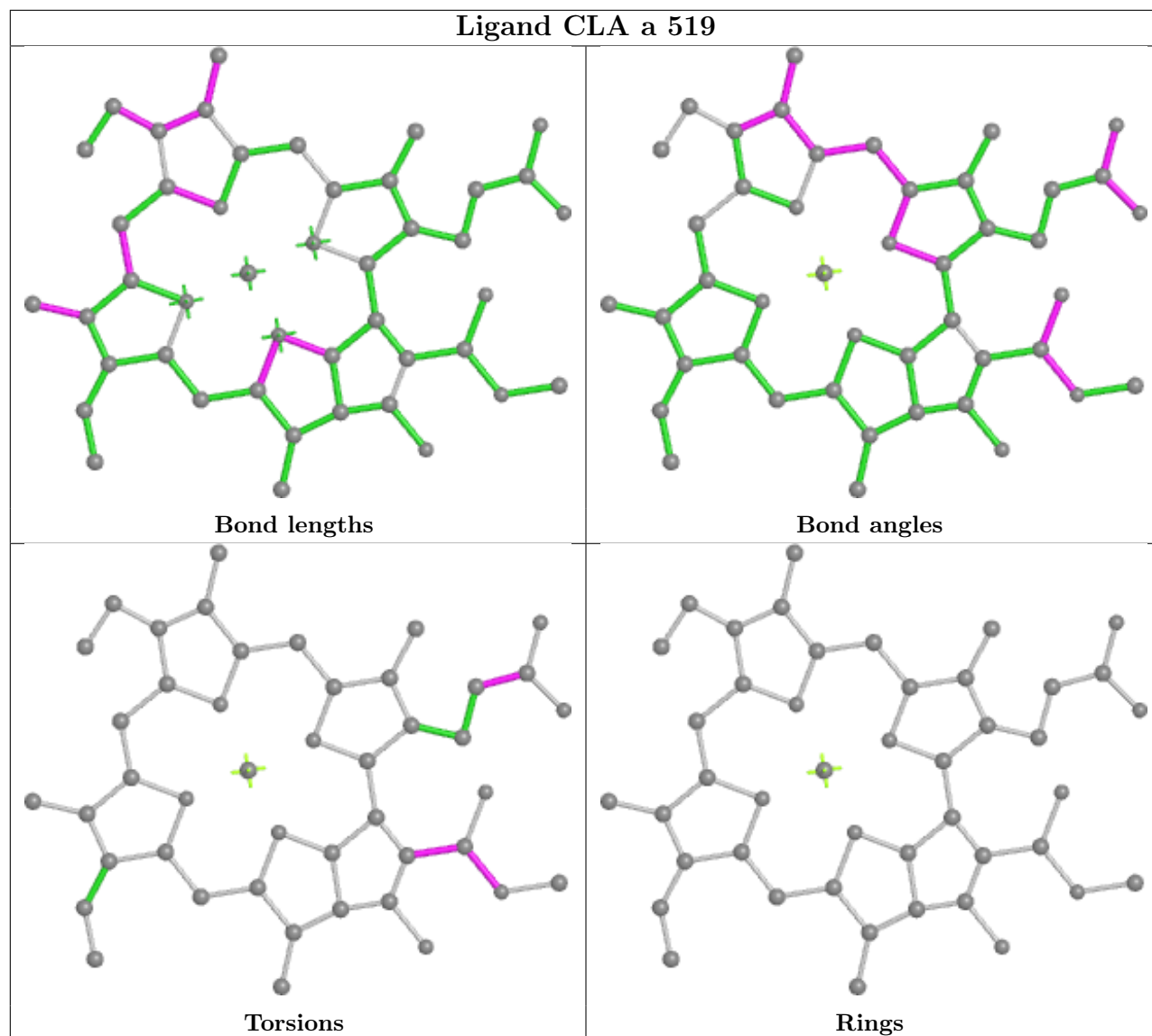


Ligand CLA A 1237

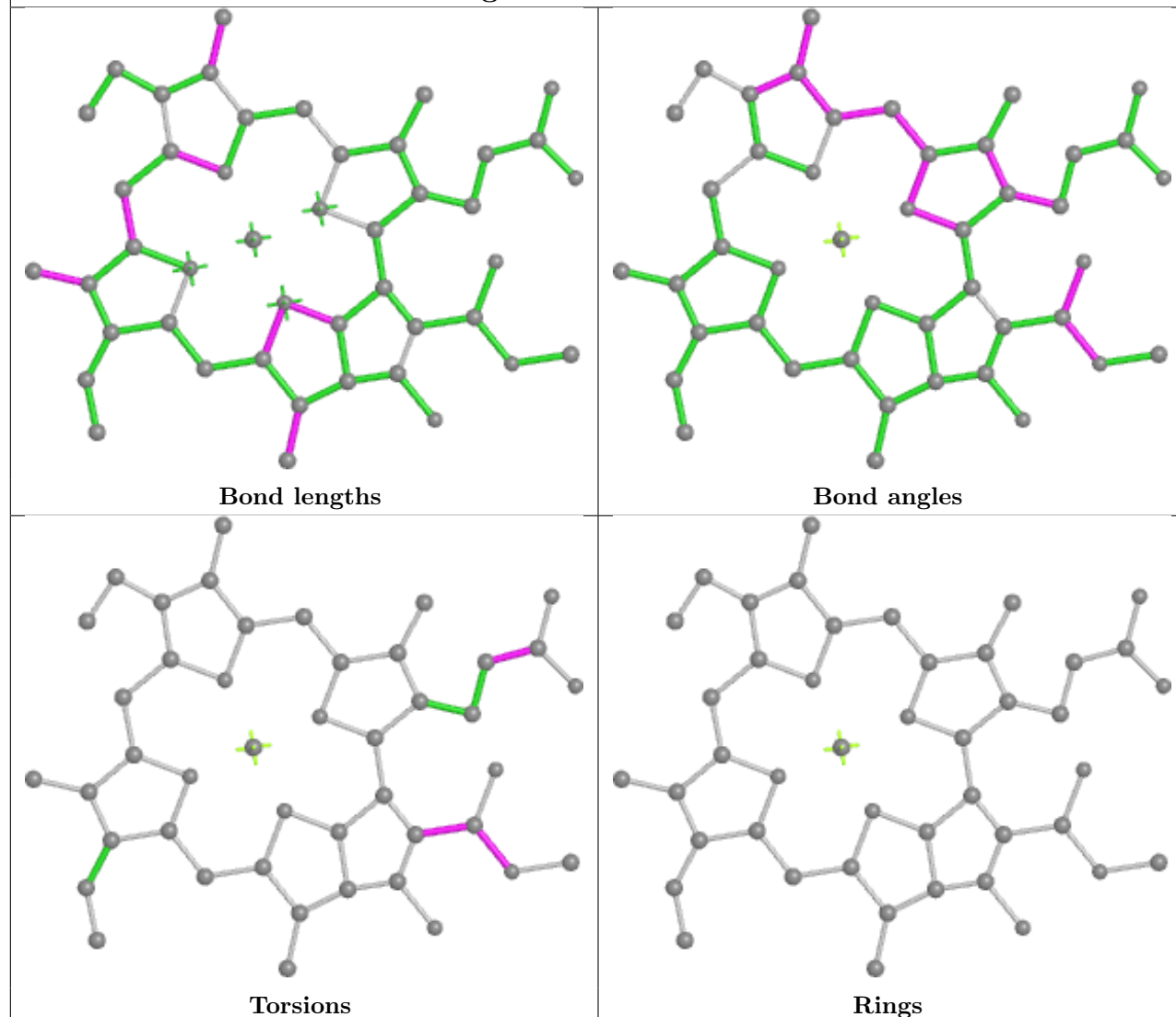




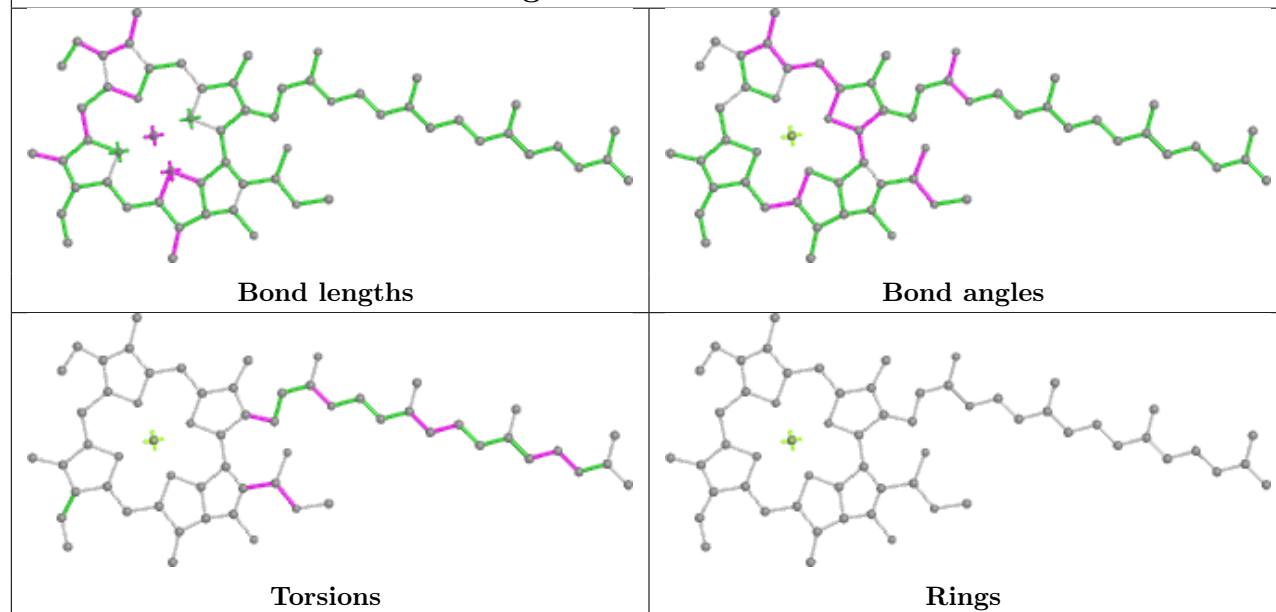
Ligand CLA a 519

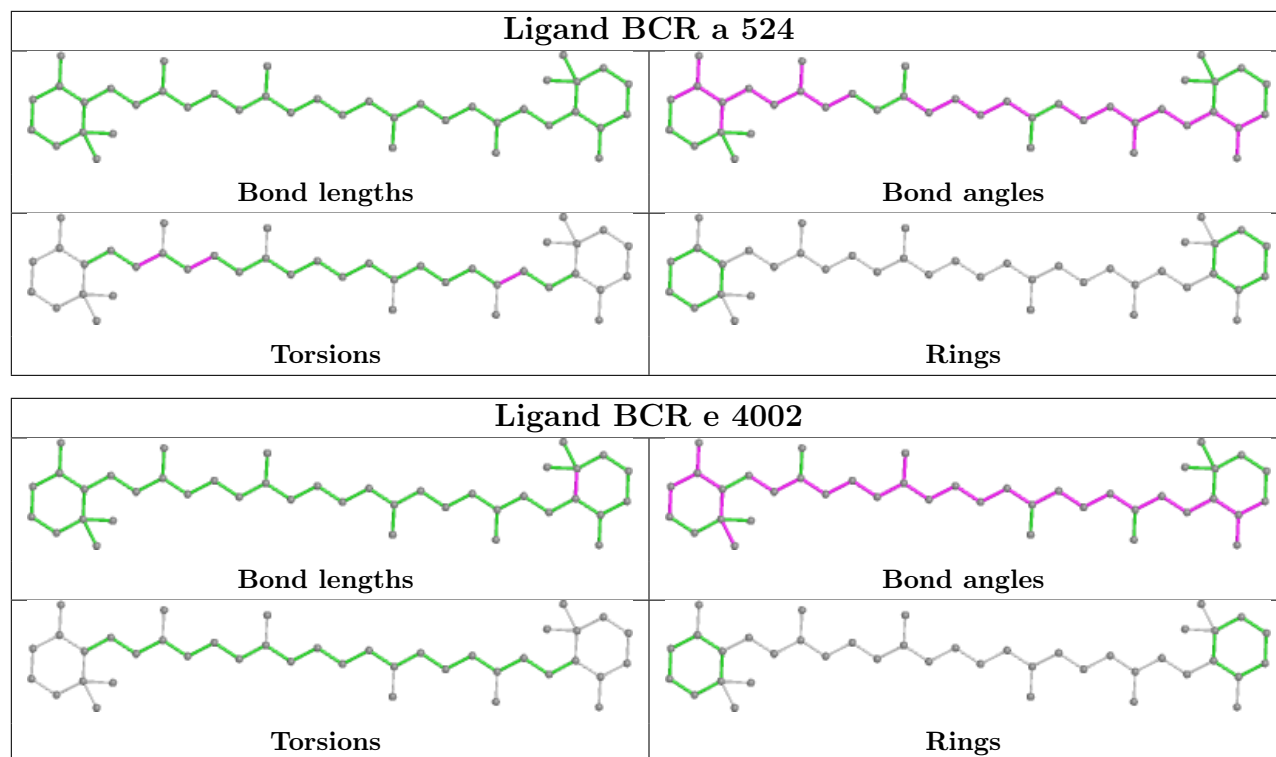


Ligand CLA A 1801

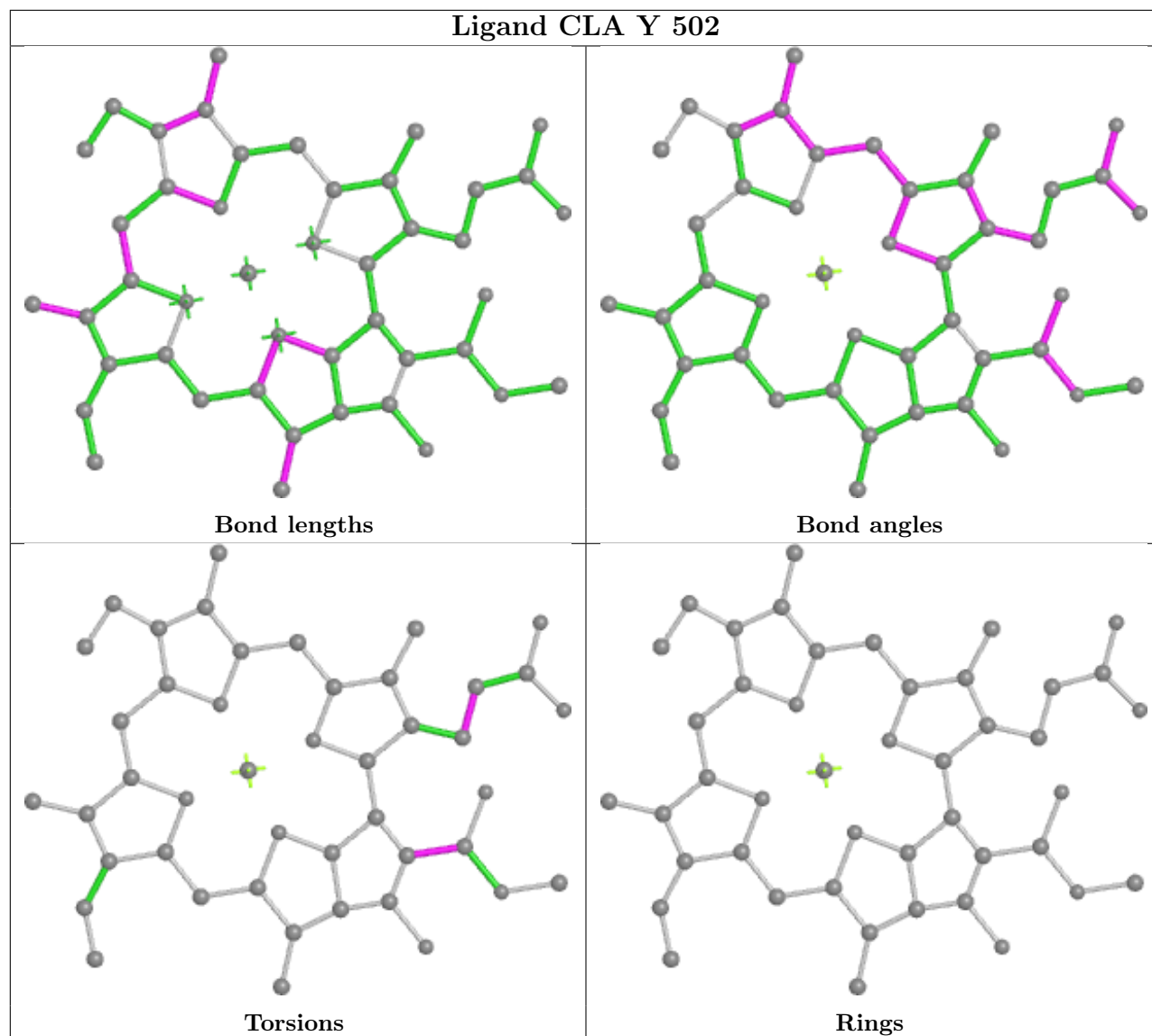


Ligand CLA A 1122

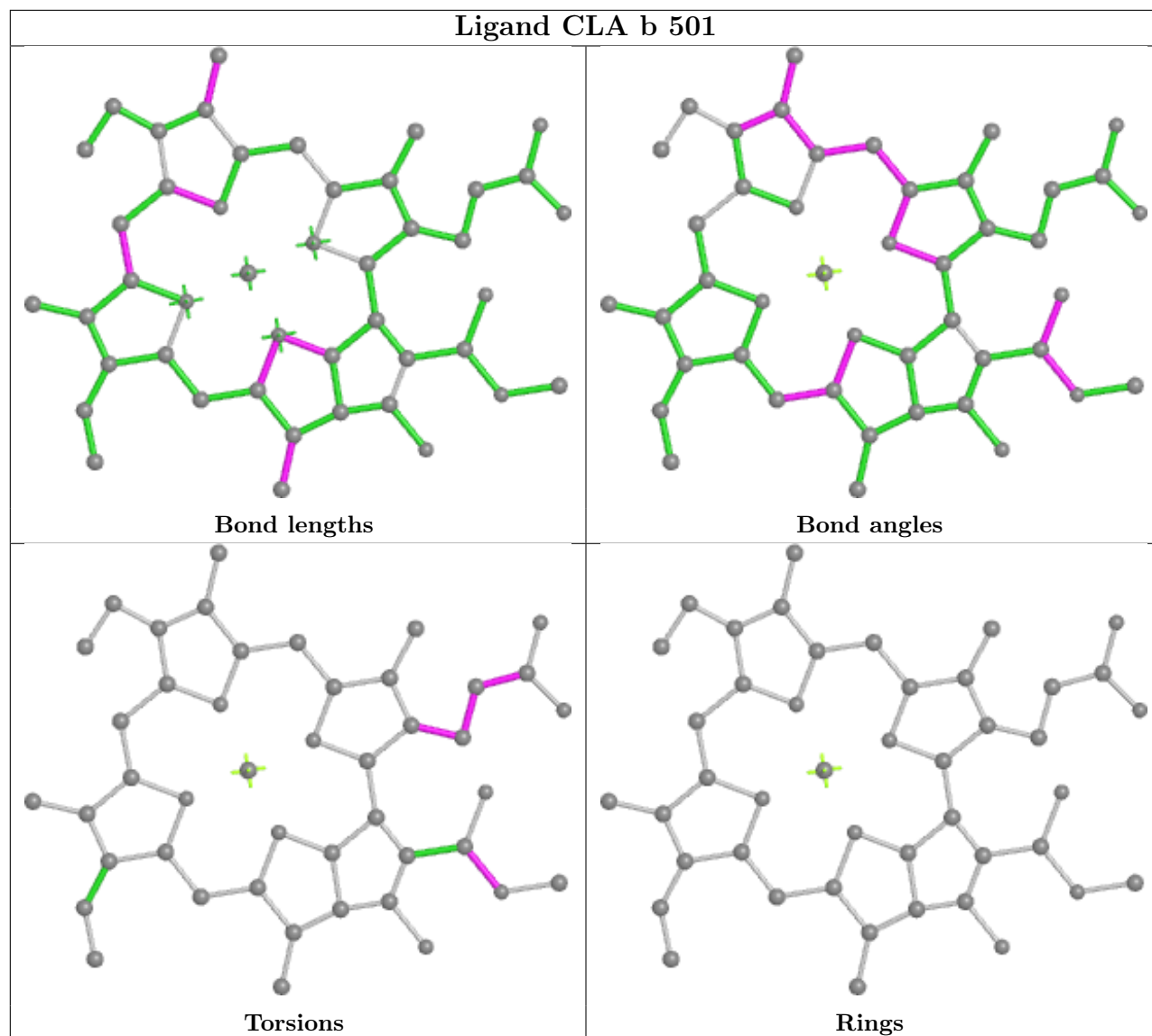




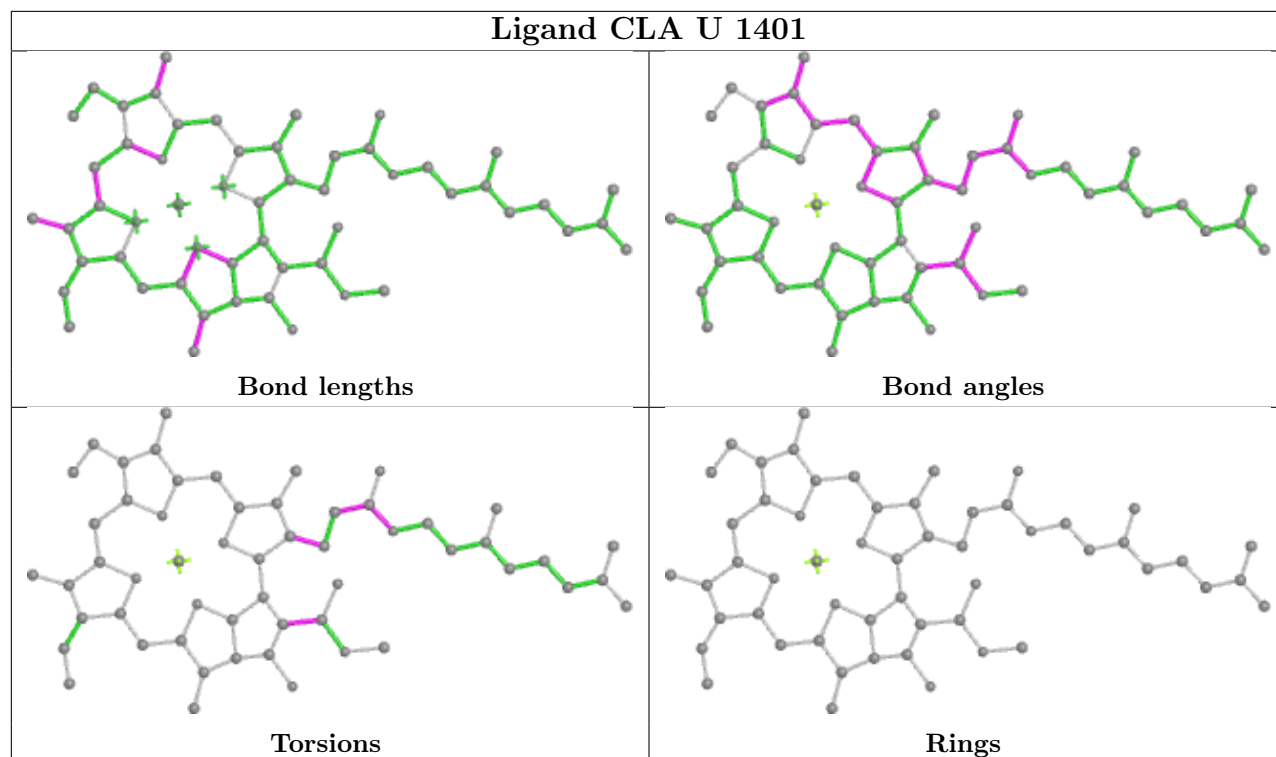
Ligand CLA Y 502



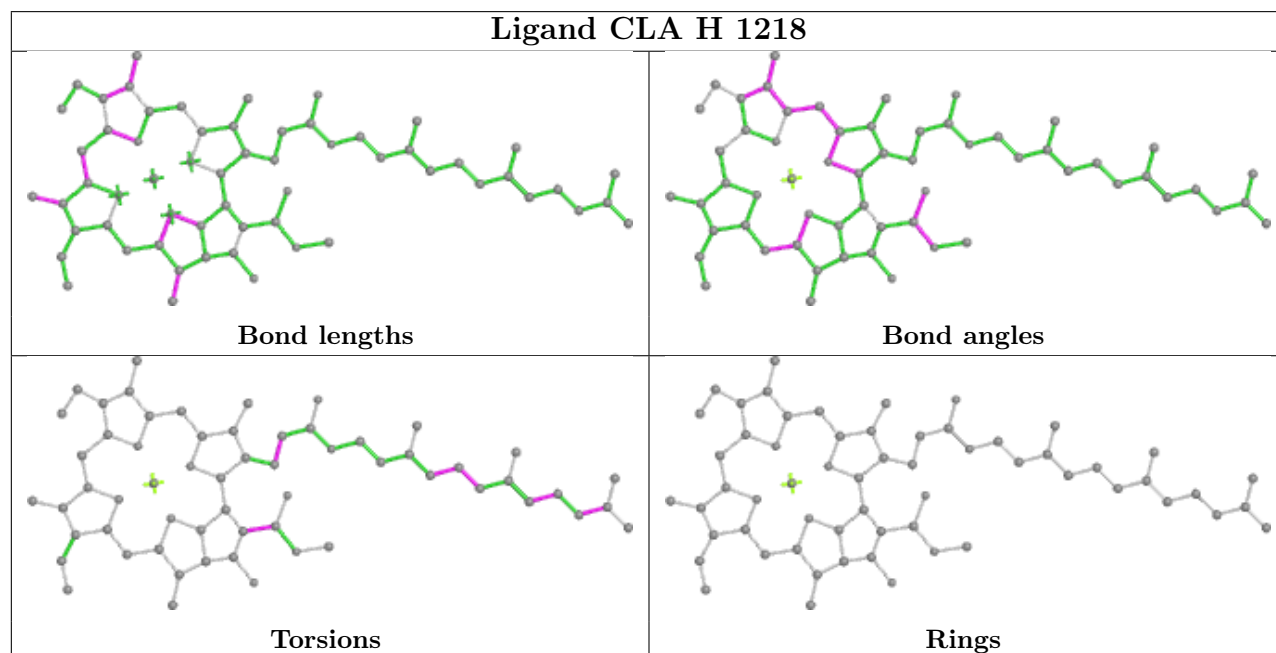
Ligand CLA b 501

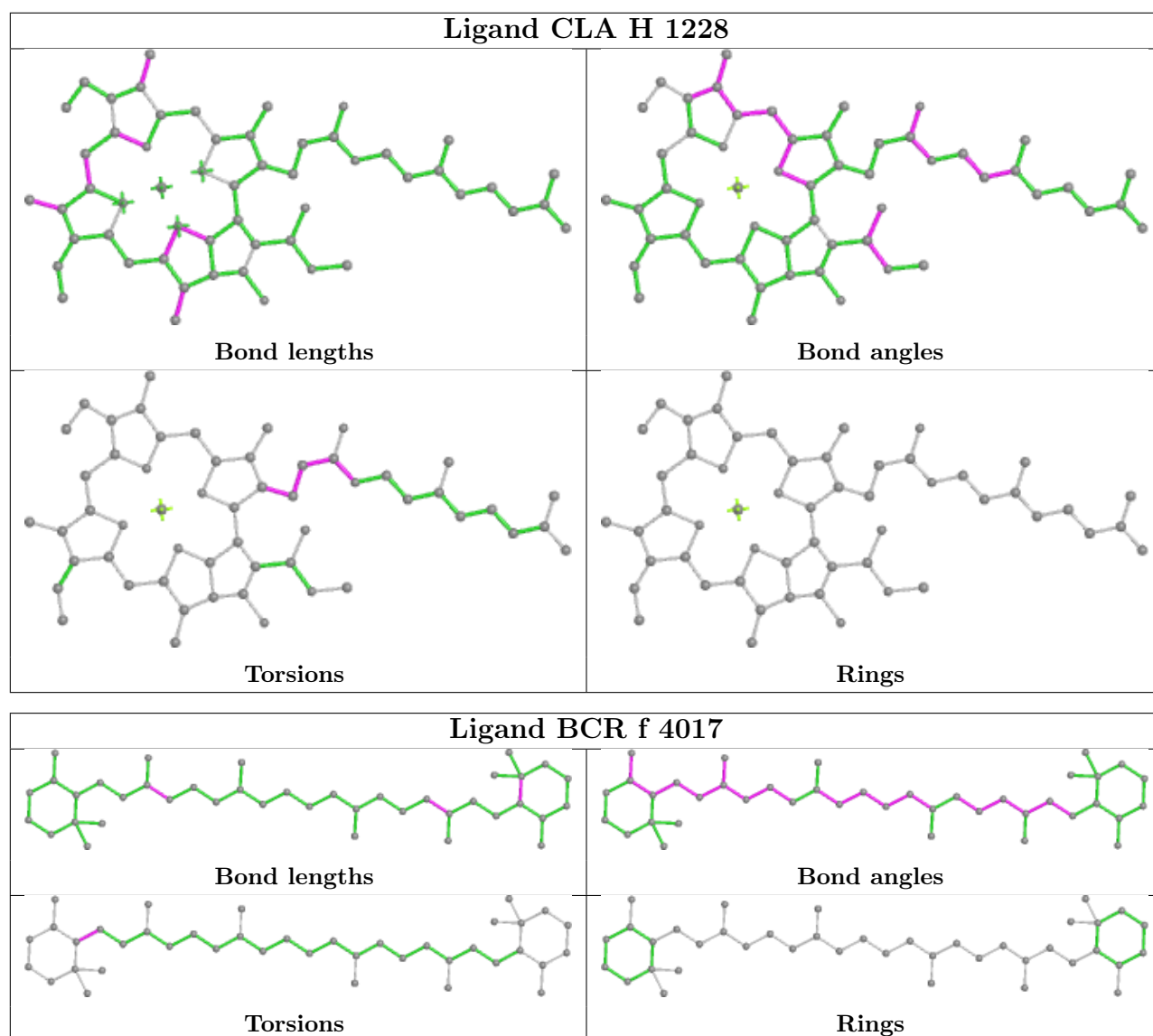


Ligand CLA U 1401

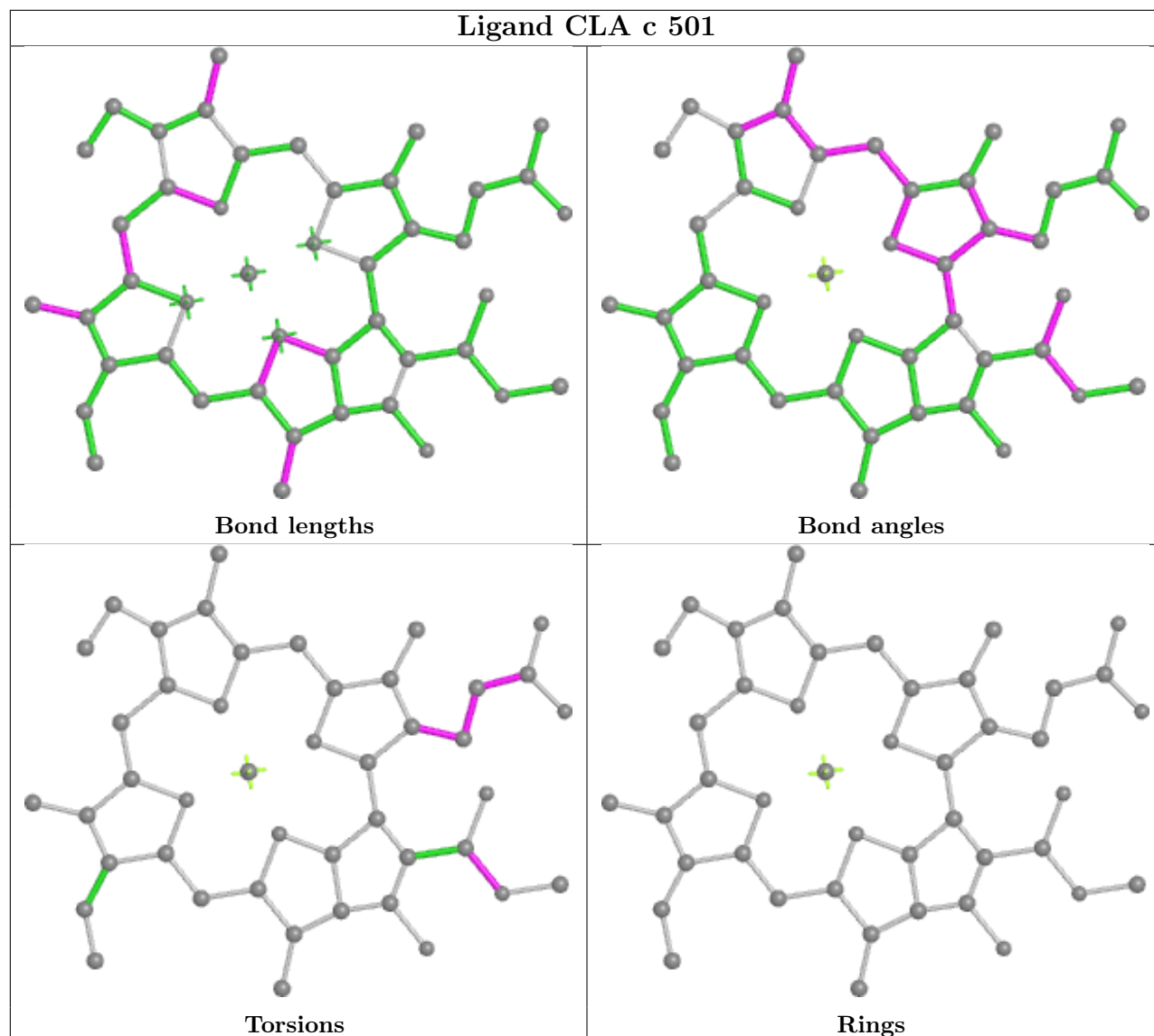


Ligand CLA H 1218

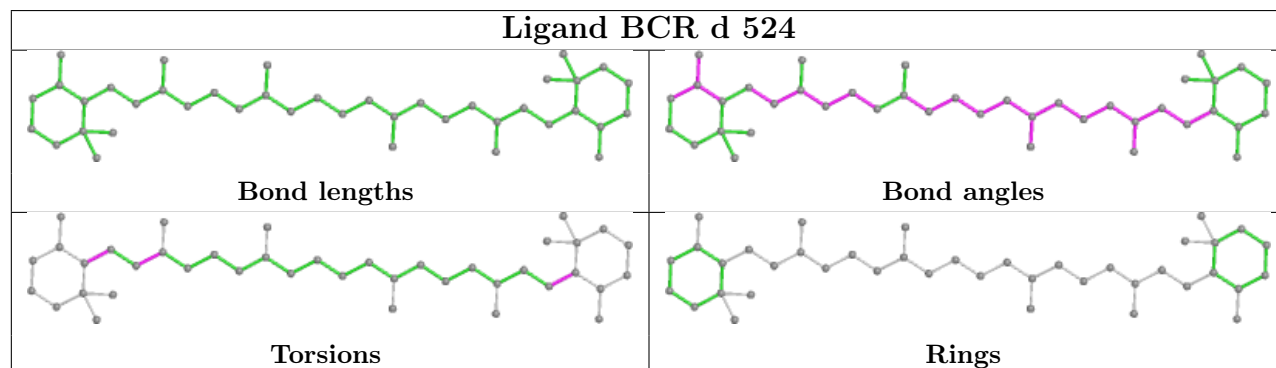


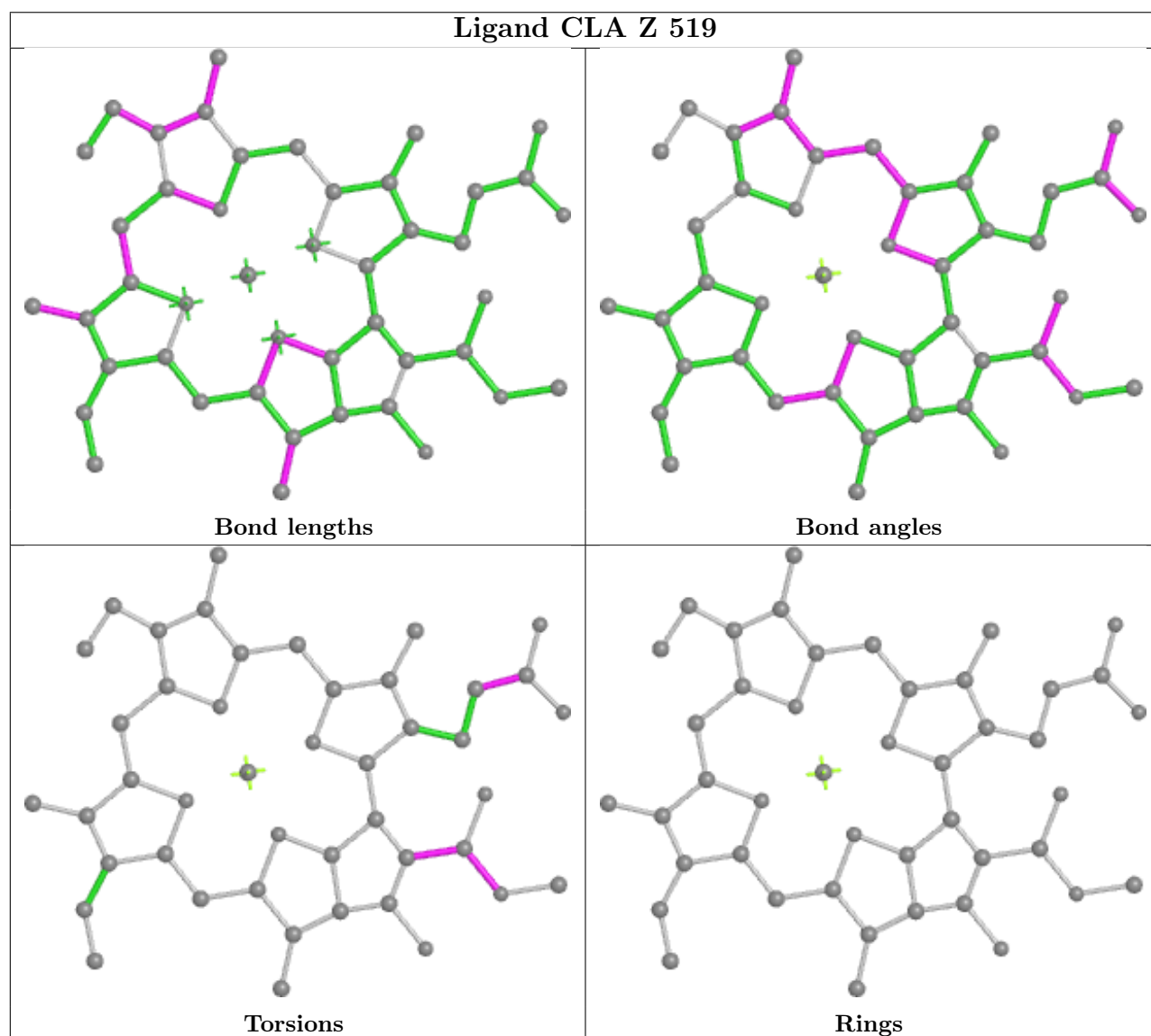
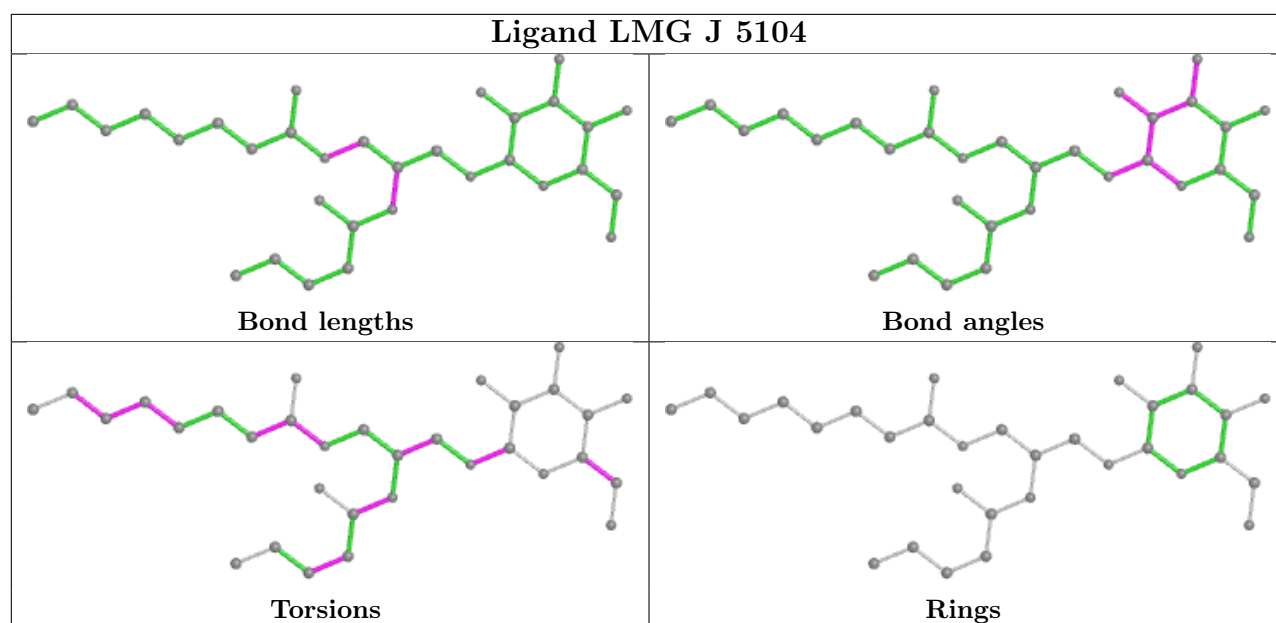


Ligand CLA c 501

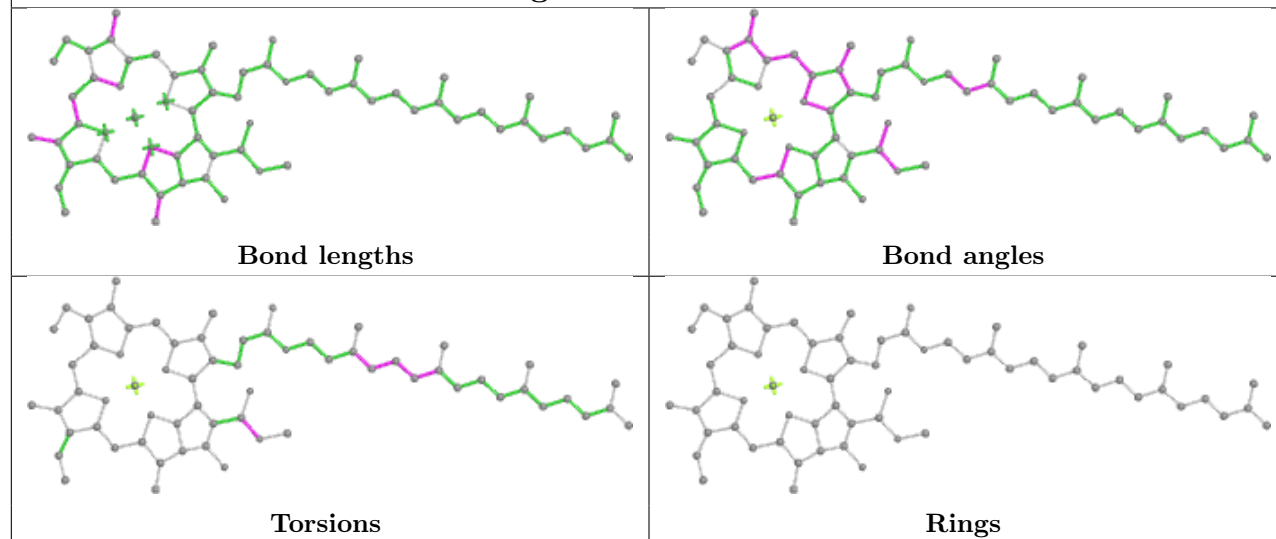


Ligand BCR d 524

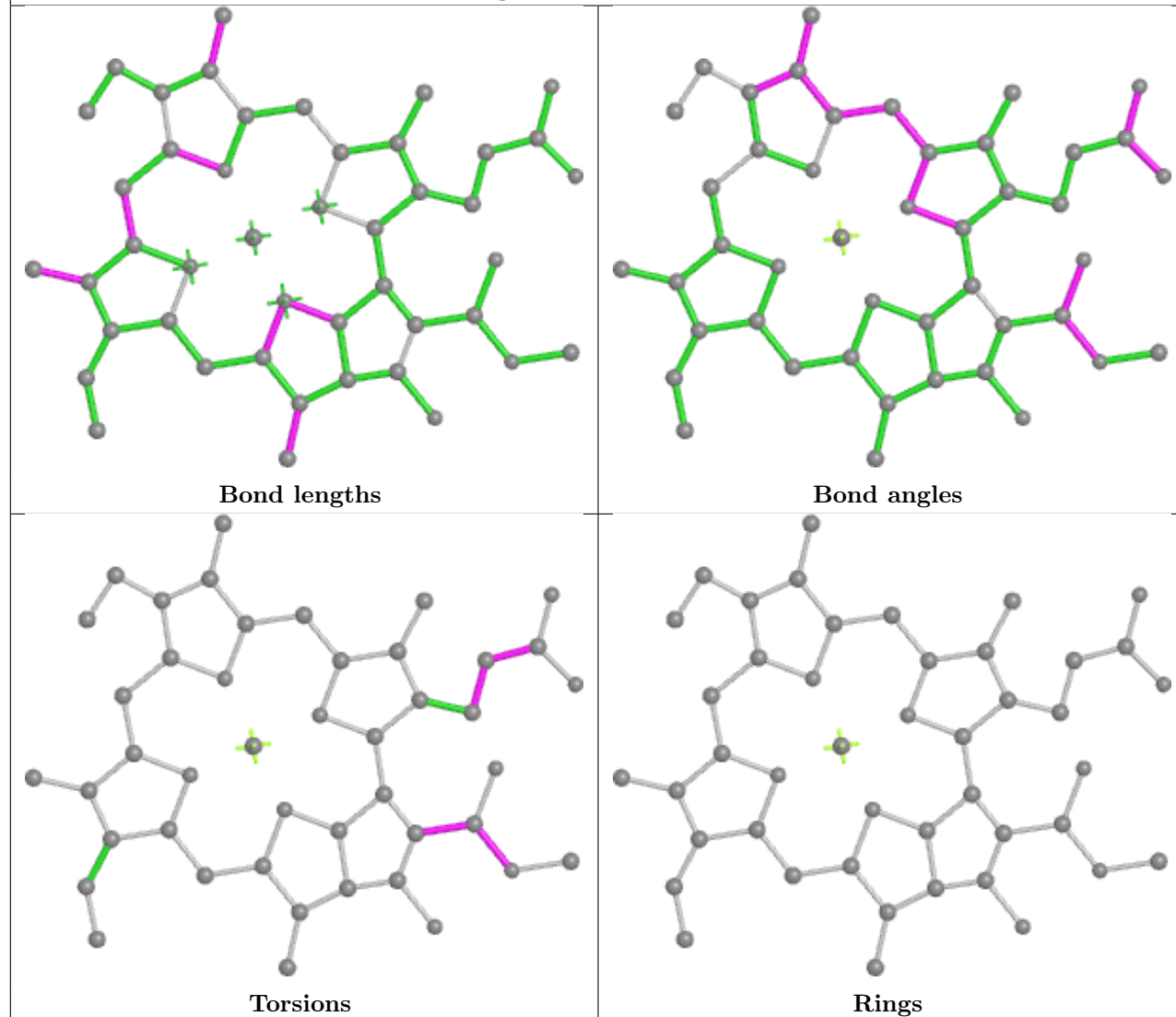




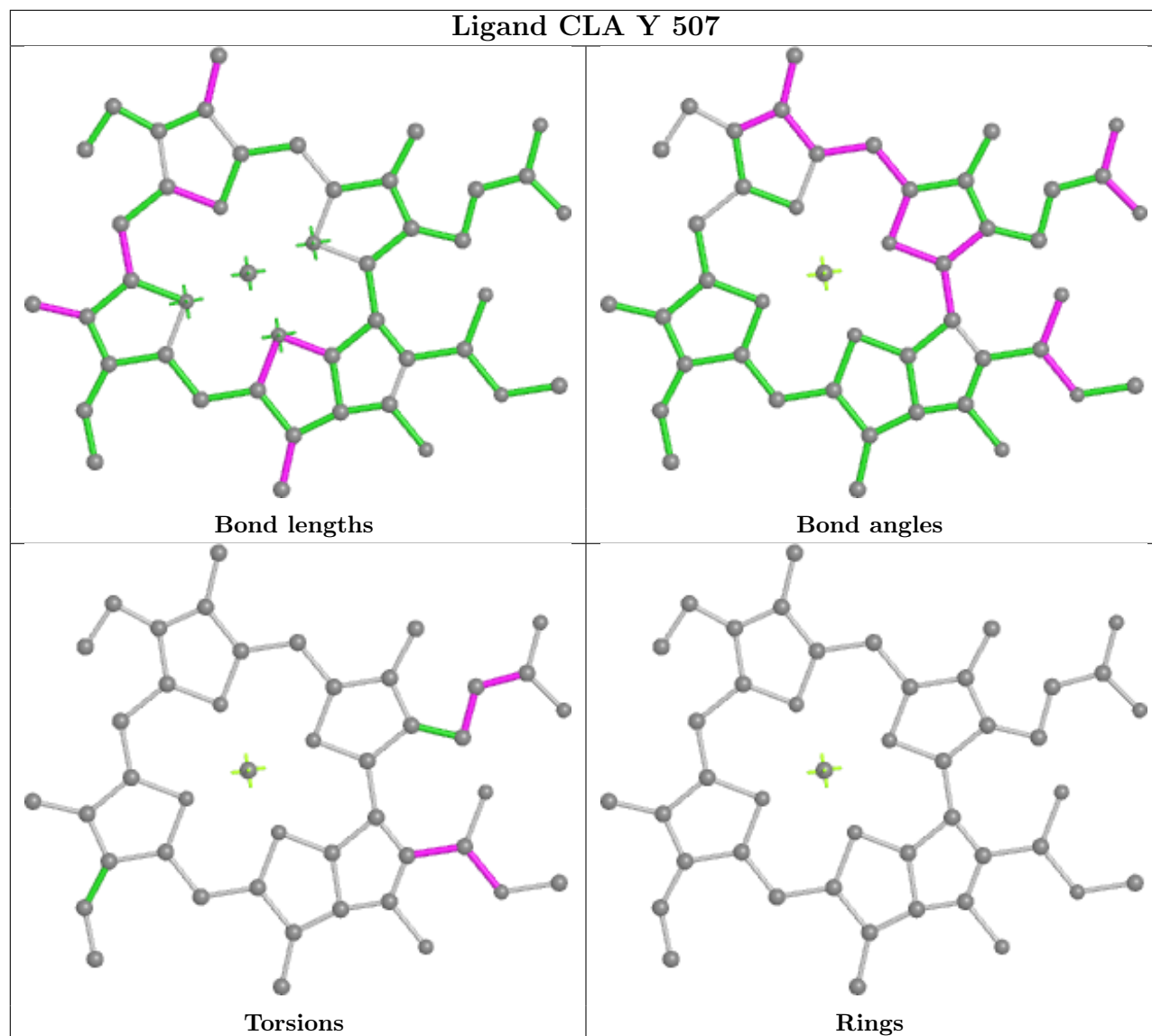
Ligand CLA f 1231

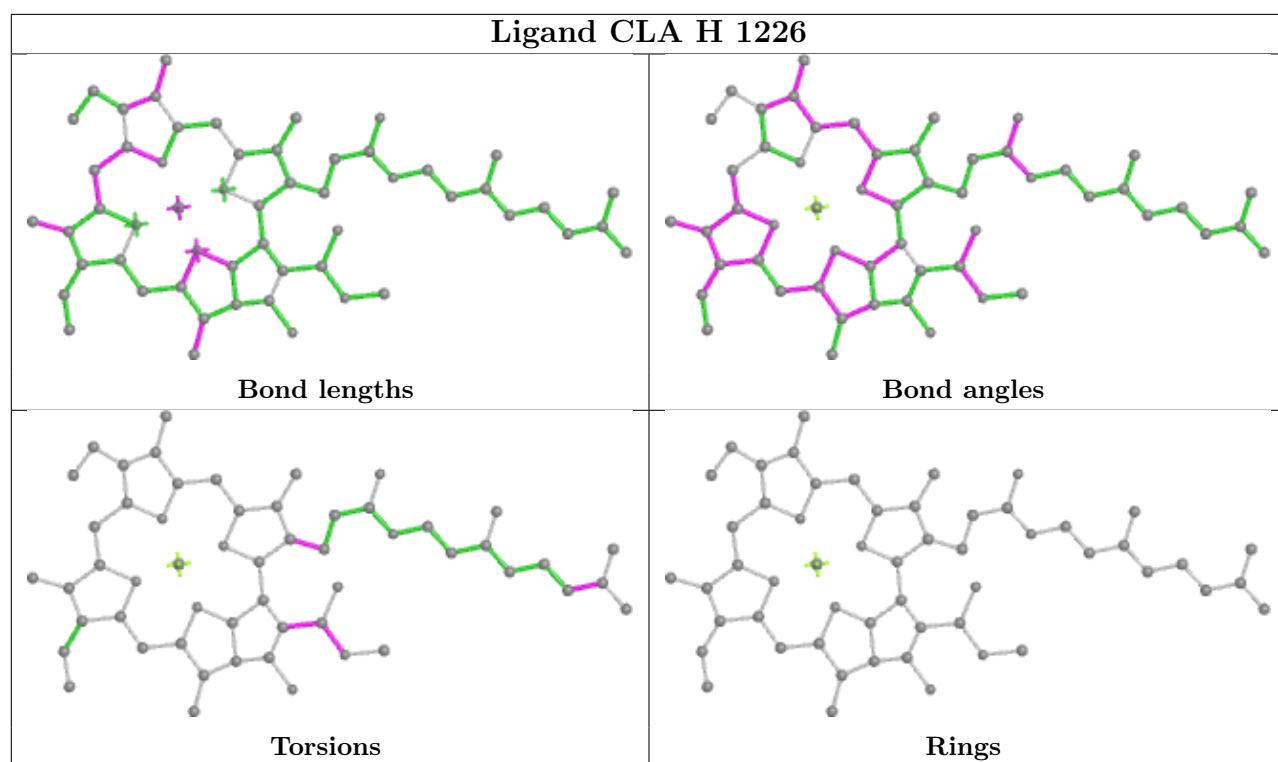


Ligand CLA 1 517

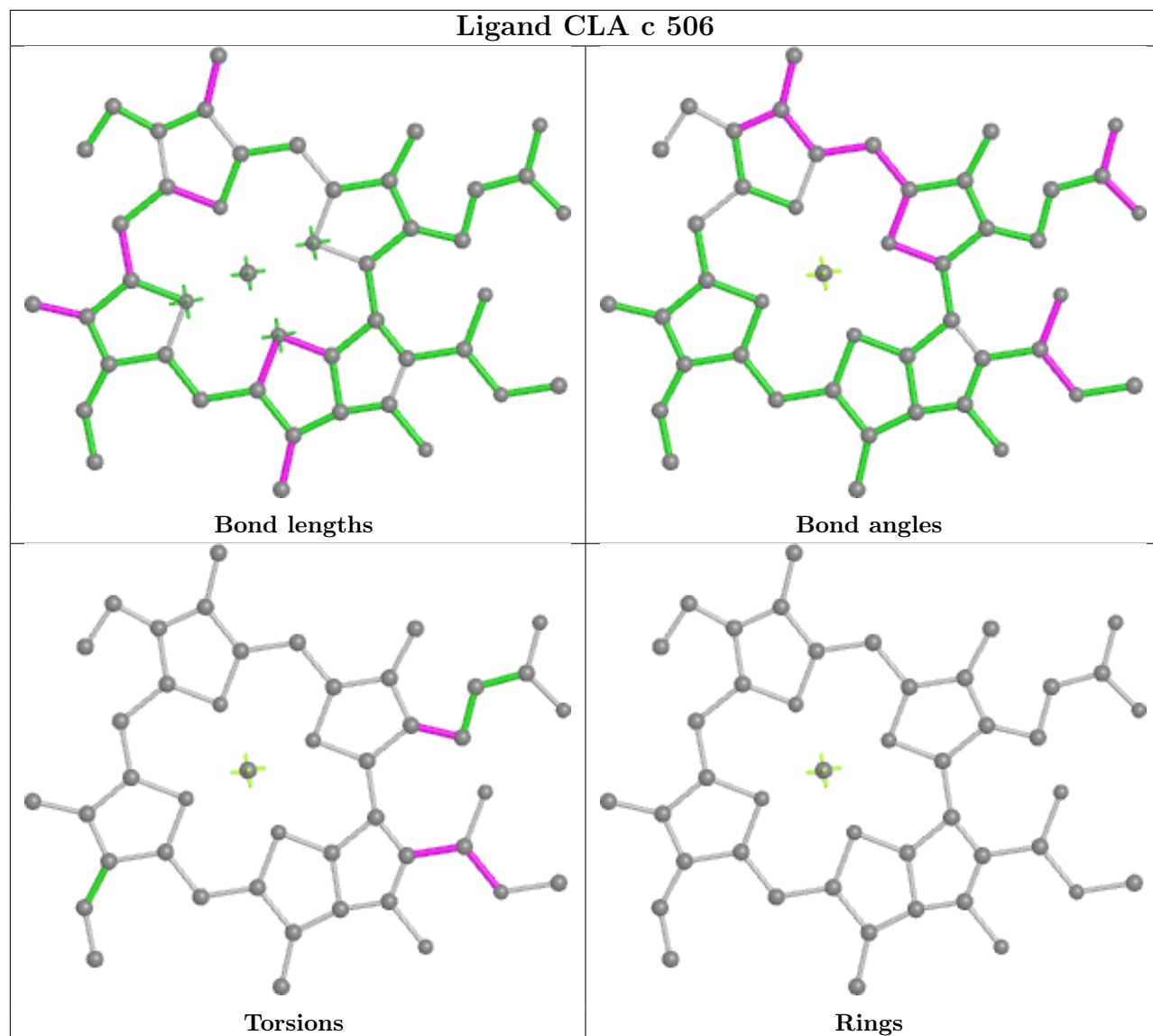


Ligand CLA Y 507

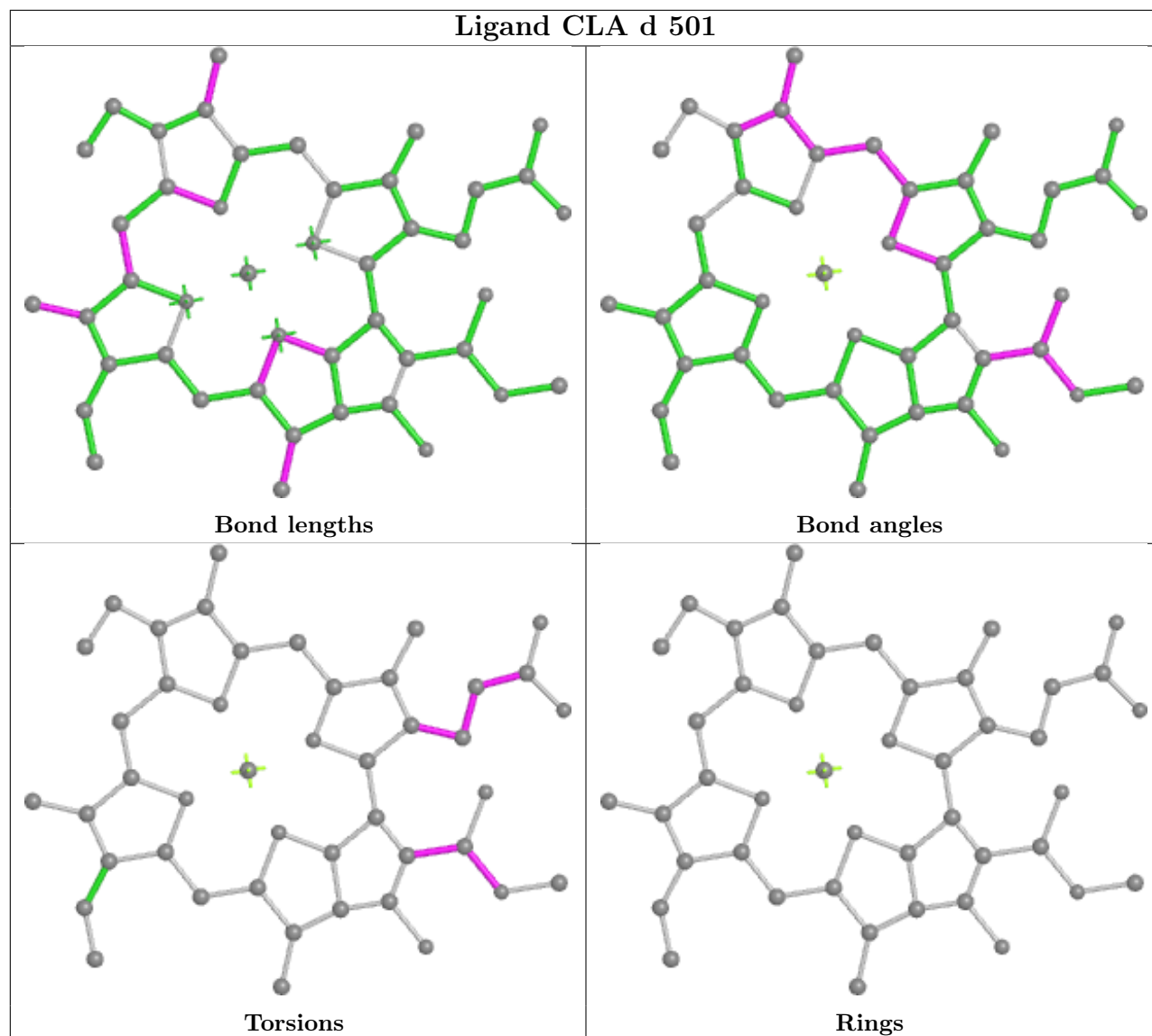




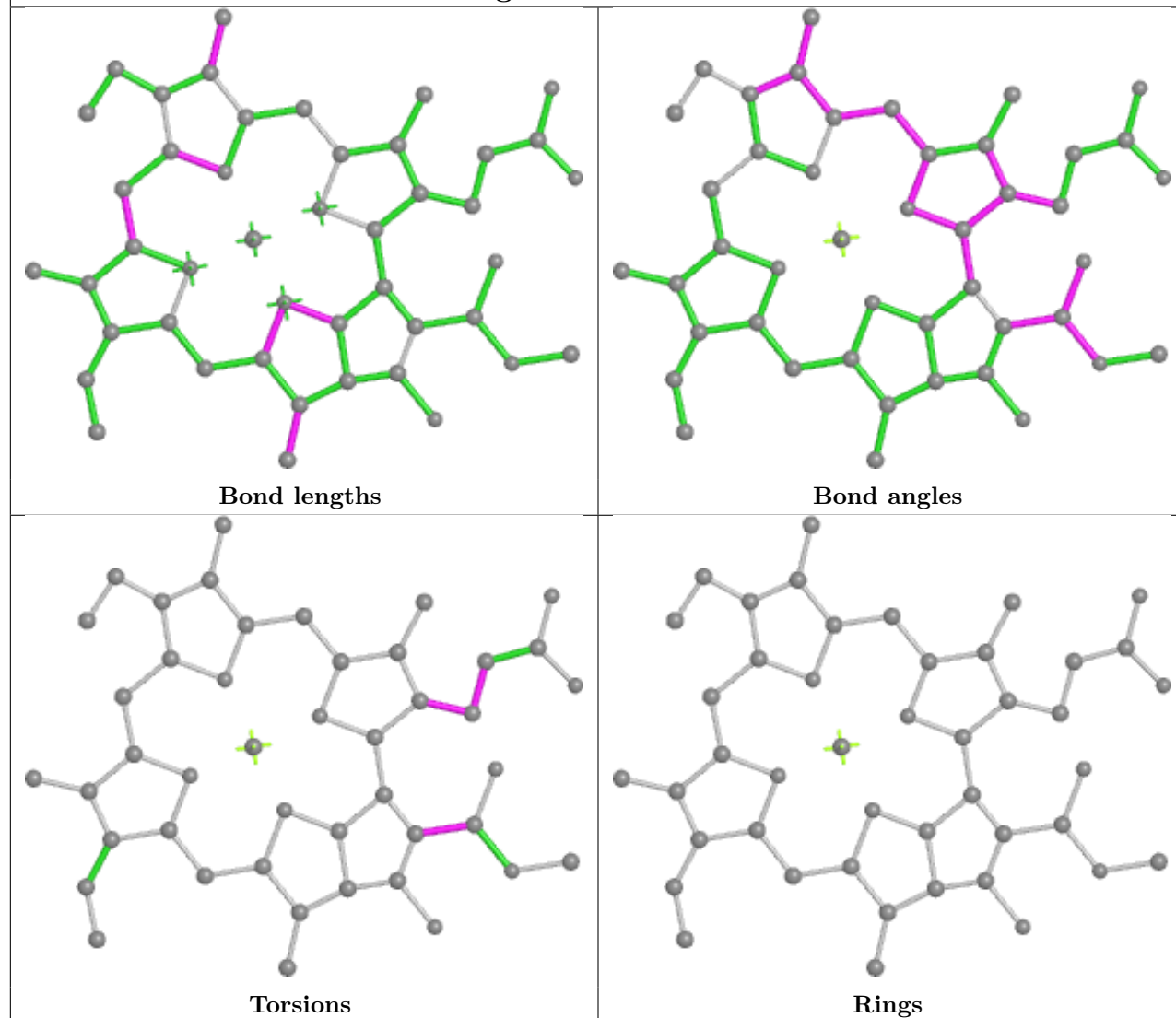
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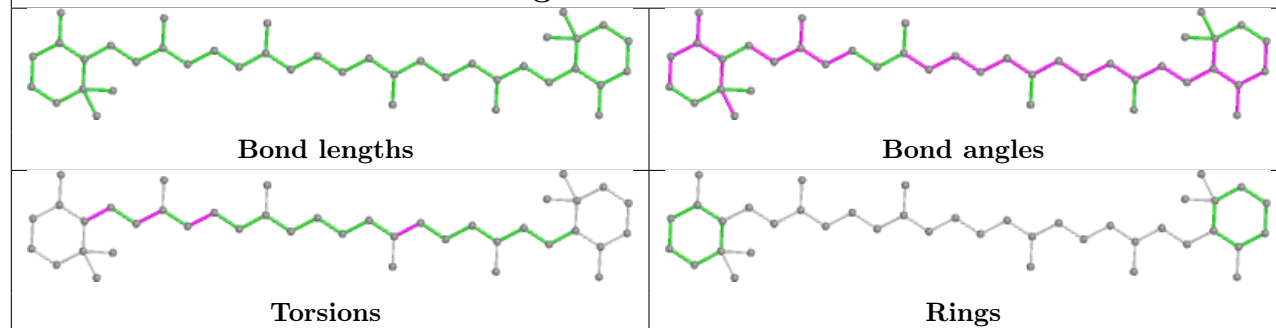
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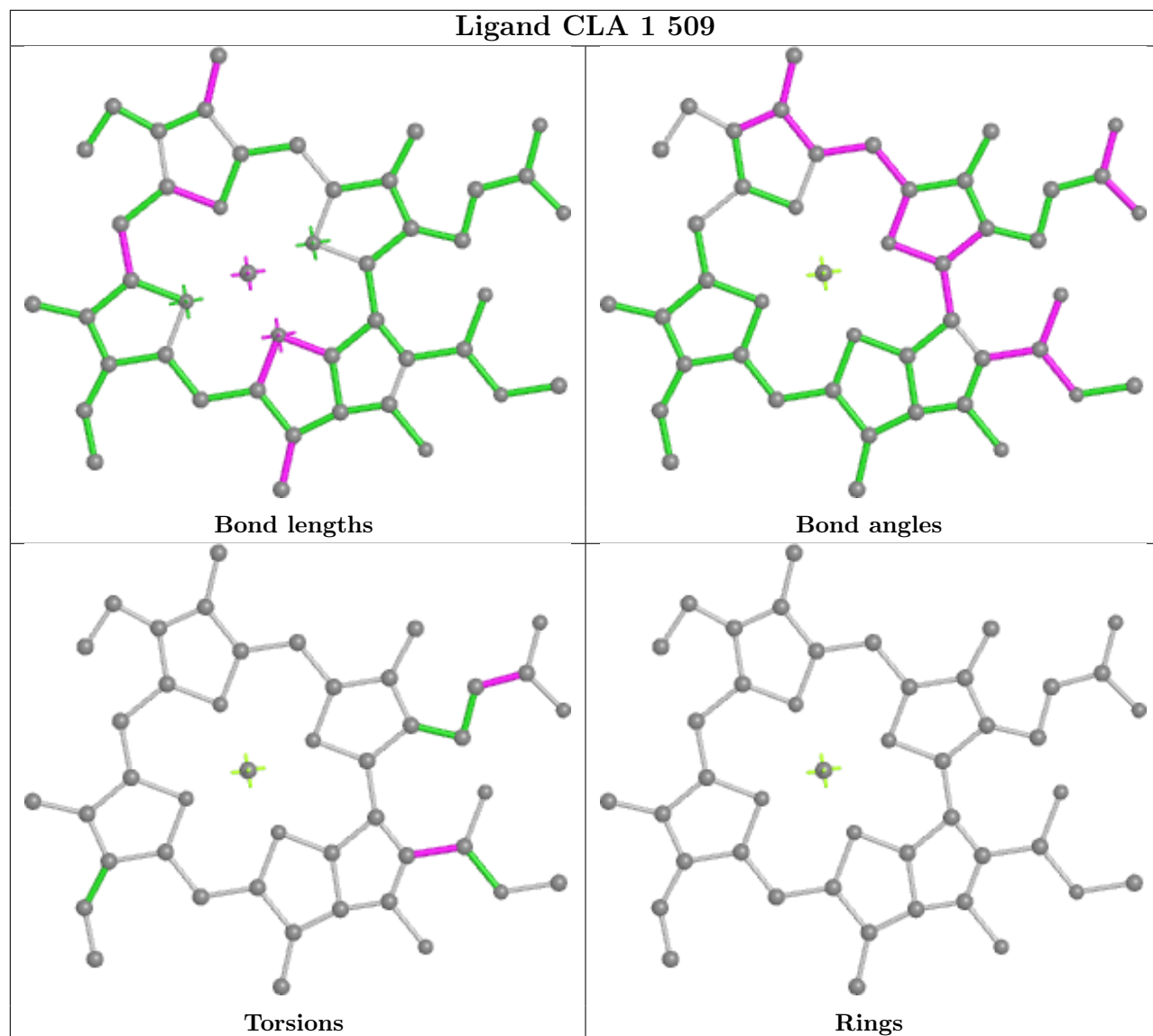
Ligand CLA s 504

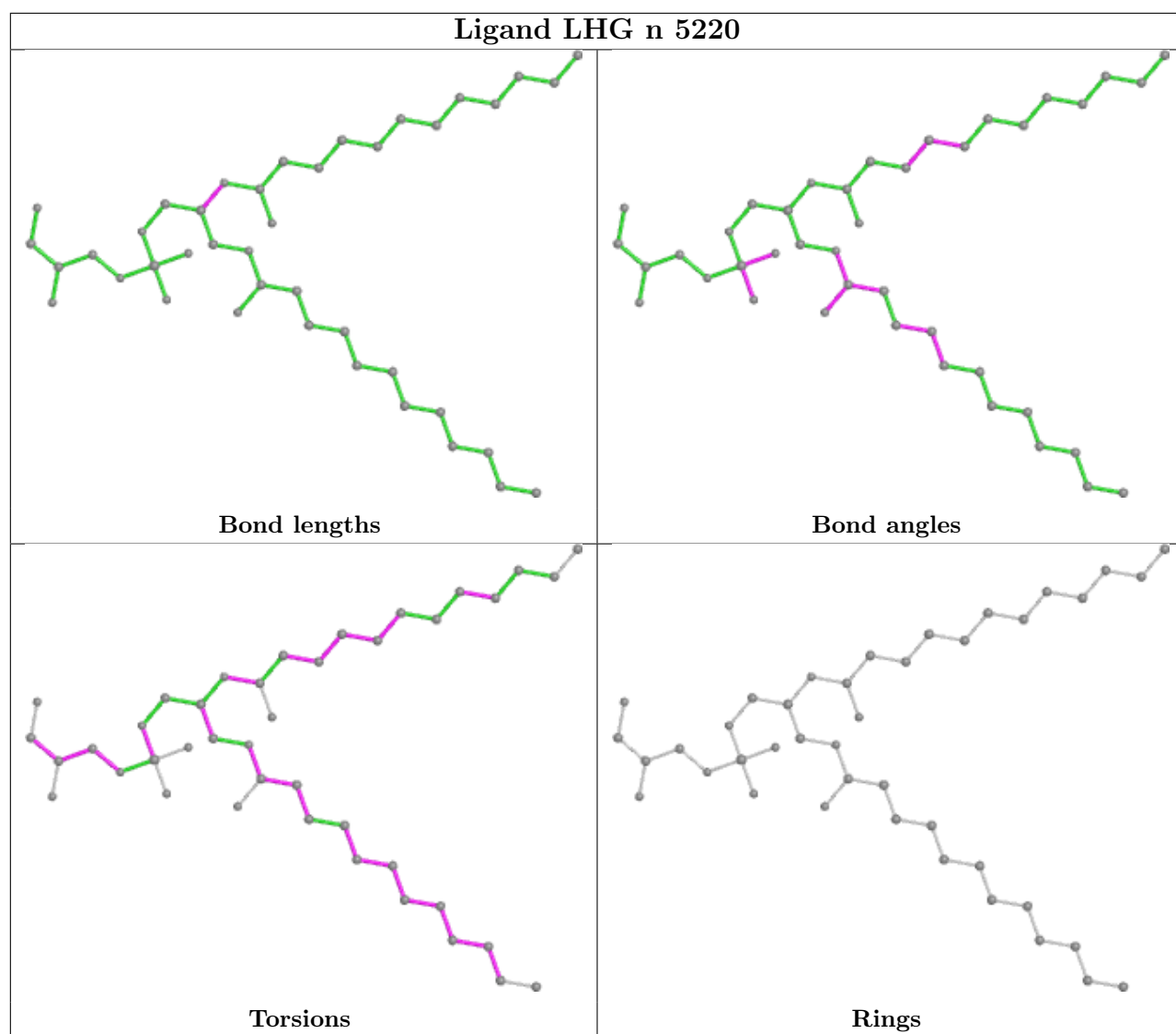


Ligand BCR u 521

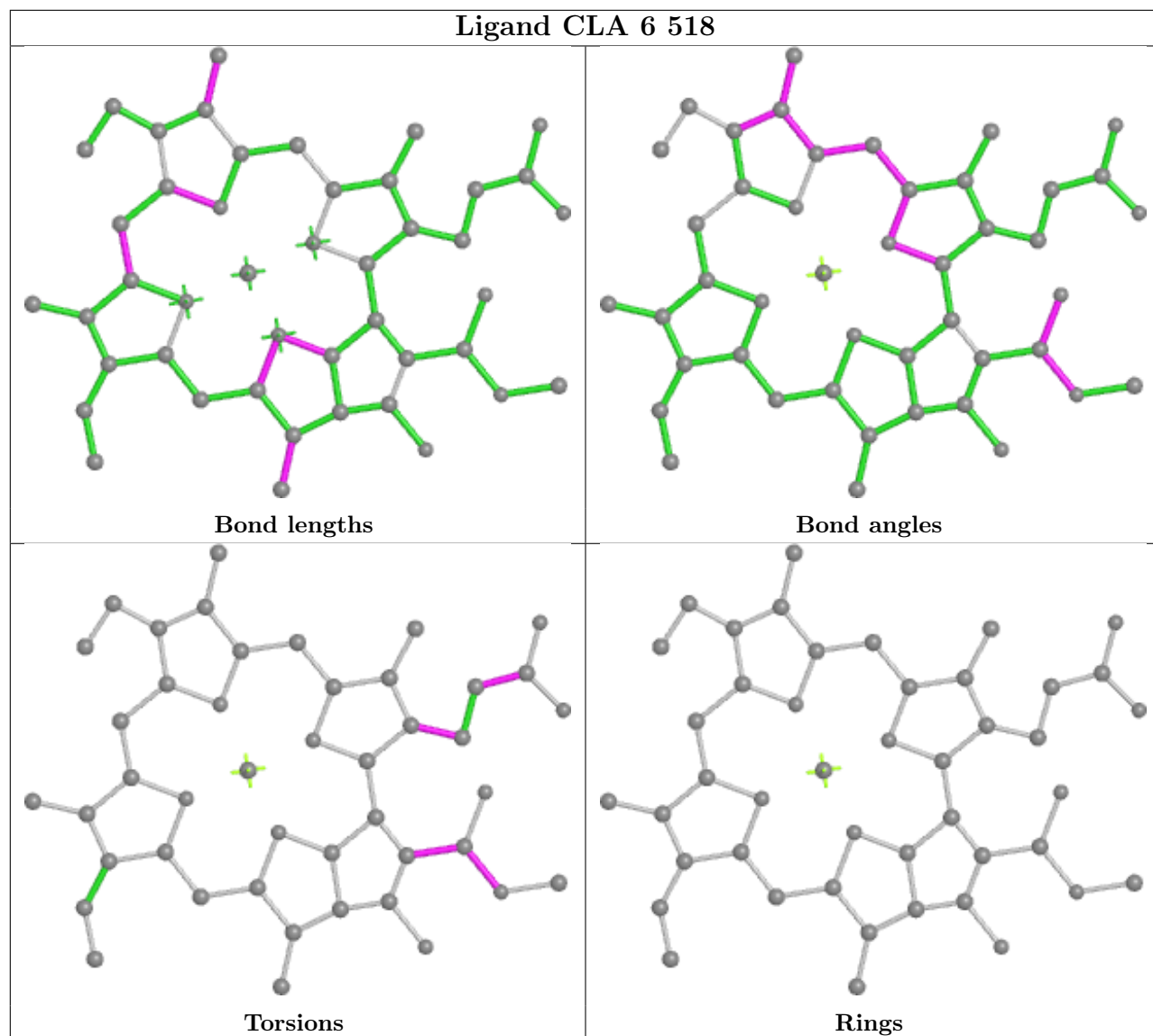


Ligand CLA 1 509

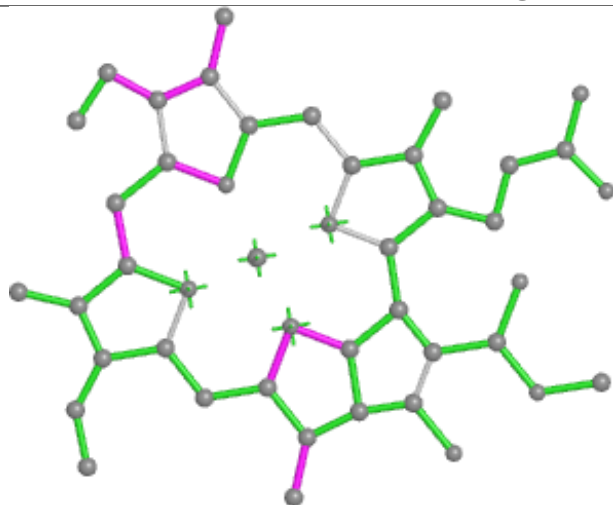




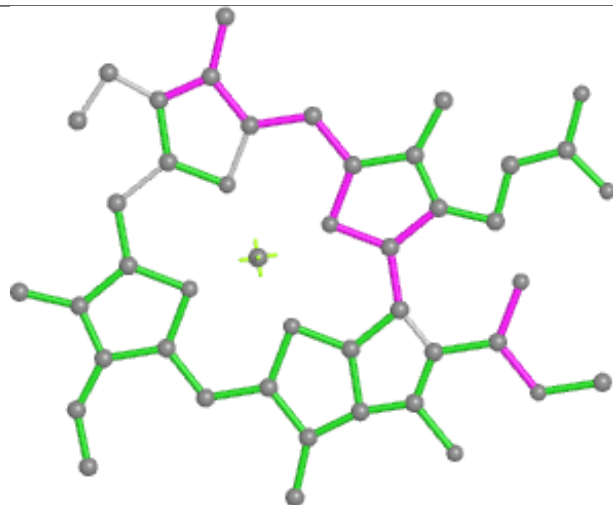
Ligand CLA 6 518



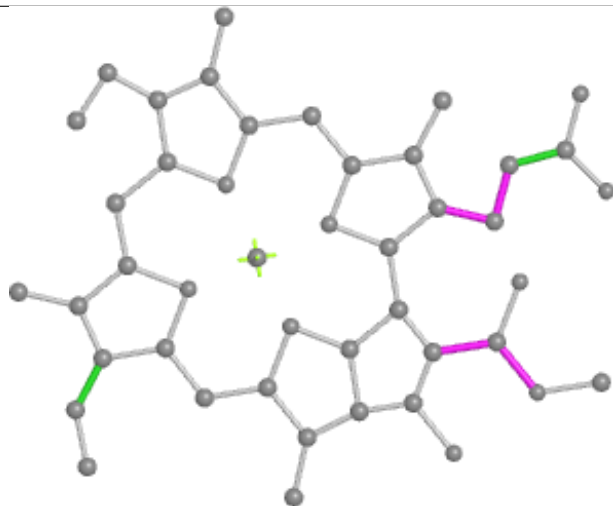
Ligand CLA Y 503



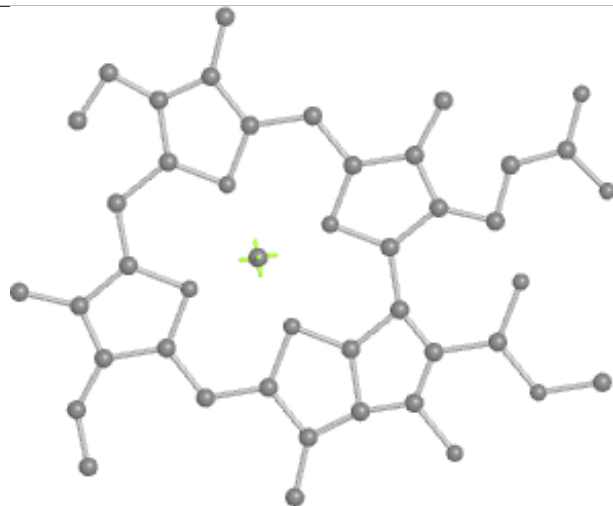
Bond lengths



Bond angles

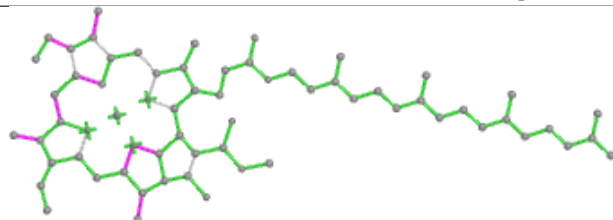


Torsions

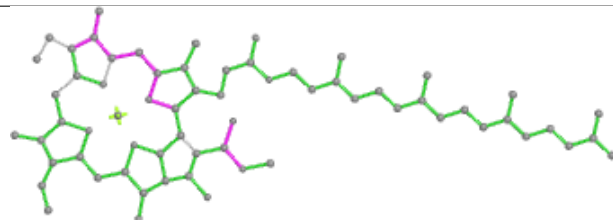


Rings

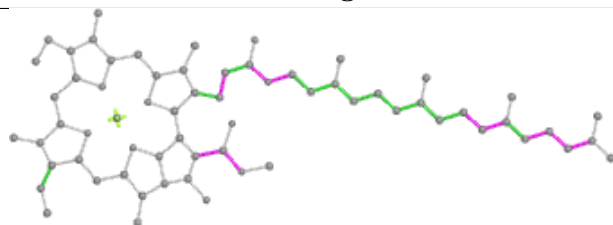
Ligand CLA f 1207



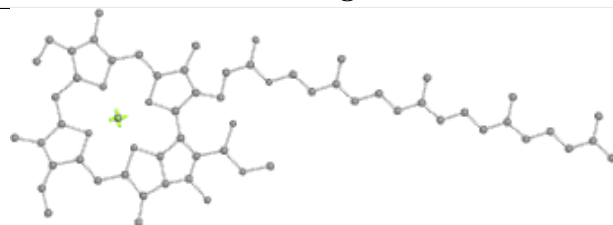
Bond lengths



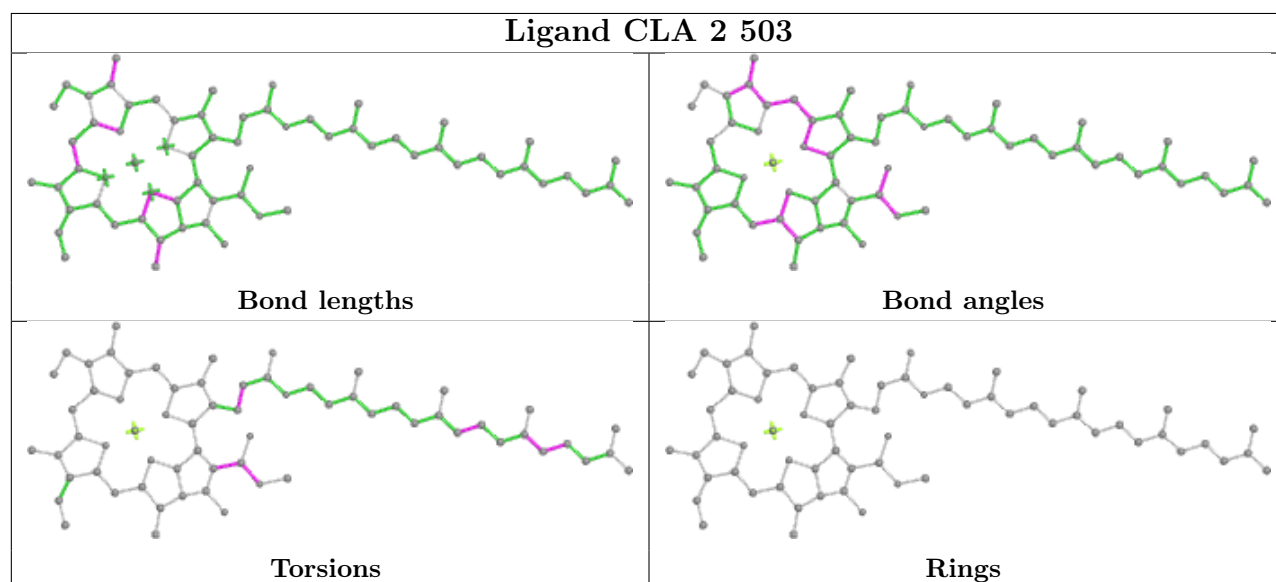
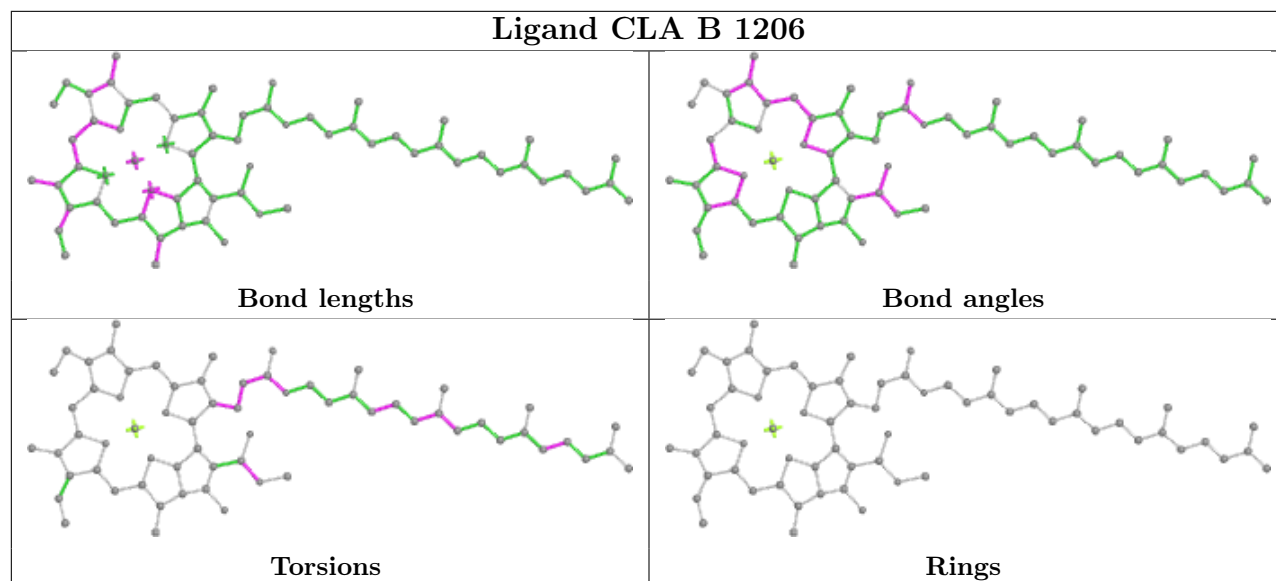
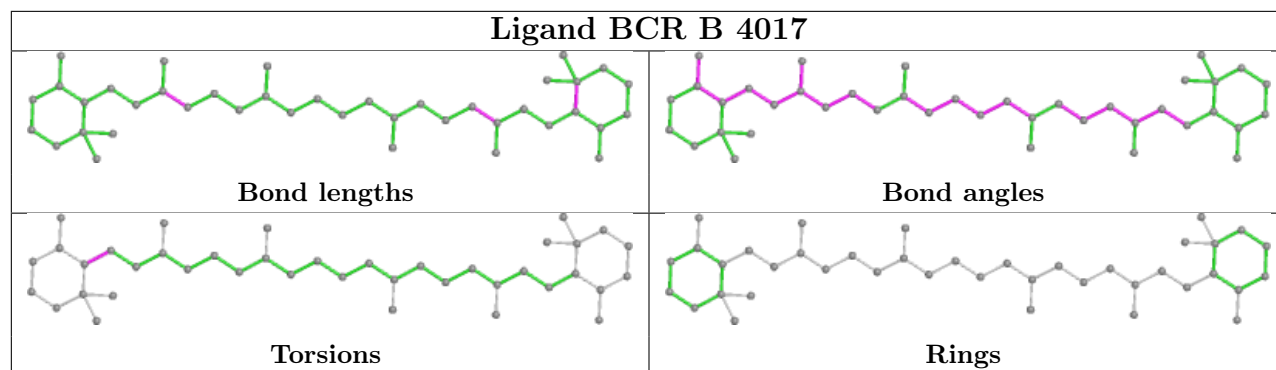
Bond angles

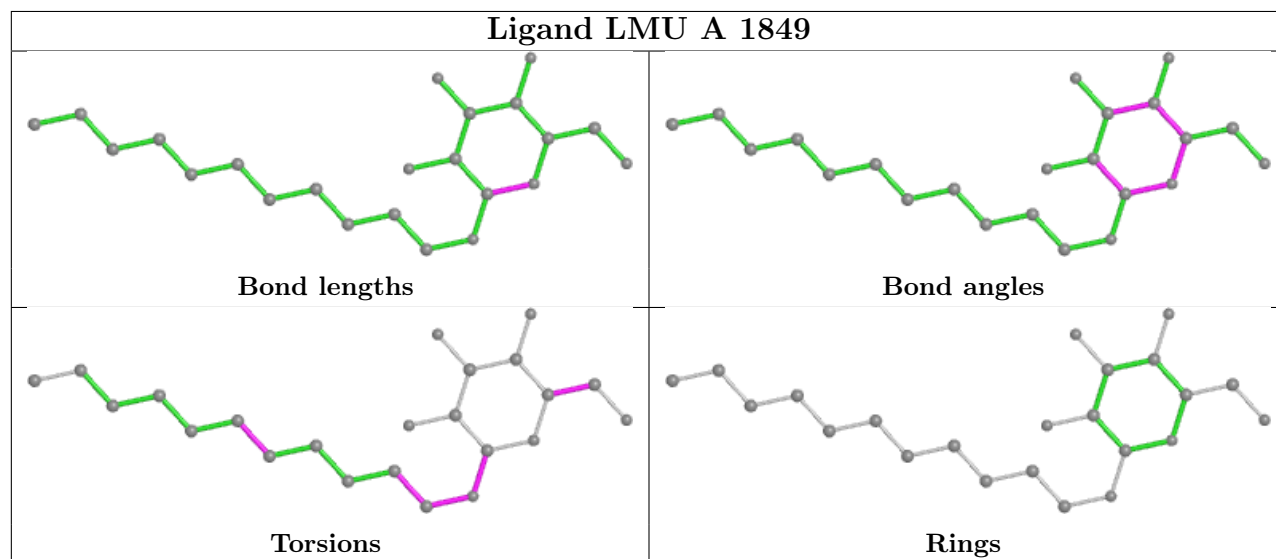
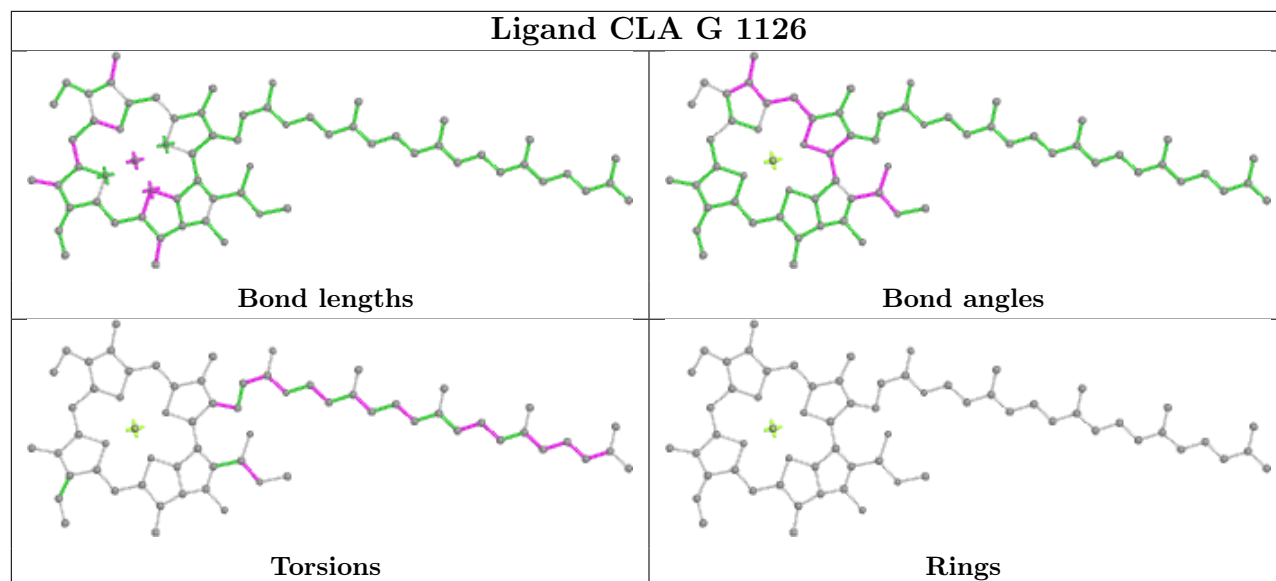
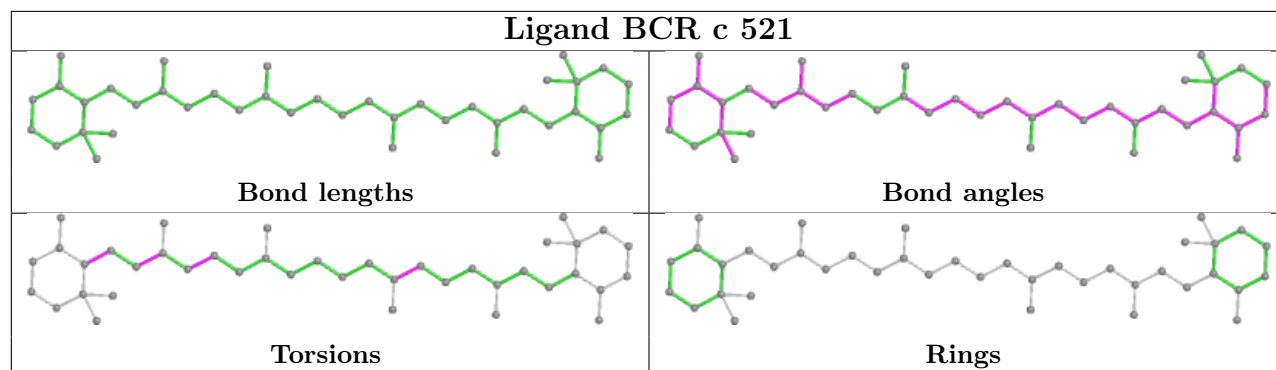


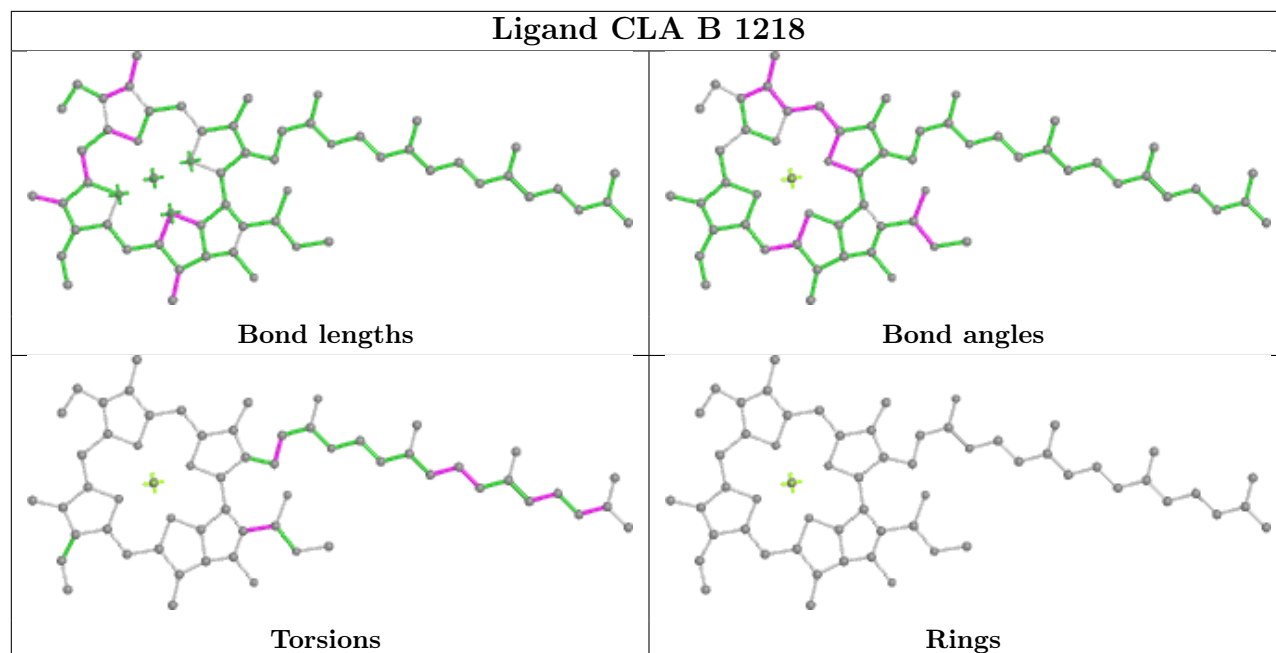
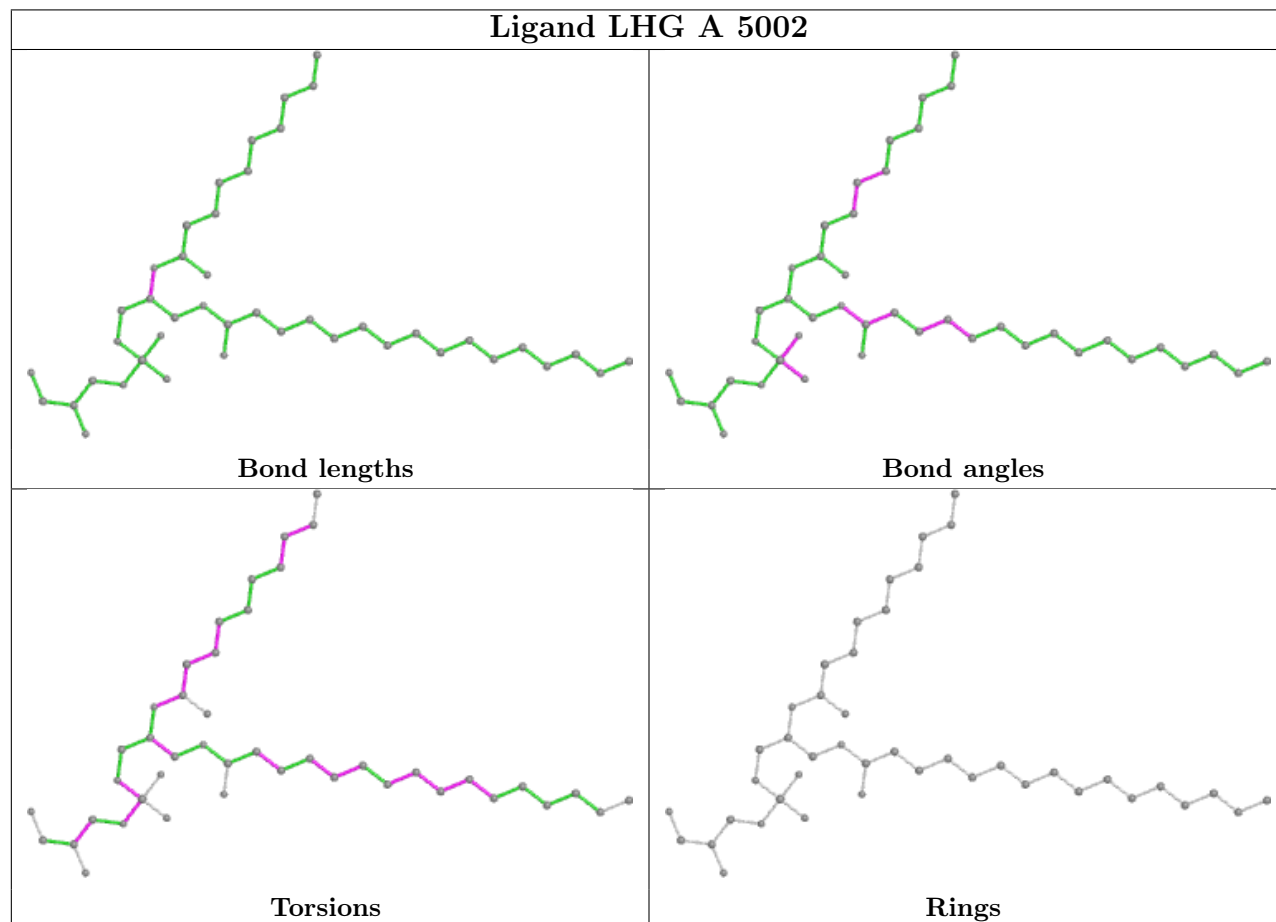
Torsions



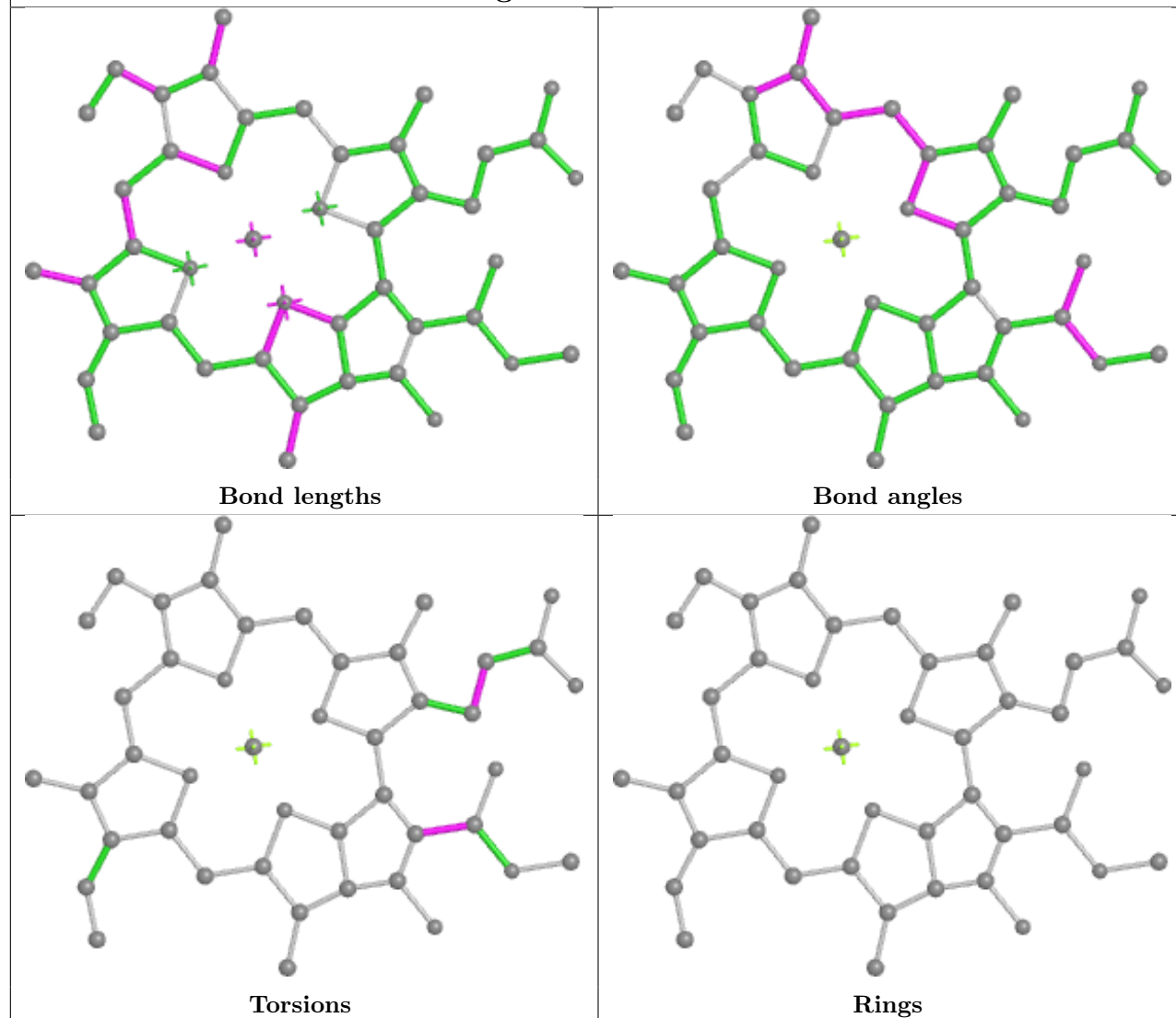
Rings



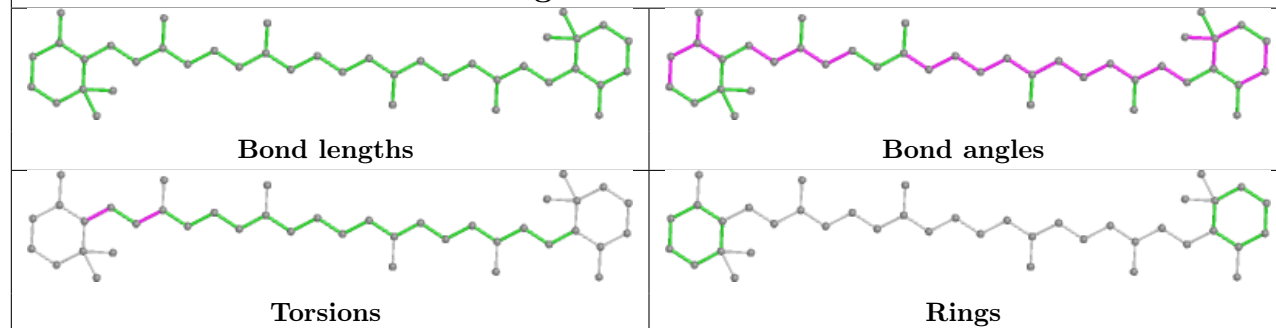


Ligand CLA B 1218**Ligand LHG A 5002**

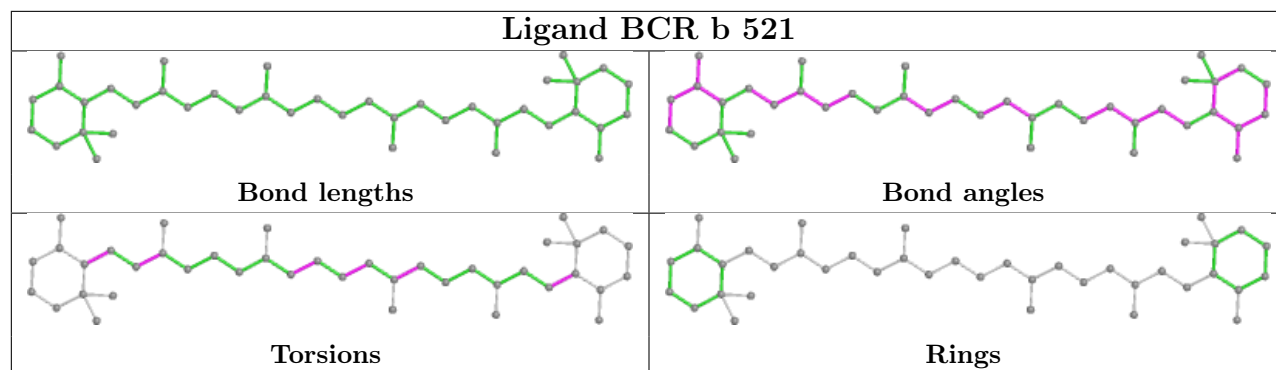
Ligand CLA t 505



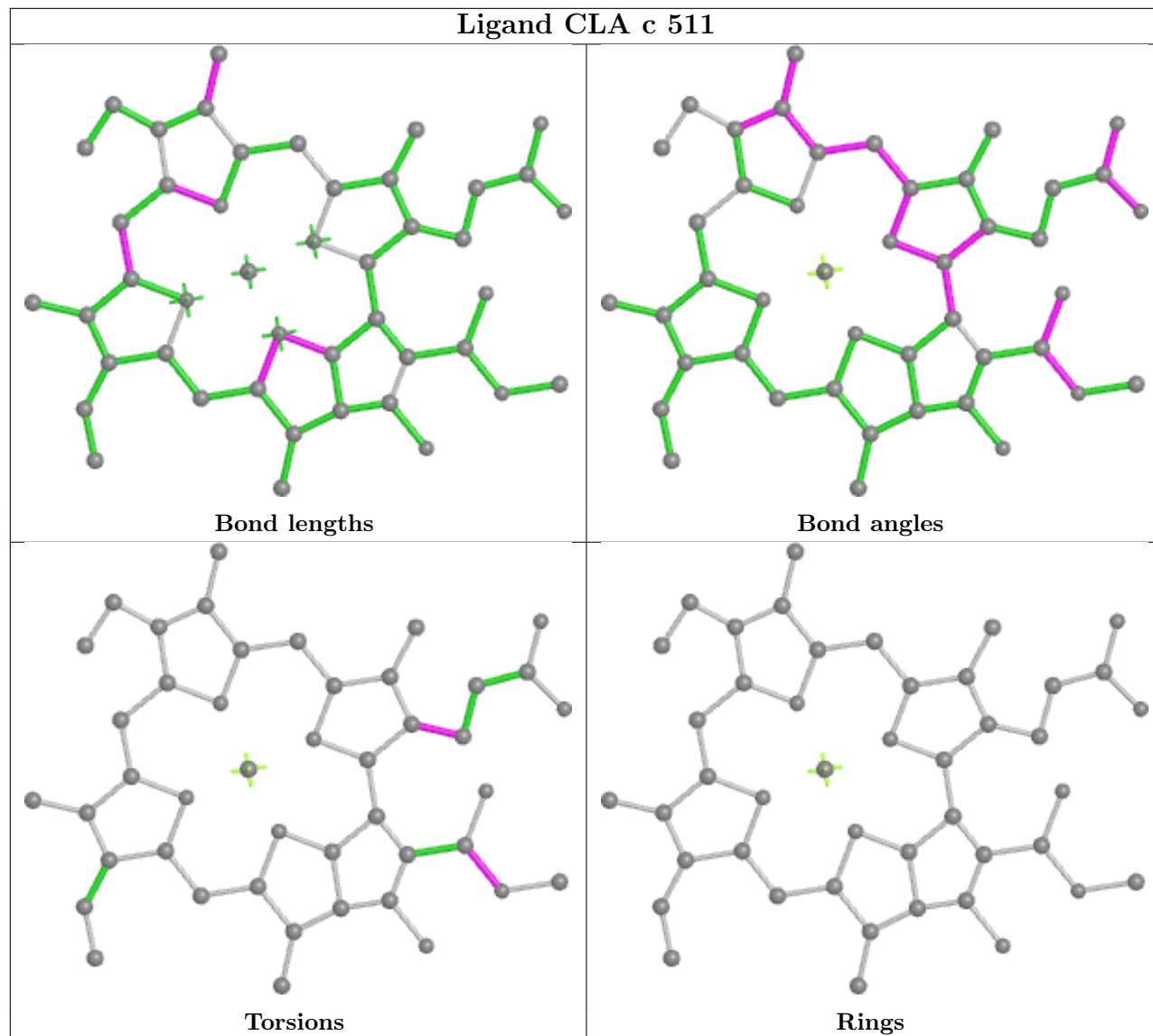
Ligand BCR 2 521



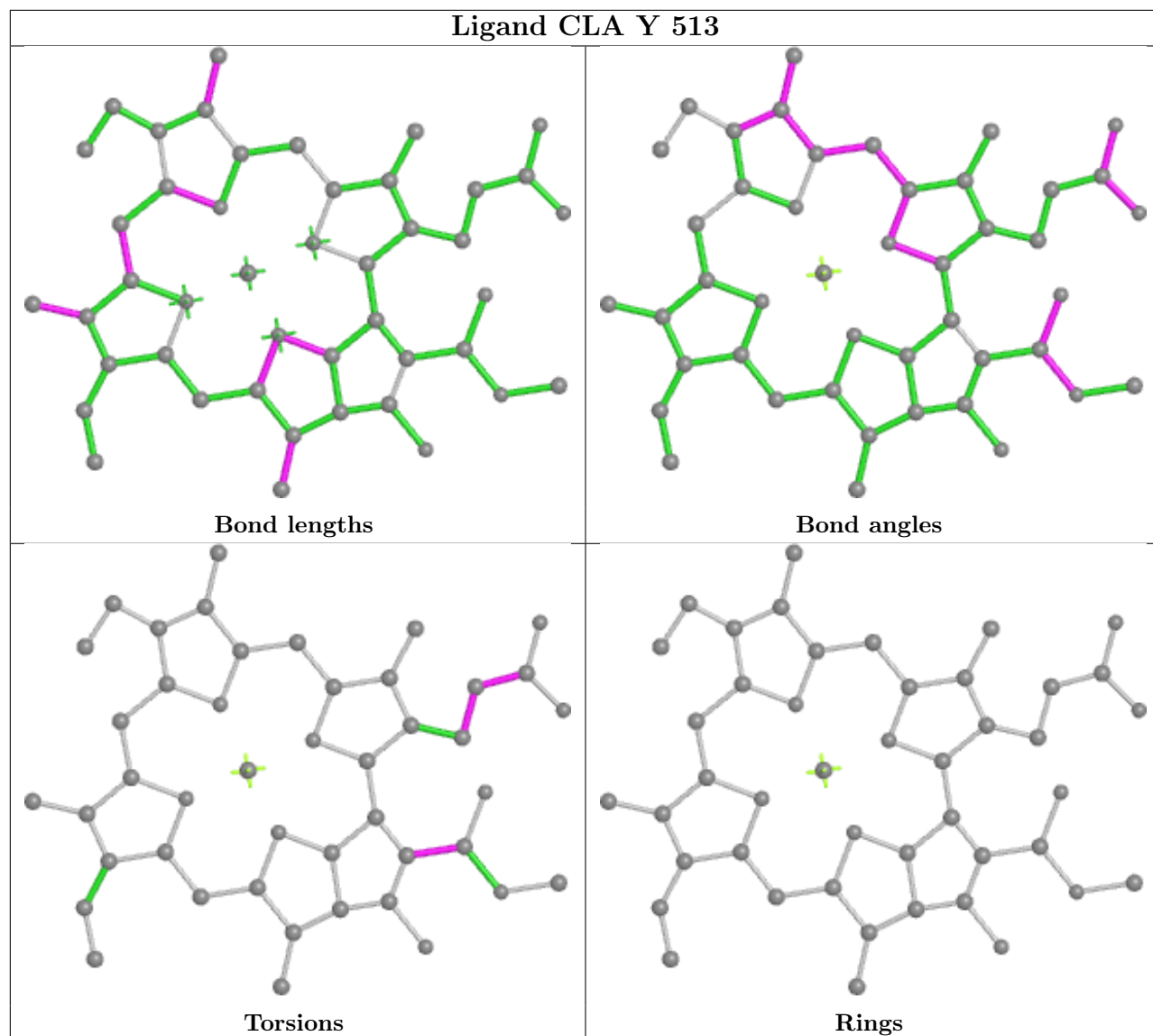
Ligand BCR b 521



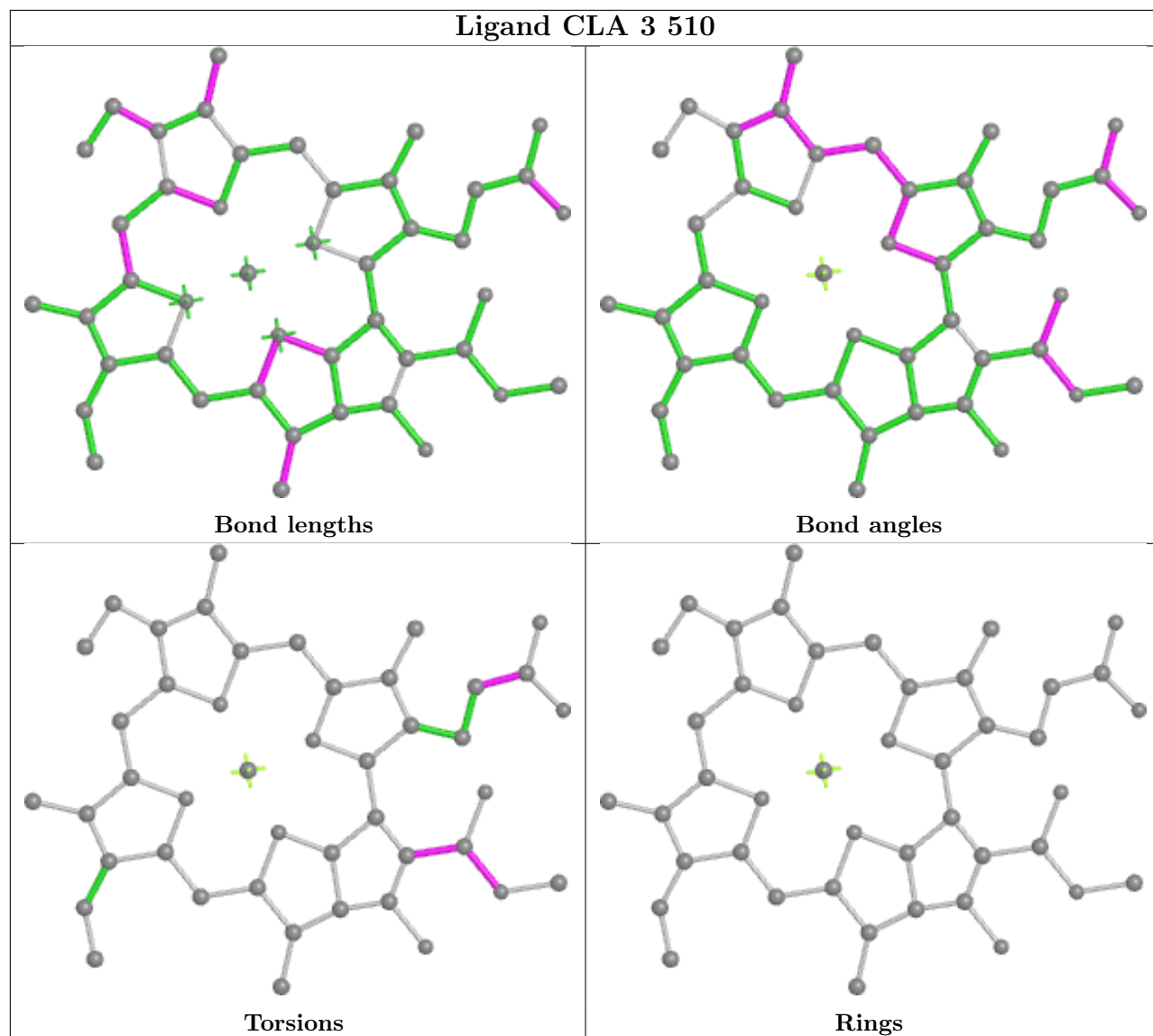
Ligand CLA c 511



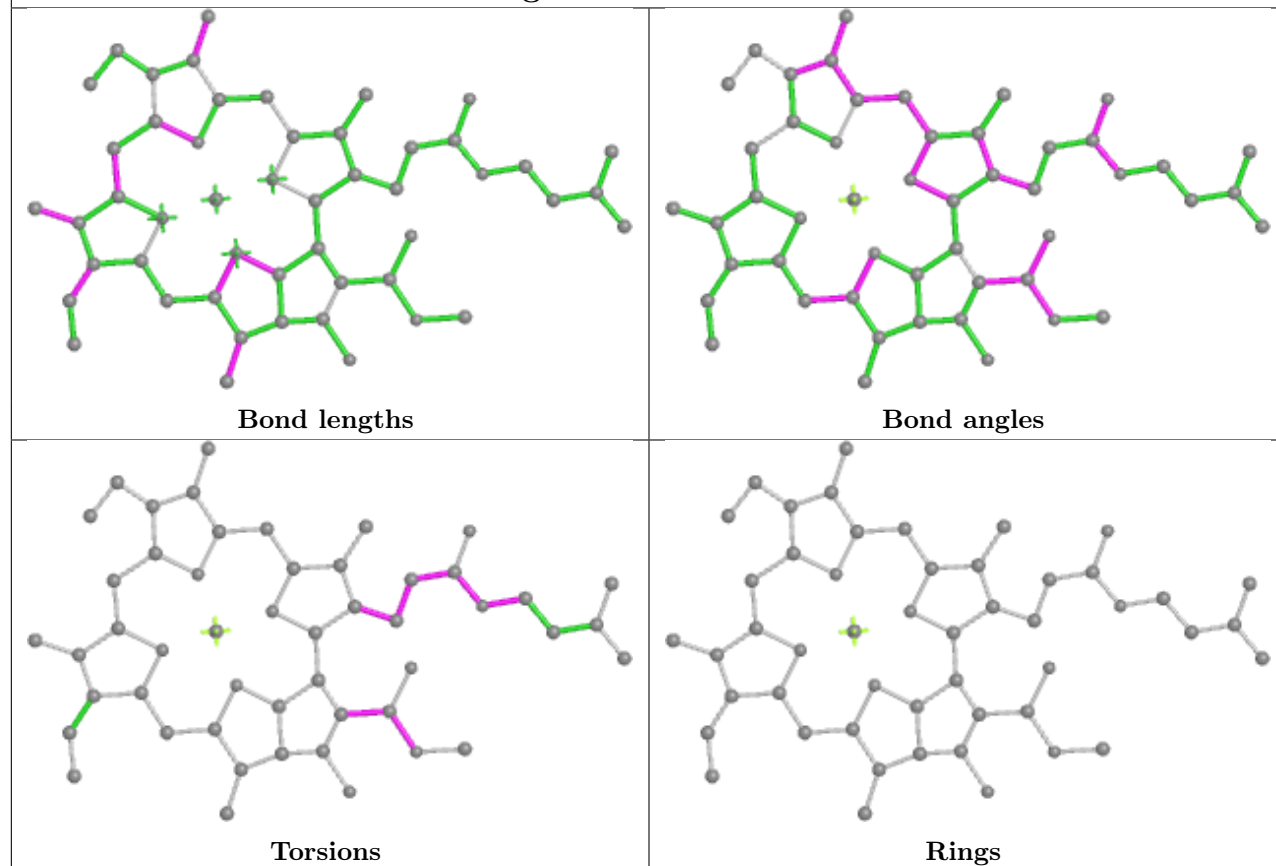
Ligand CLA Y 513



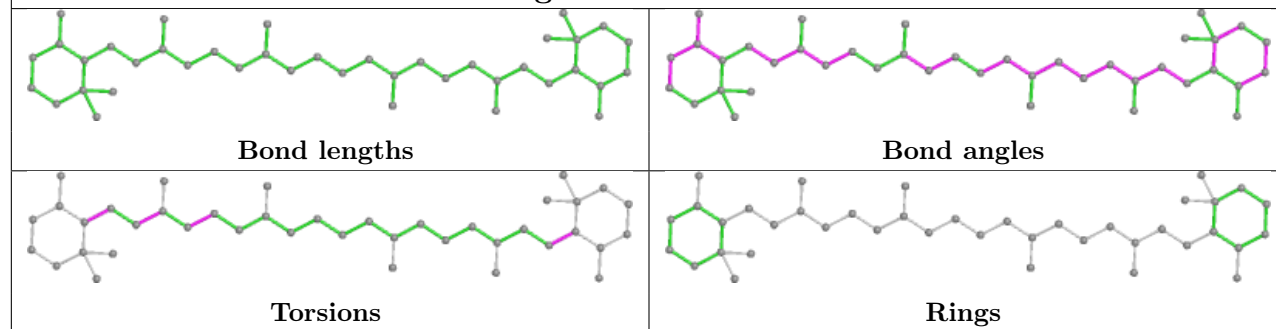
Ligand CLA 3 510

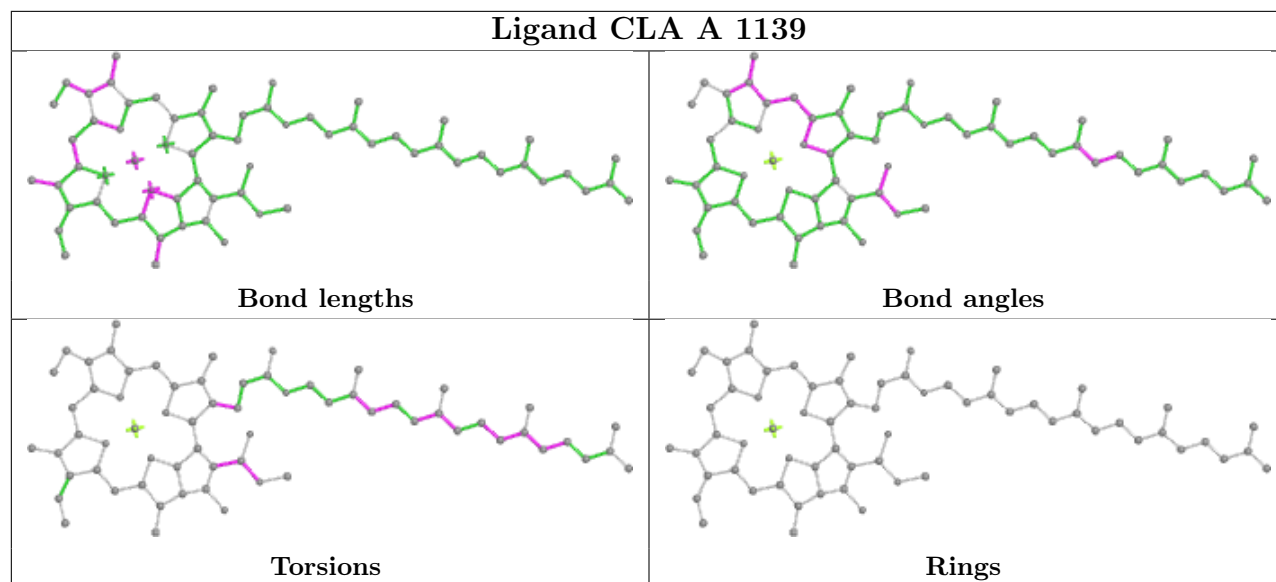
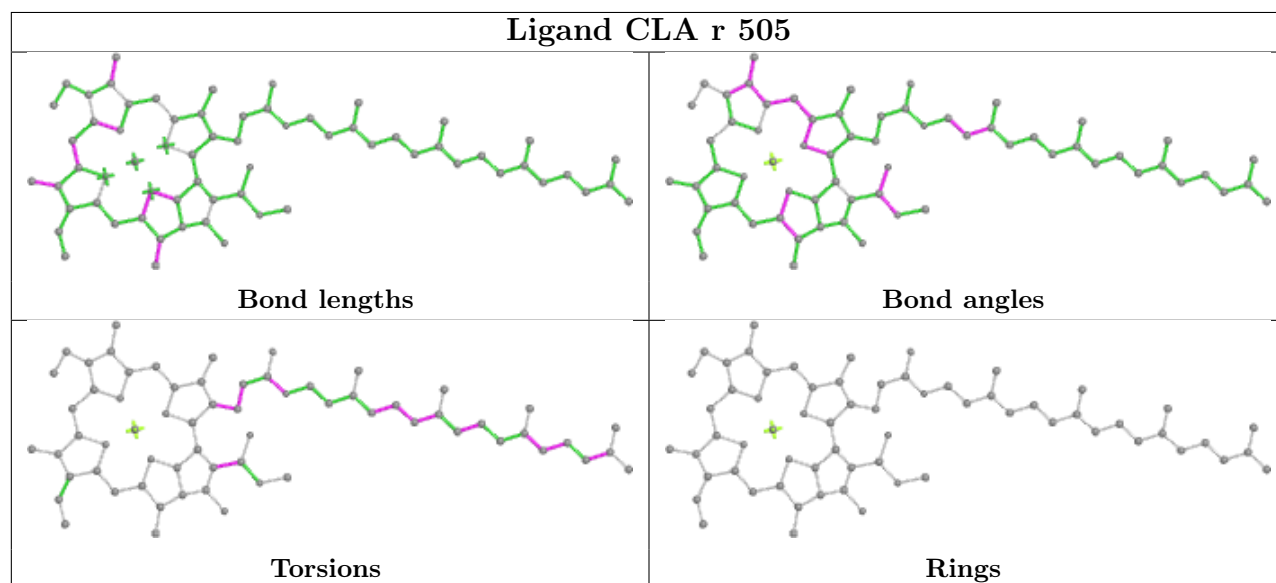


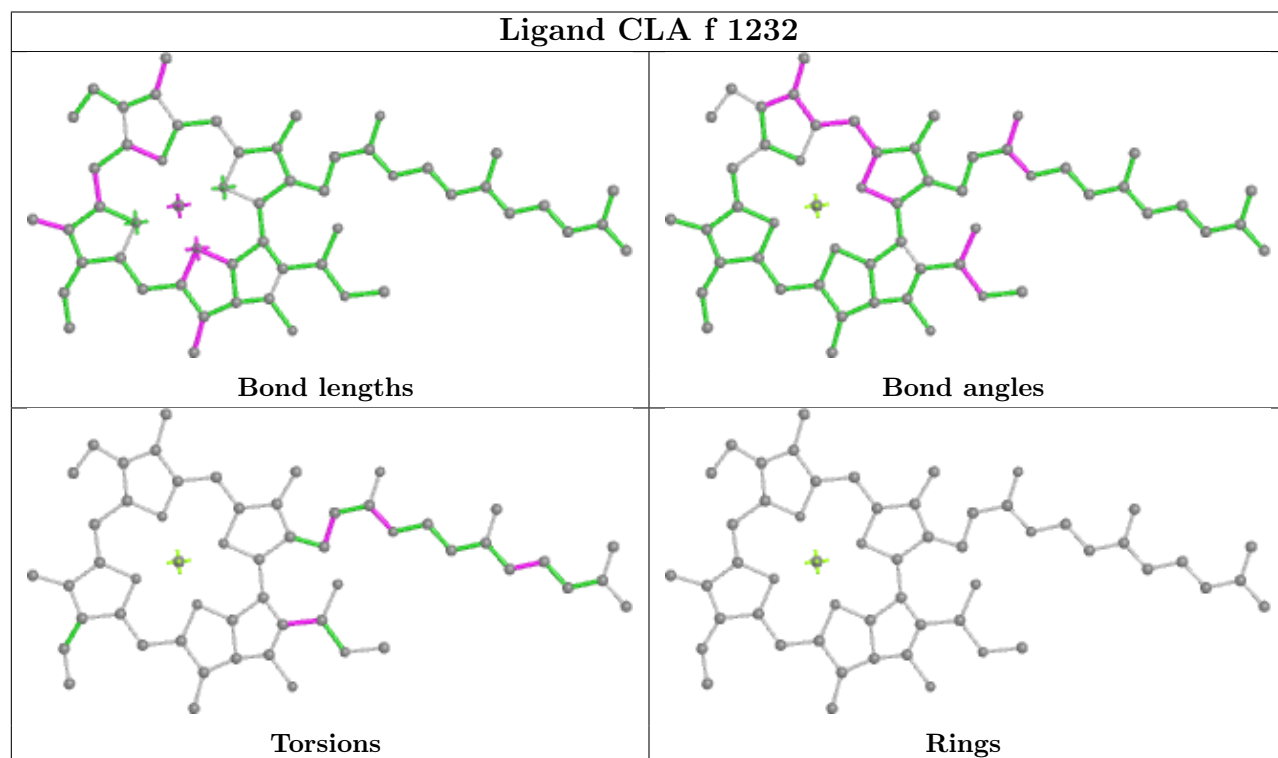
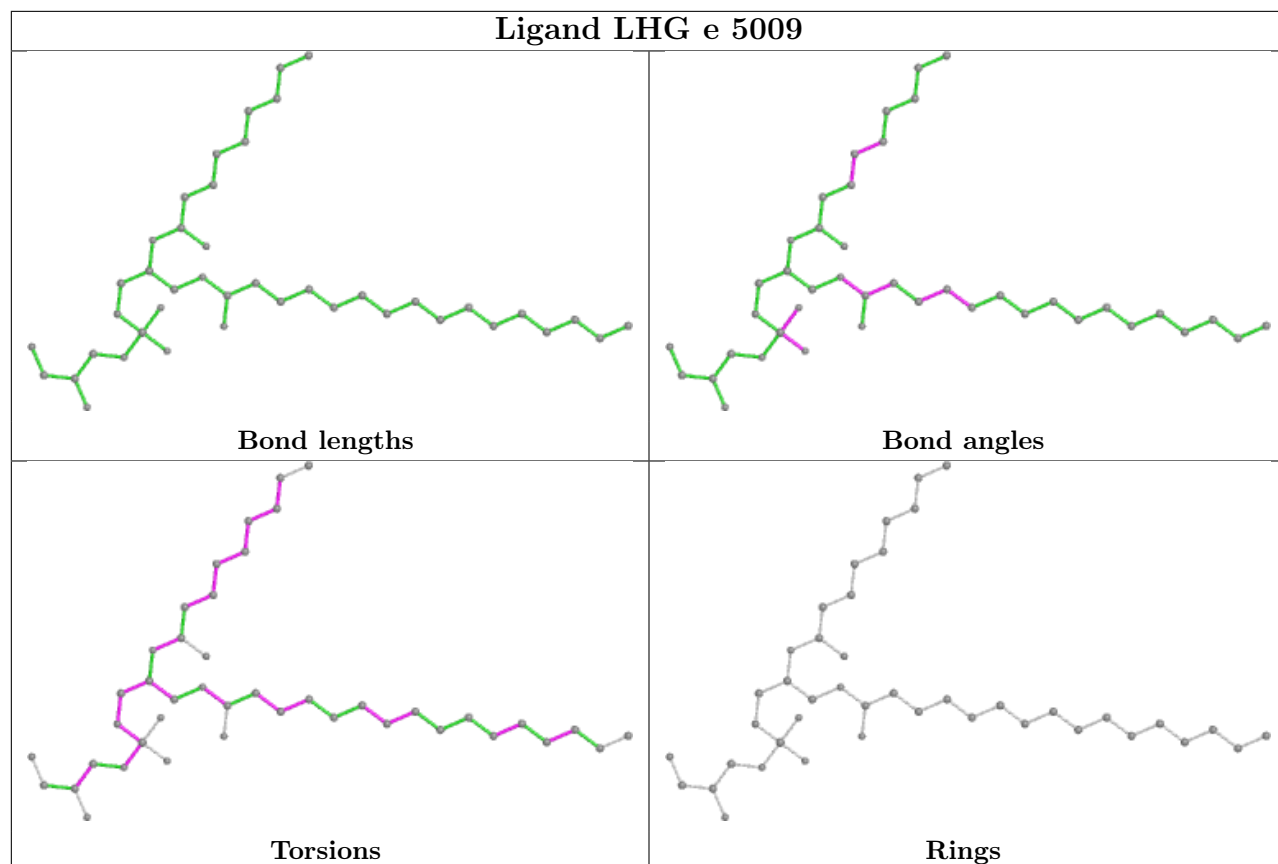
Ligand CLA A 1120



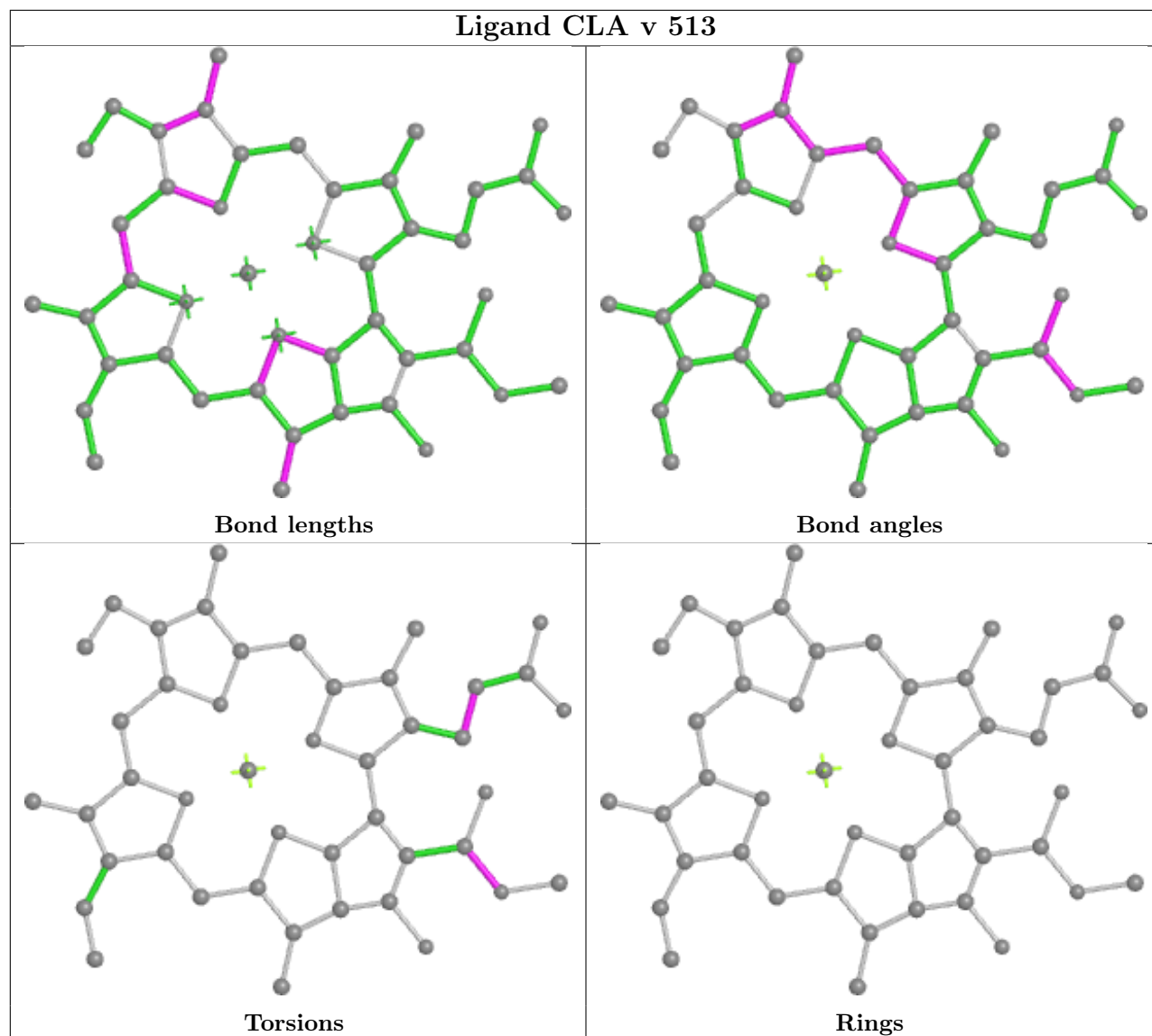
Ligand BCR a 521

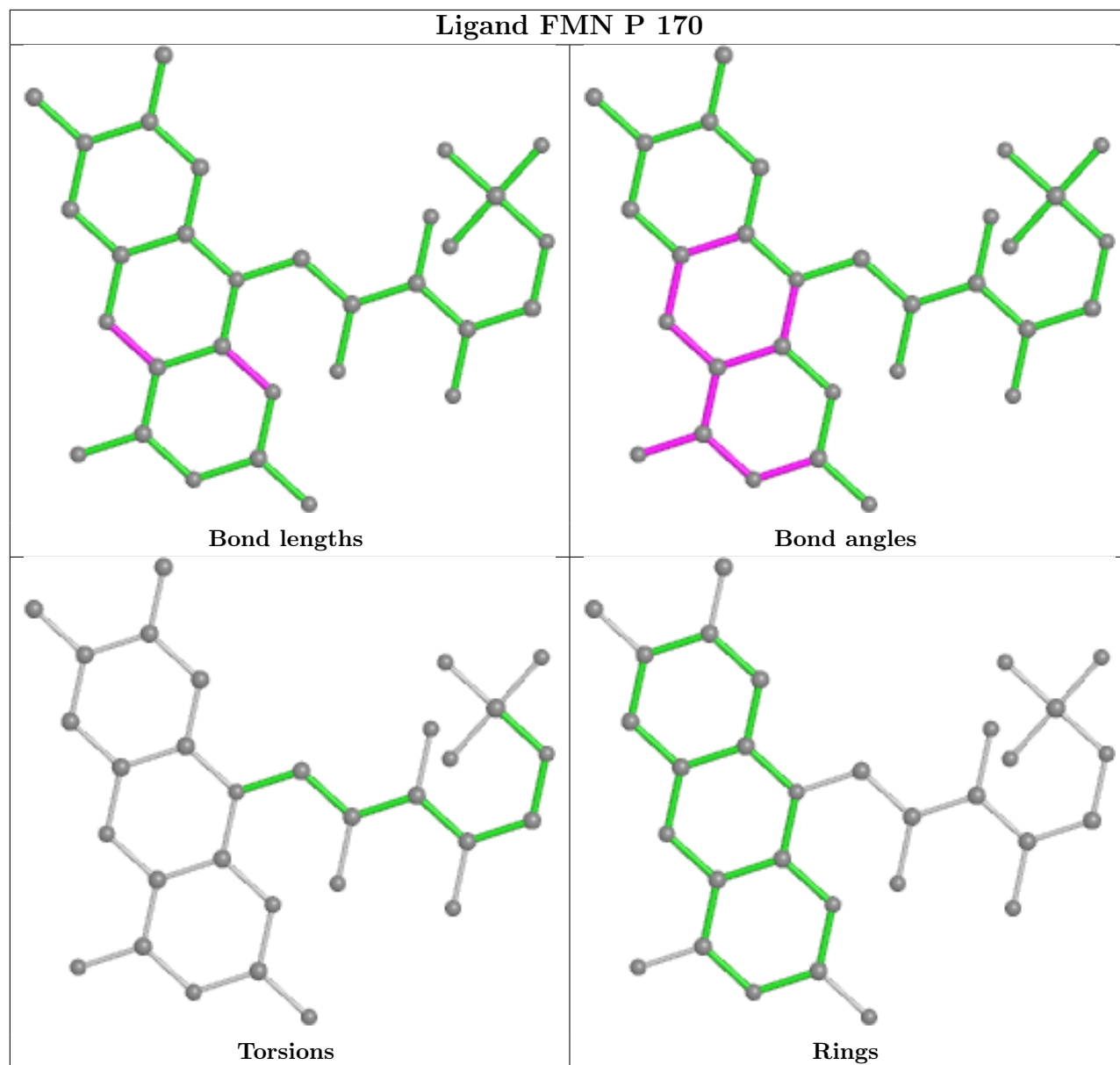


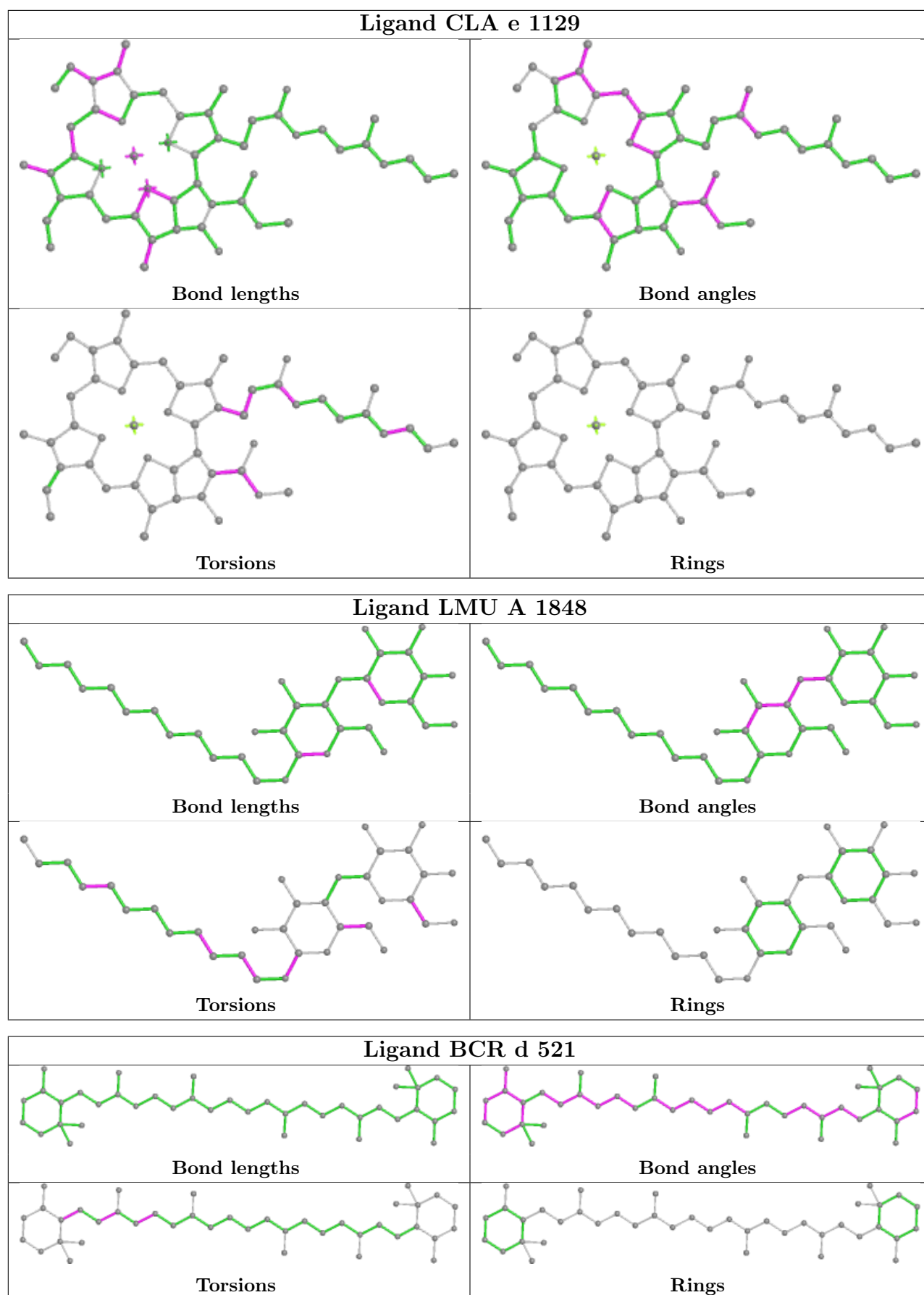
Ligand CLA A 1139**Ligand CLA r 505**



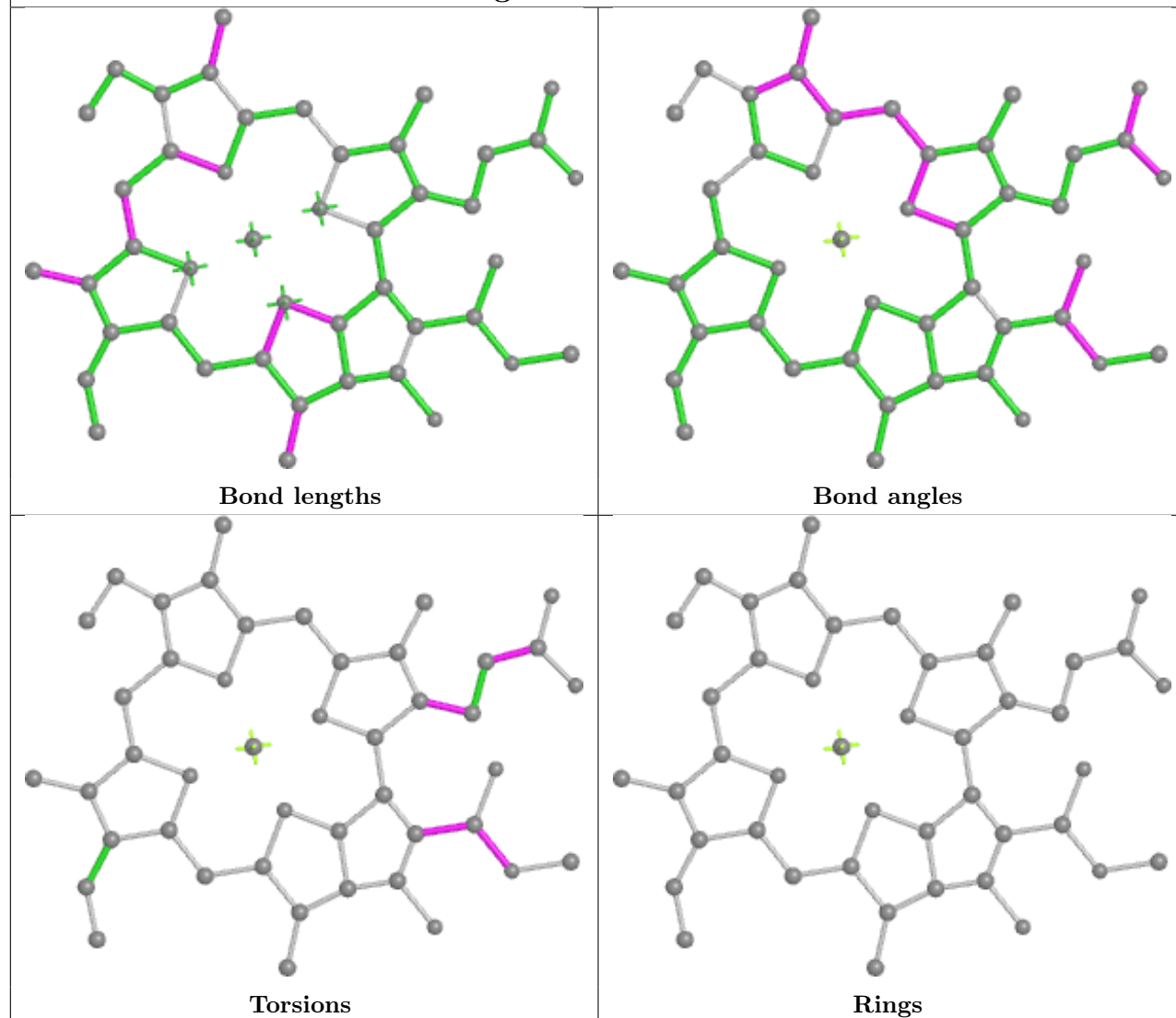
Ligand CLA v 513



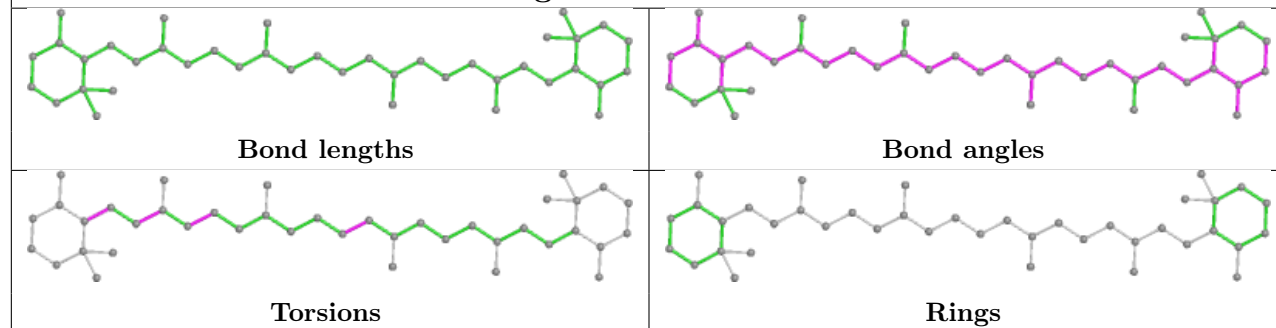




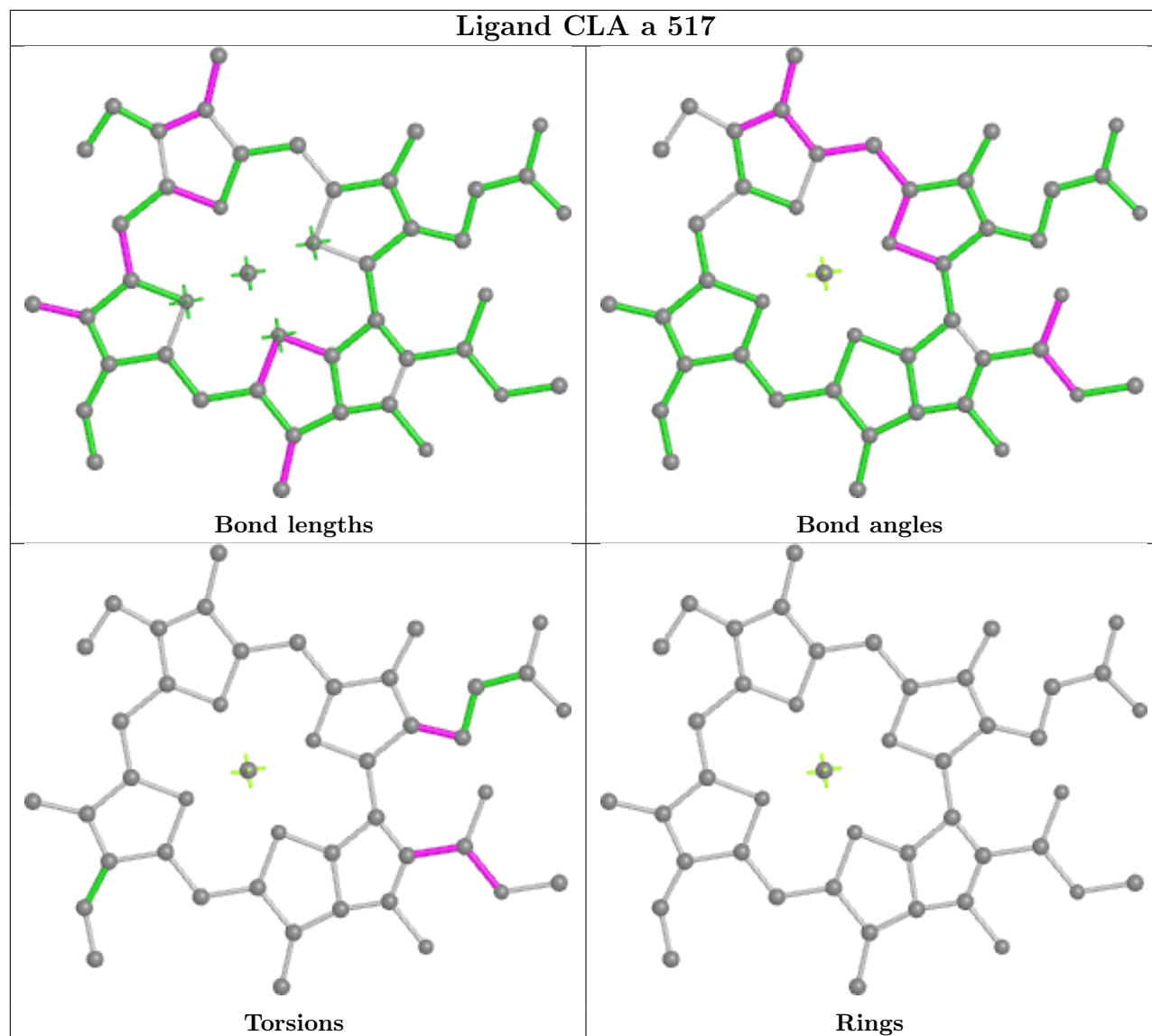
Ligand CLA 6 517

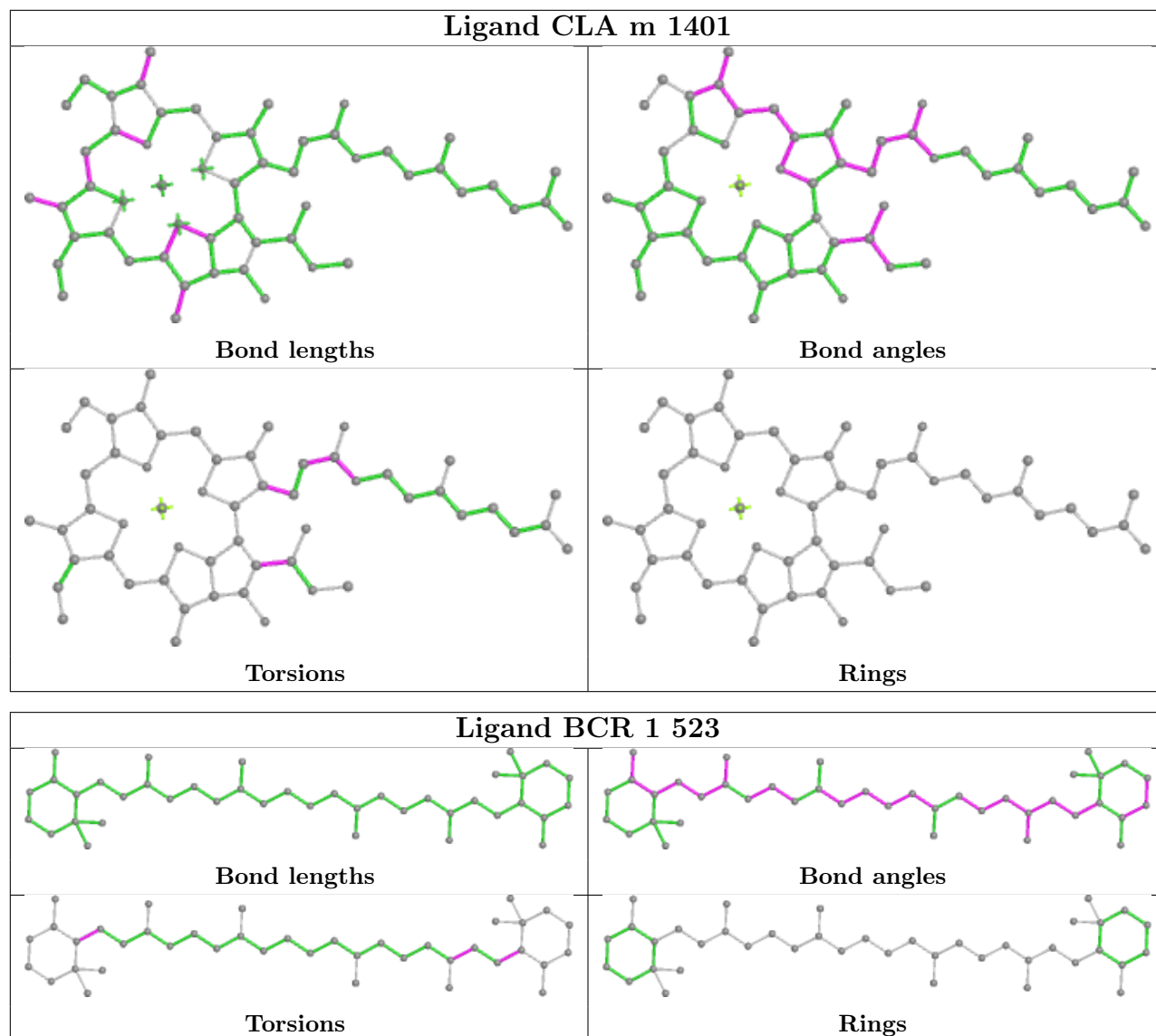


Ligand BCR 1 522

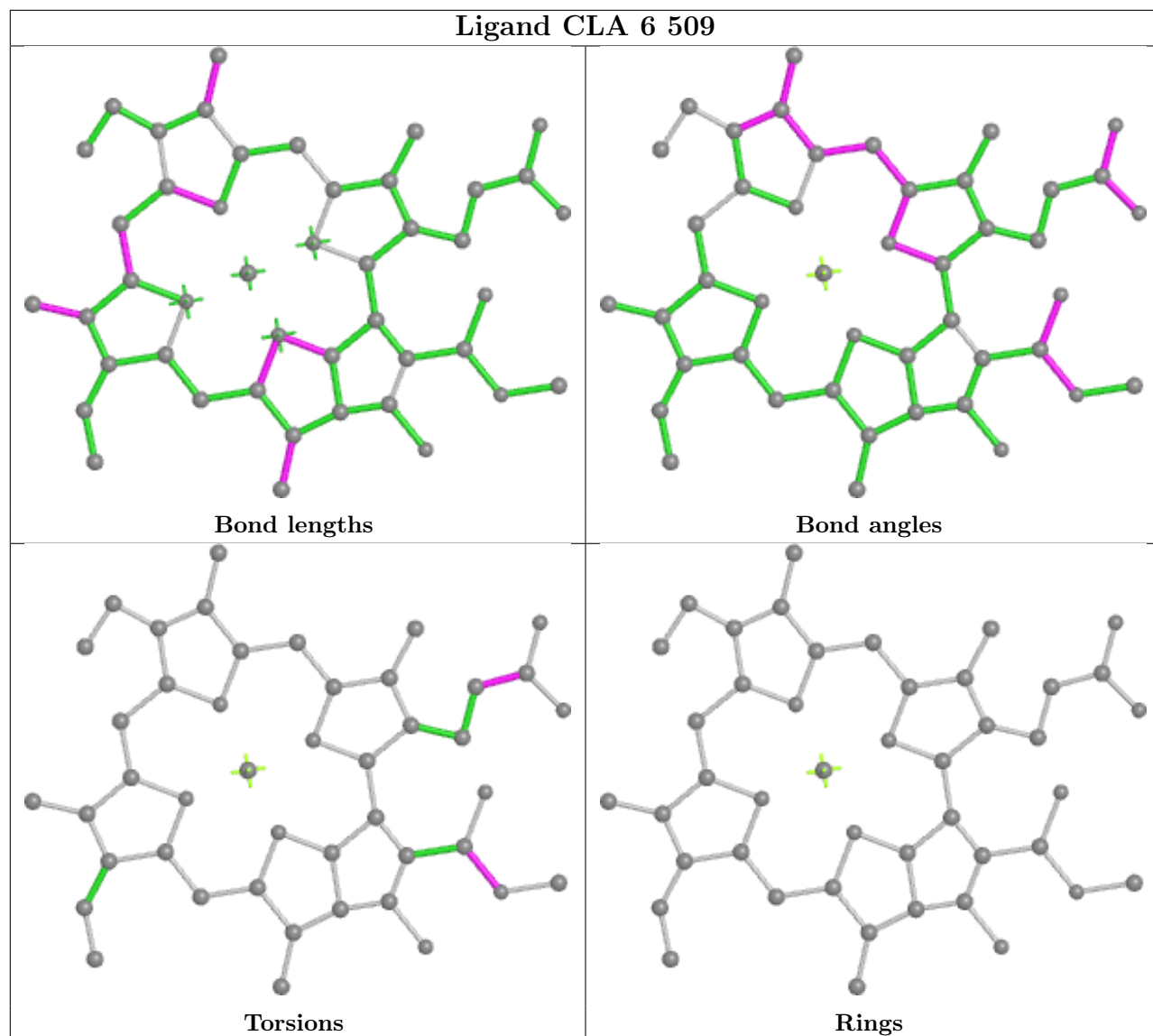


Ligand CLA a 517

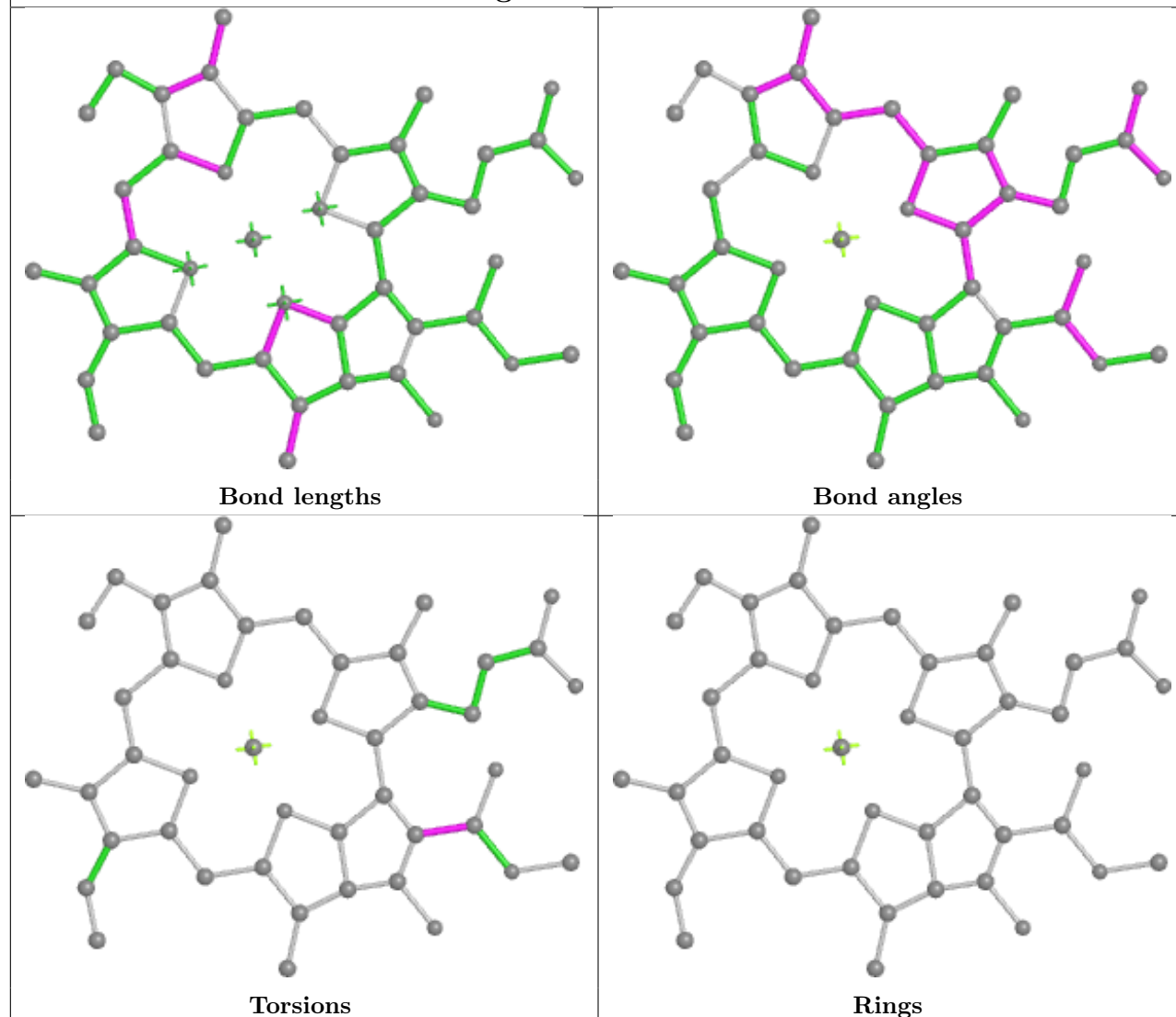




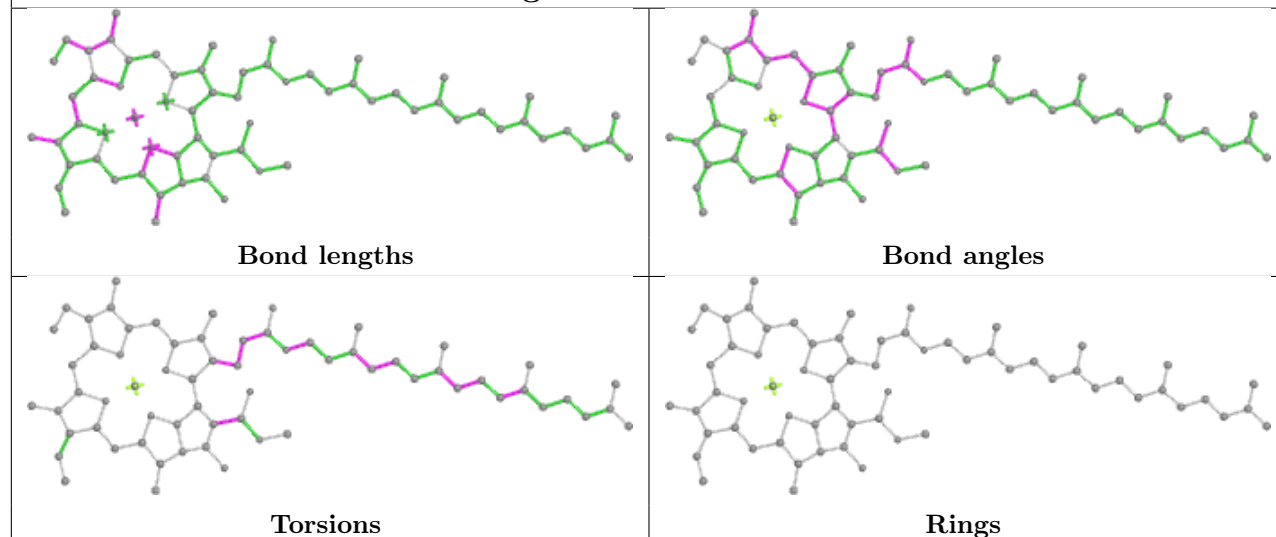
Ligand CLA 6 509

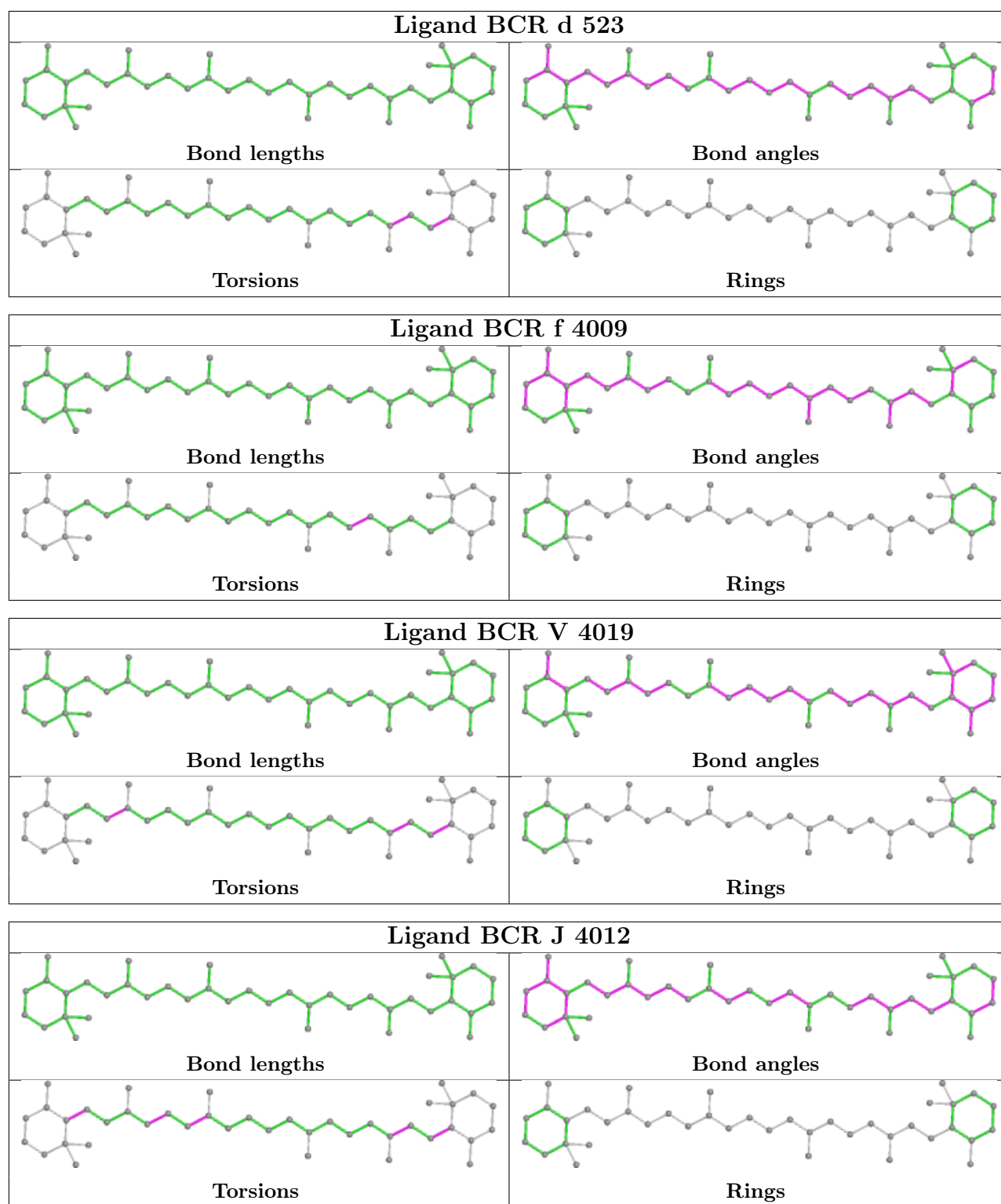


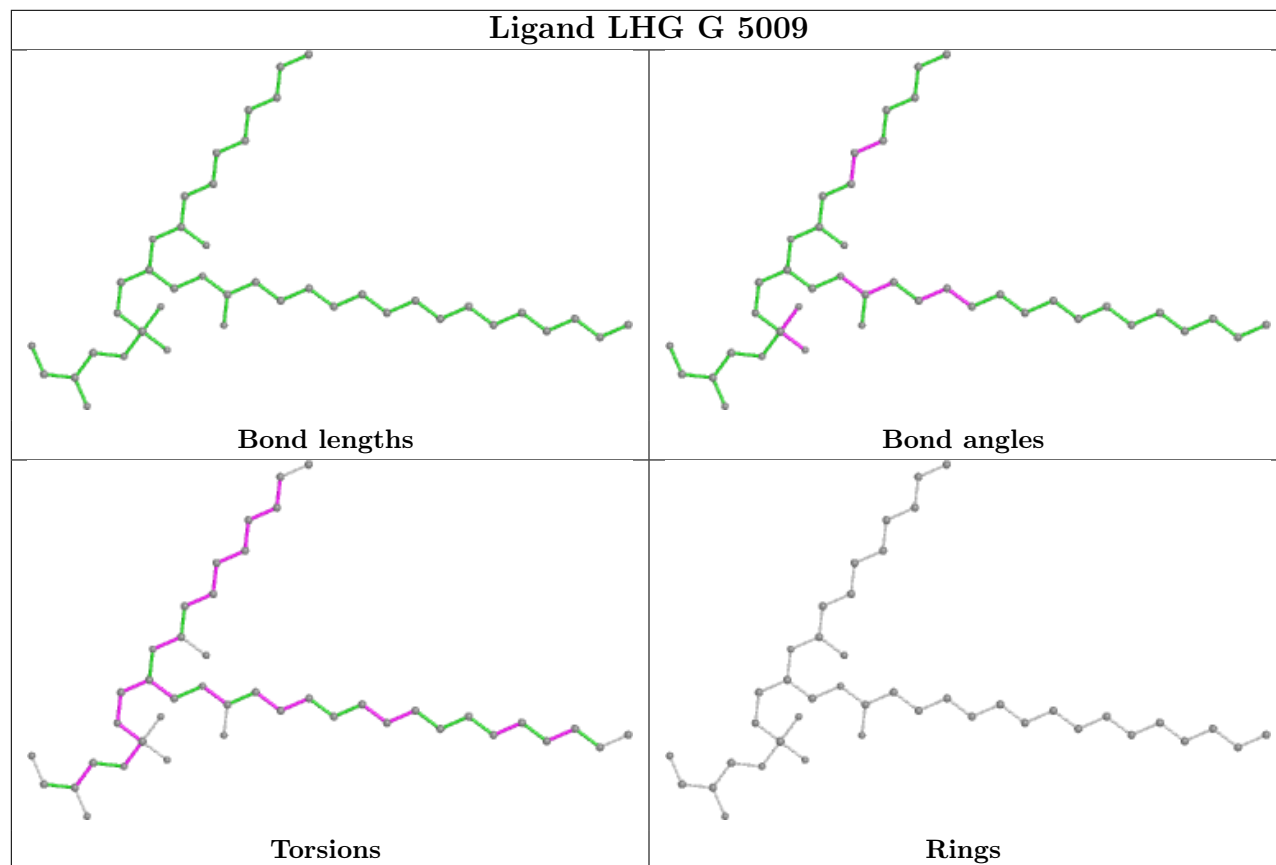
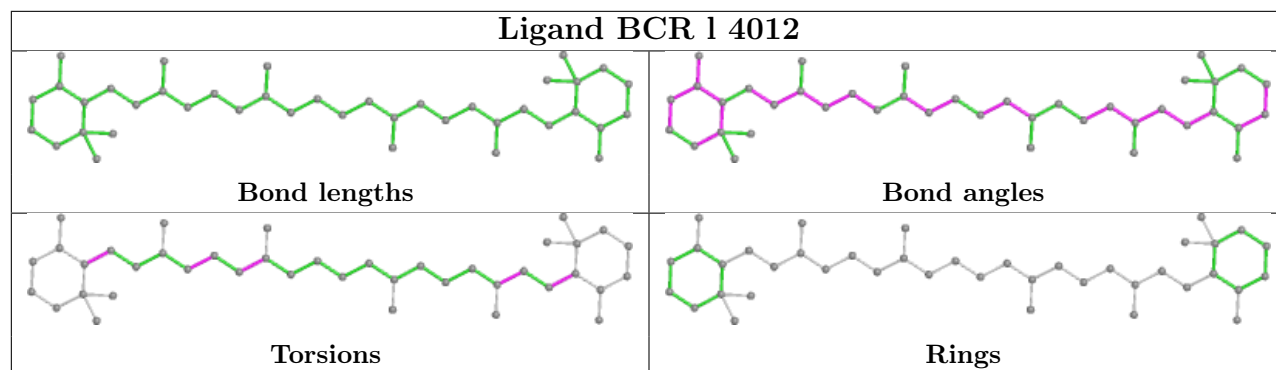
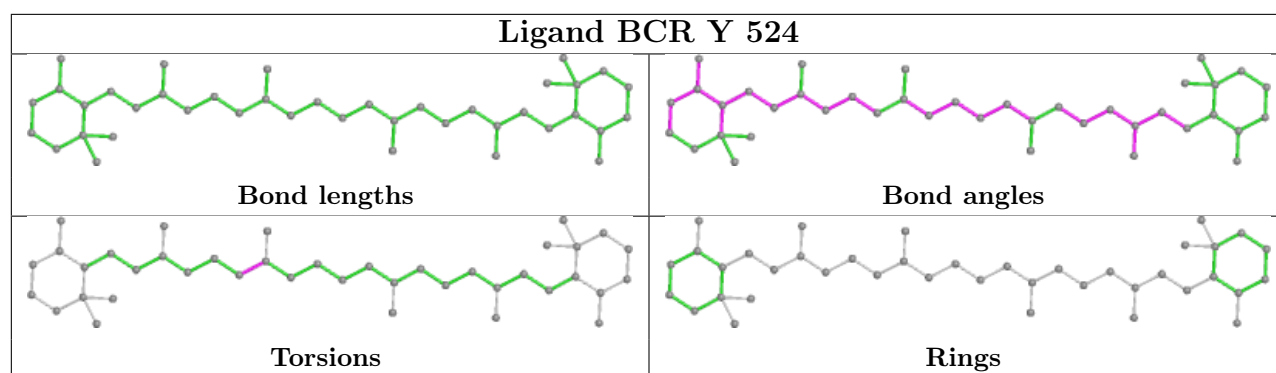
Ligand CLA r 502



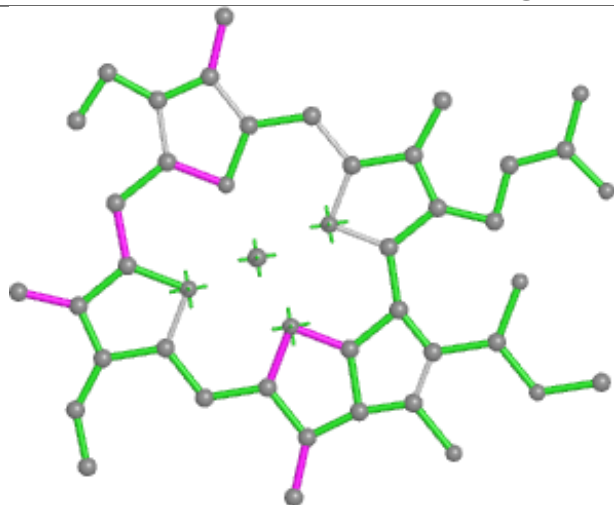
Ligand CLA A 1107



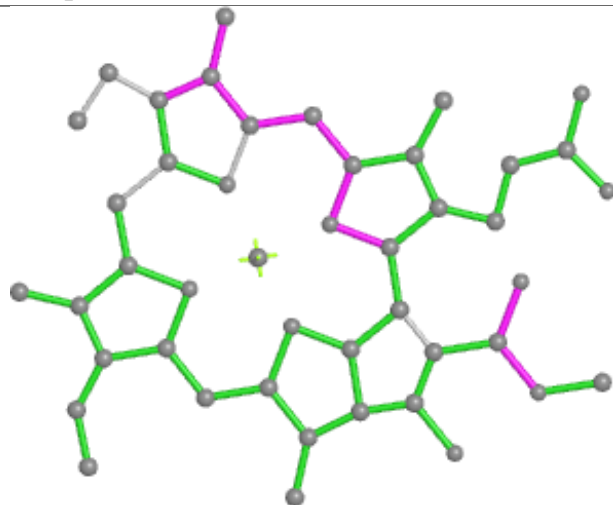




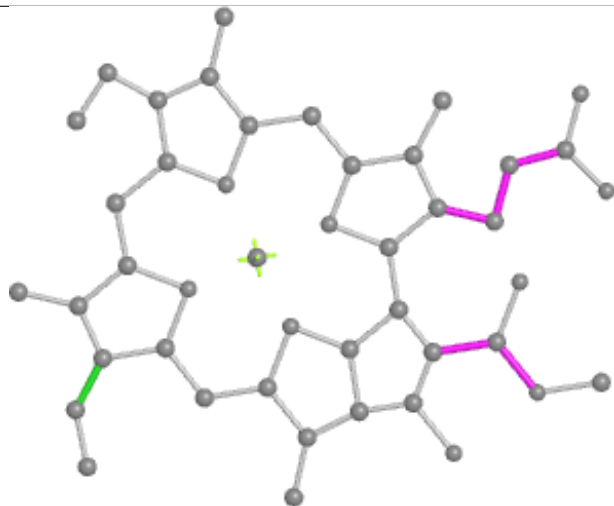
Ligand CLA q 501



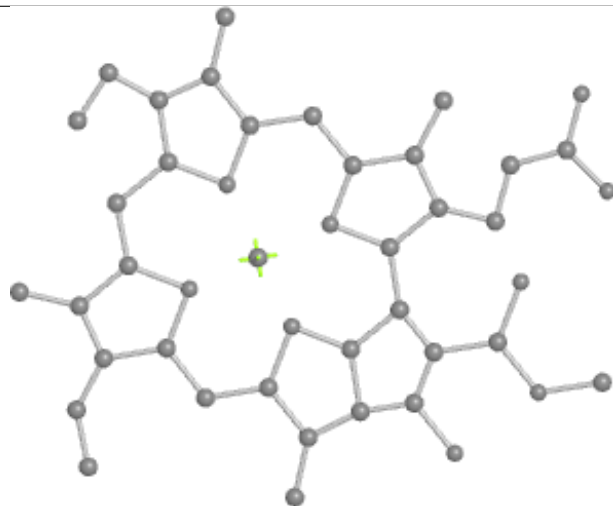
Bond lengths



Bond angles

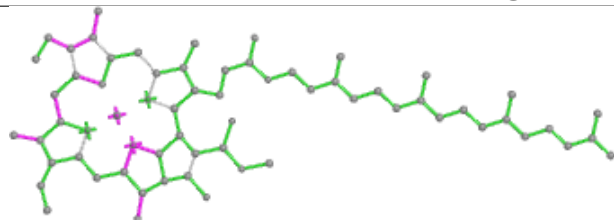


Torsions

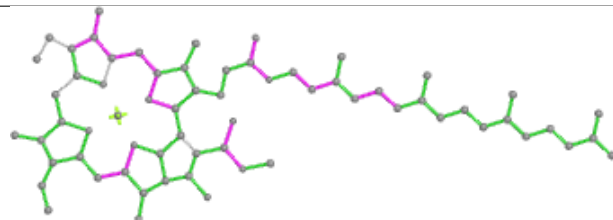


Rings

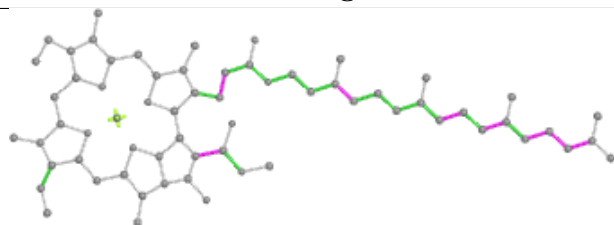
Ligand CLA A 1117



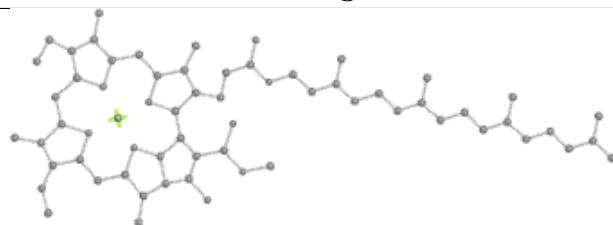
Bond lengths



Bond angles

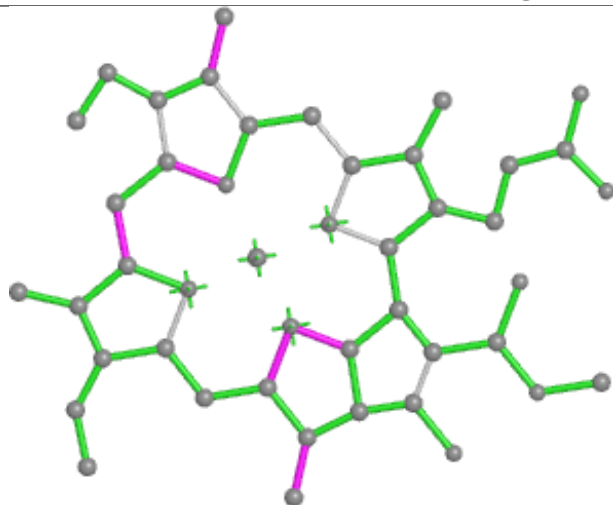


Torsions

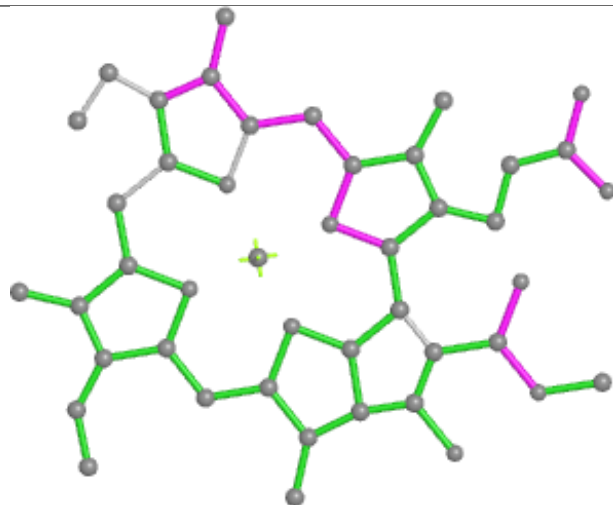


Rings

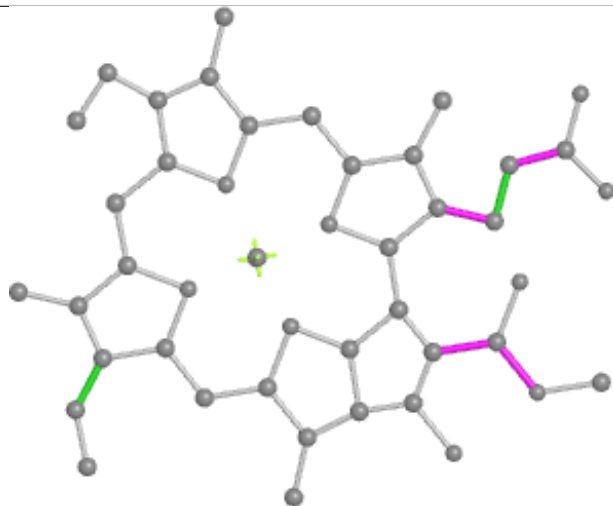
Ligand CLA d 517



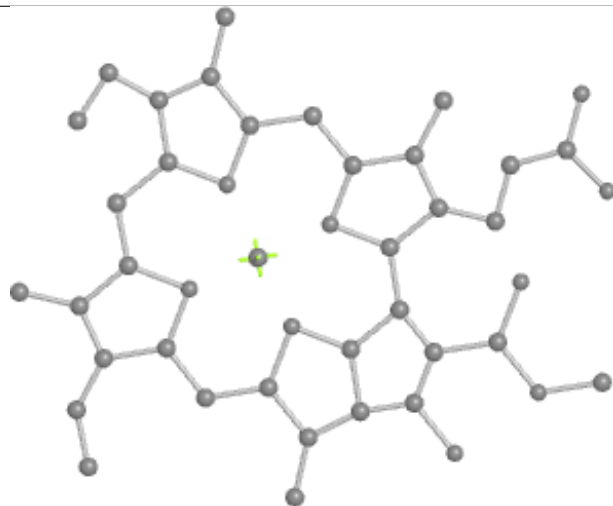
Bond lengths



Bond angles

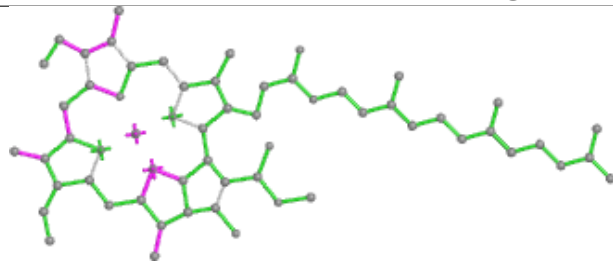


Torsions

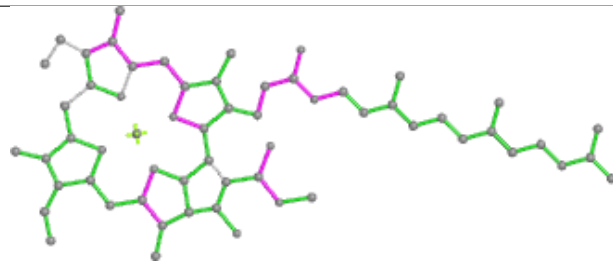


Rings

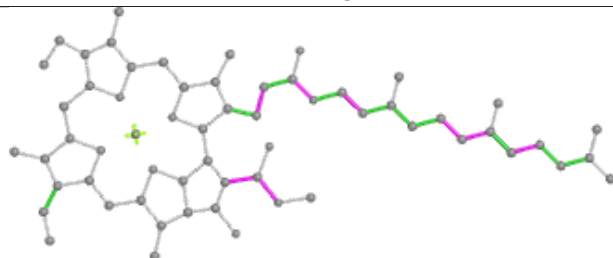
Ligand CLA H 1216



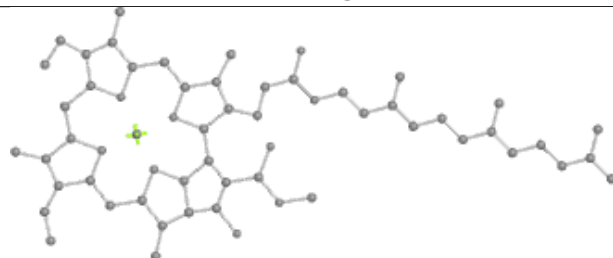
Bond lengths



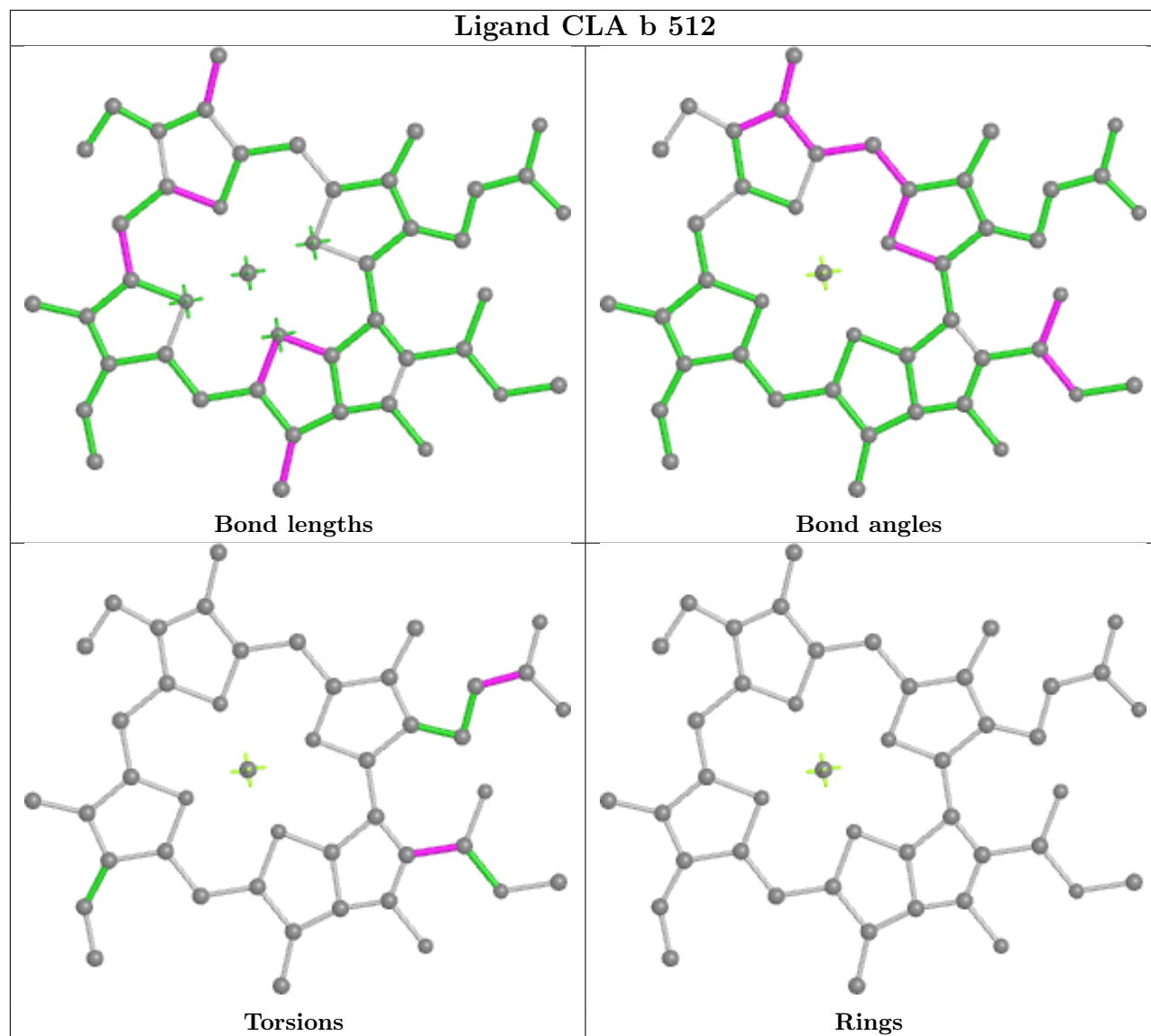
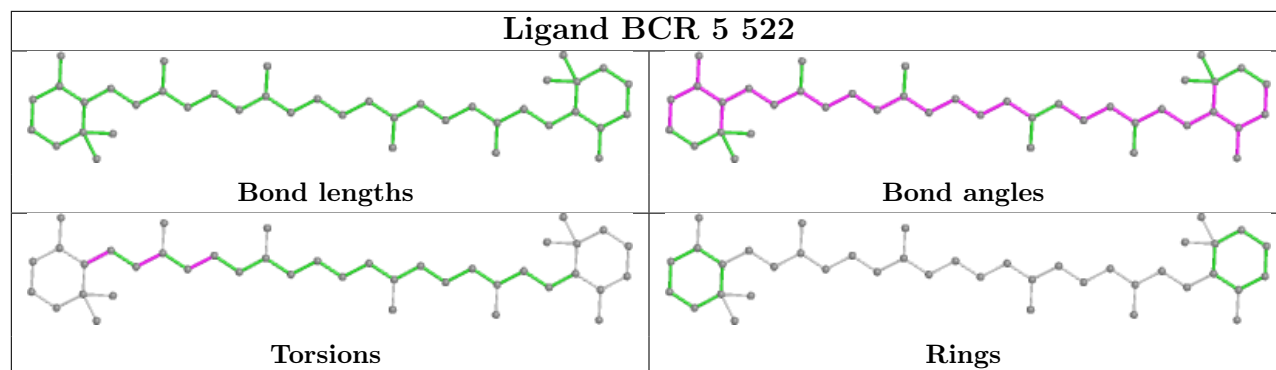
Bond angles



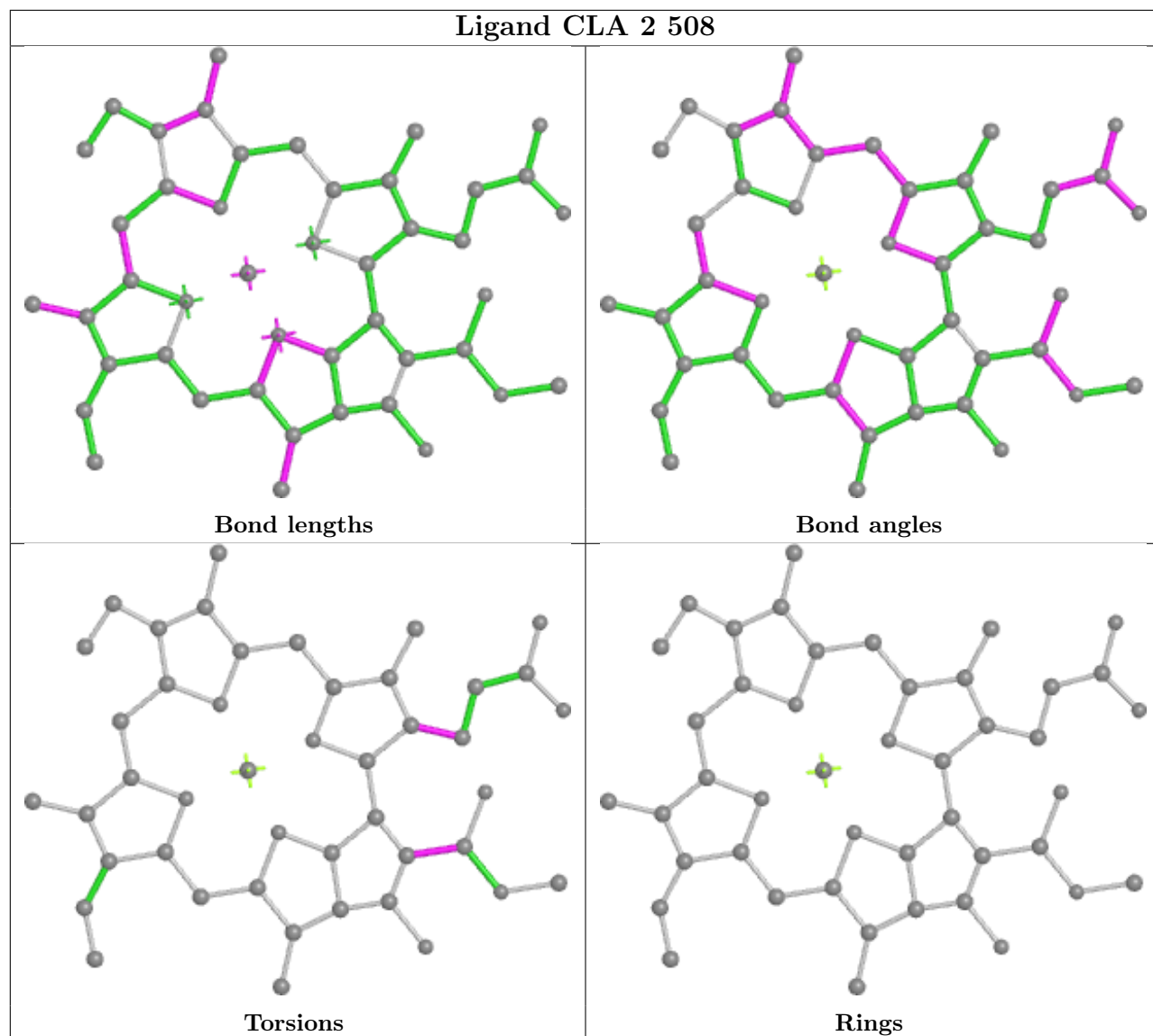
Torsions



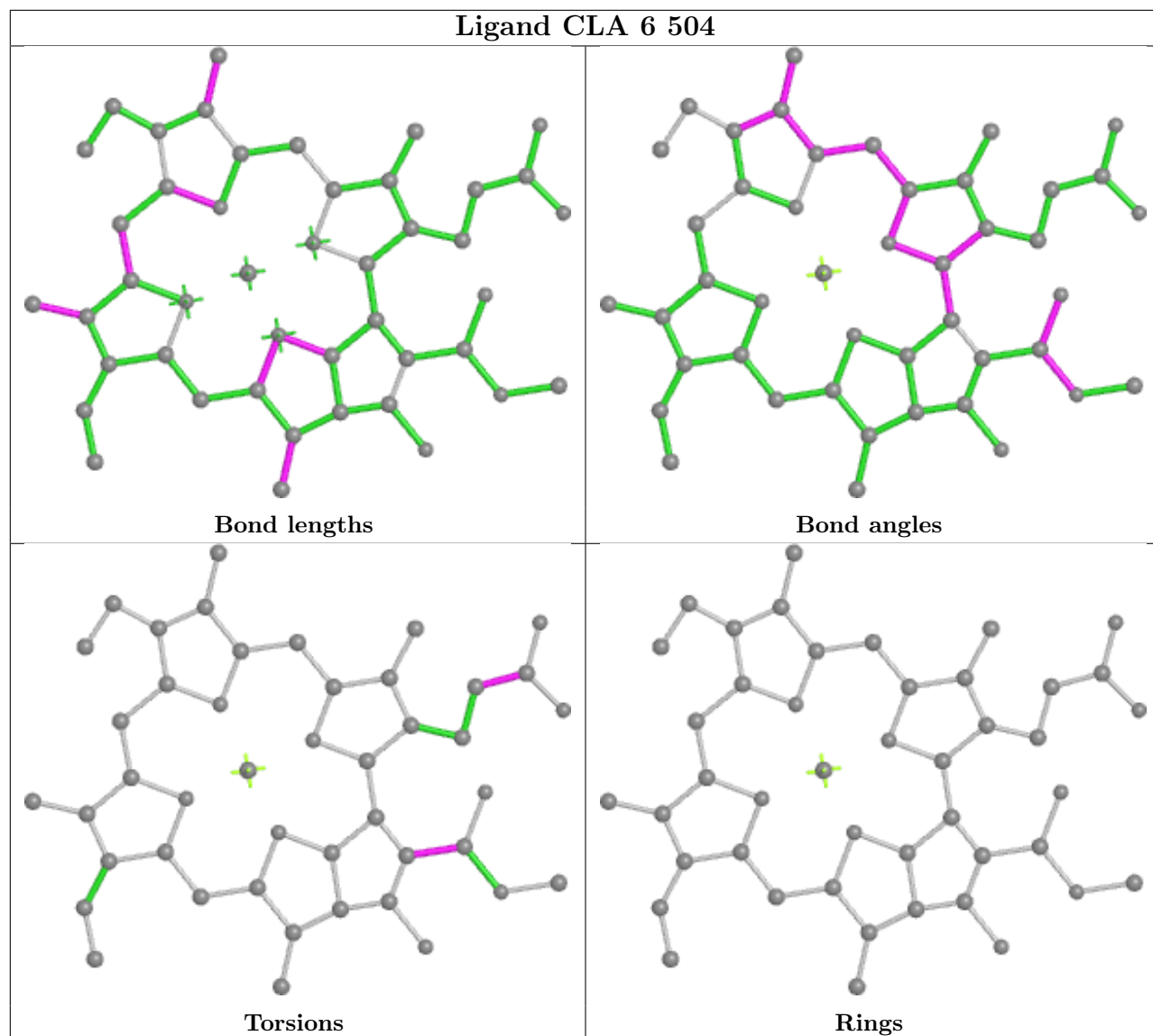
Rings



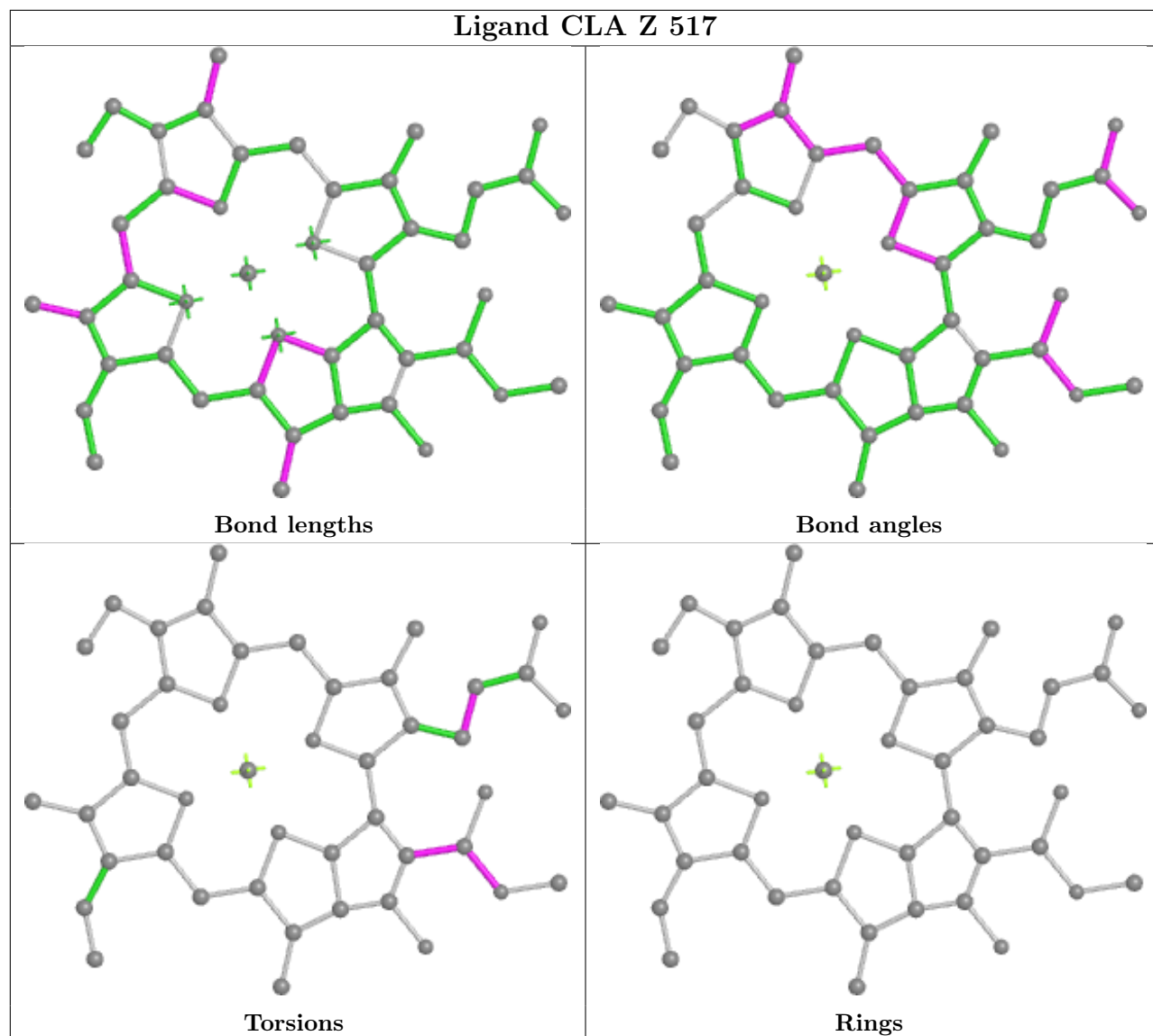
Ligand CLA 2 508

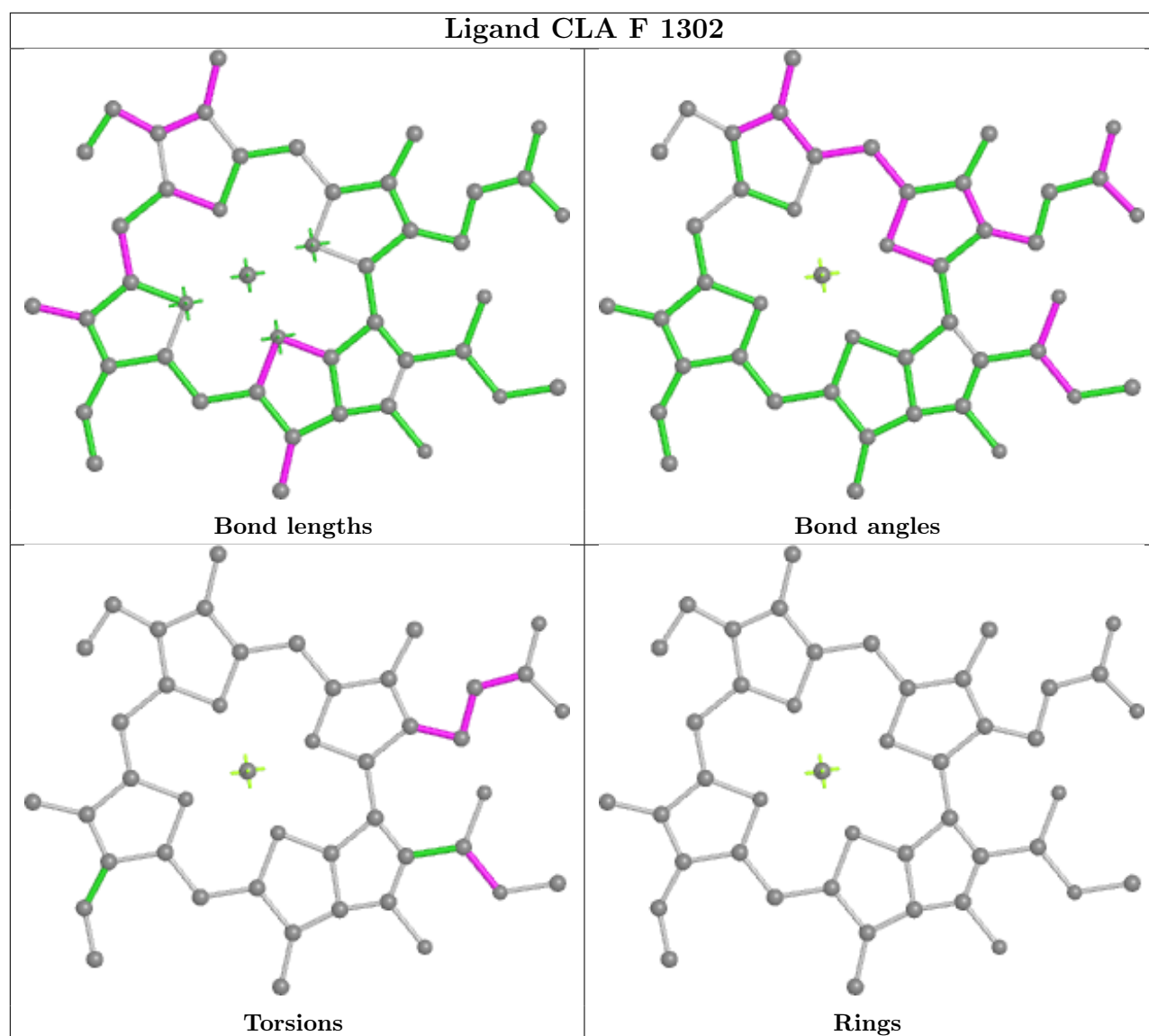


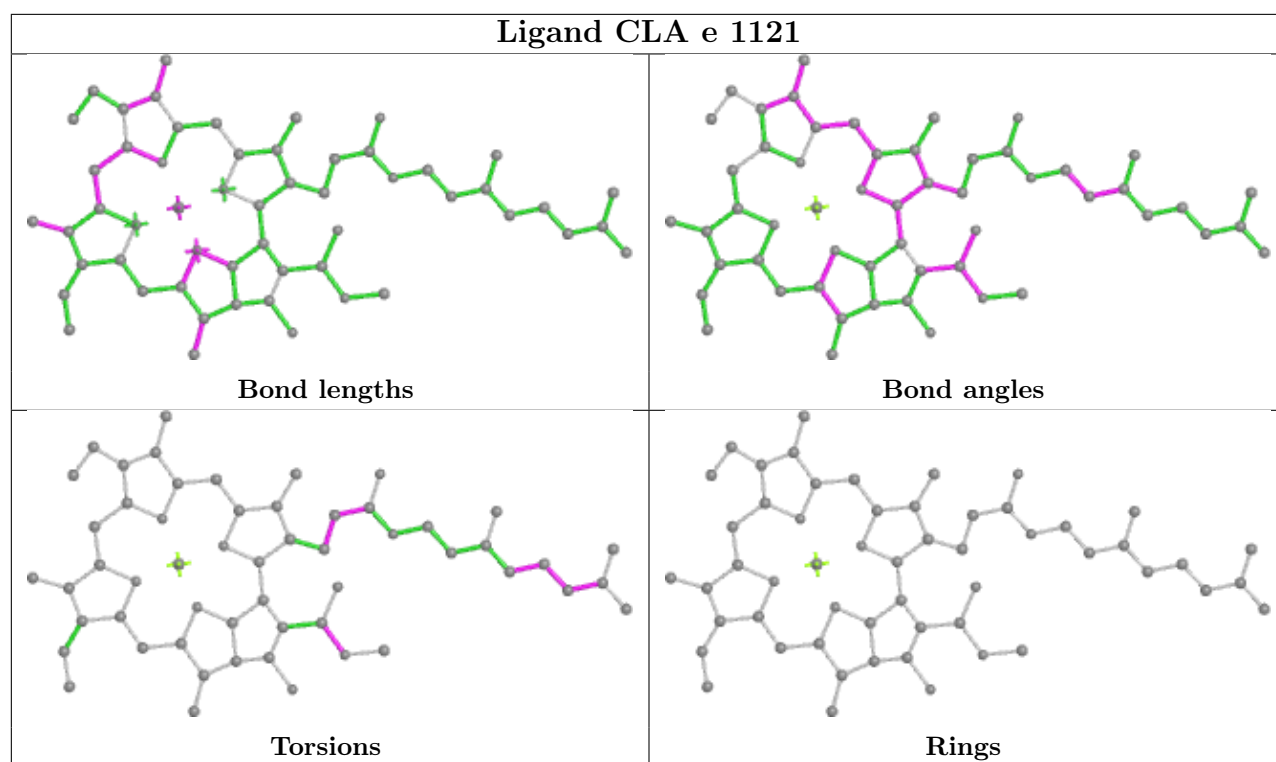
Ligand CLA 6 504



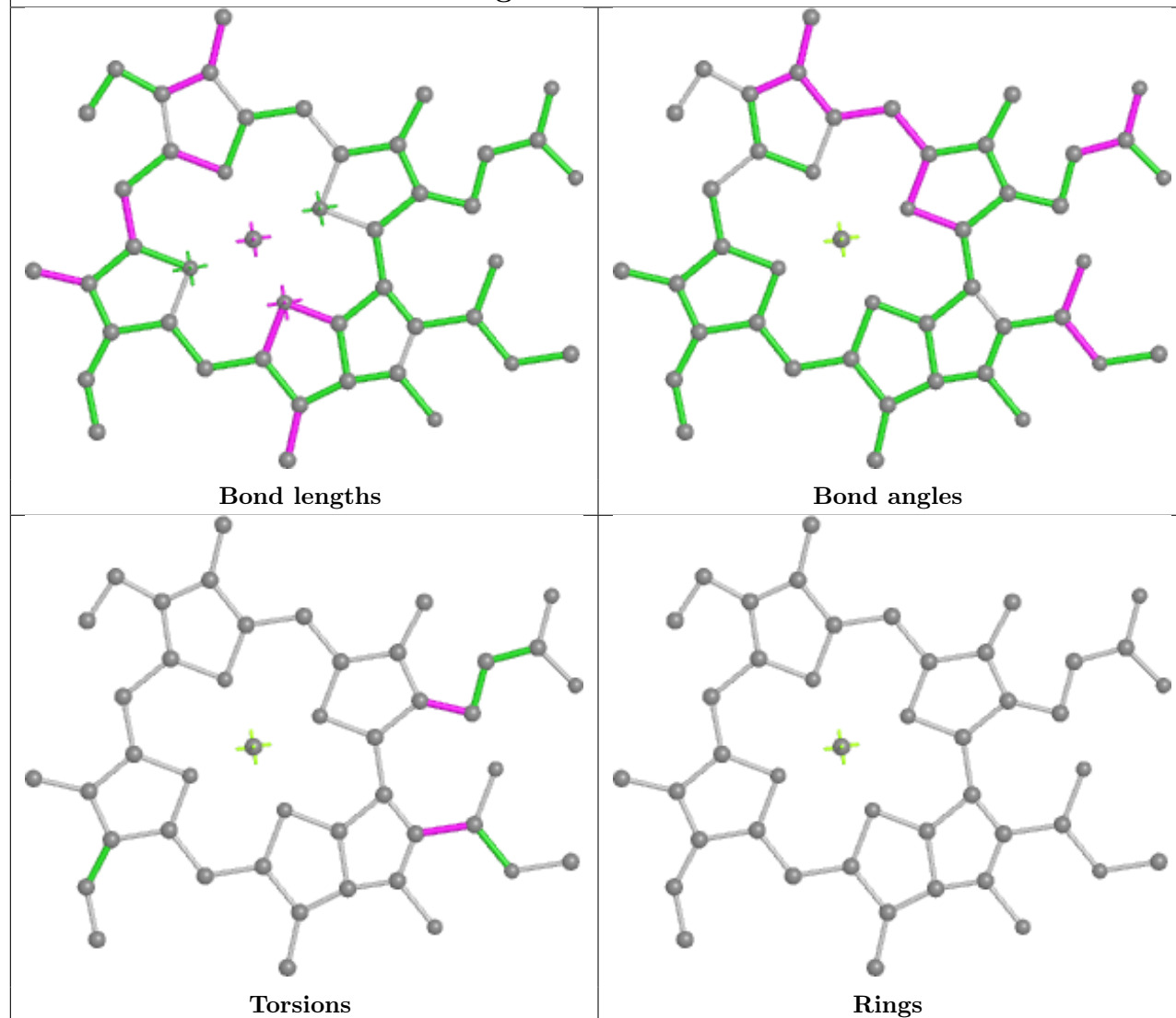
Ligand CLA Z 517



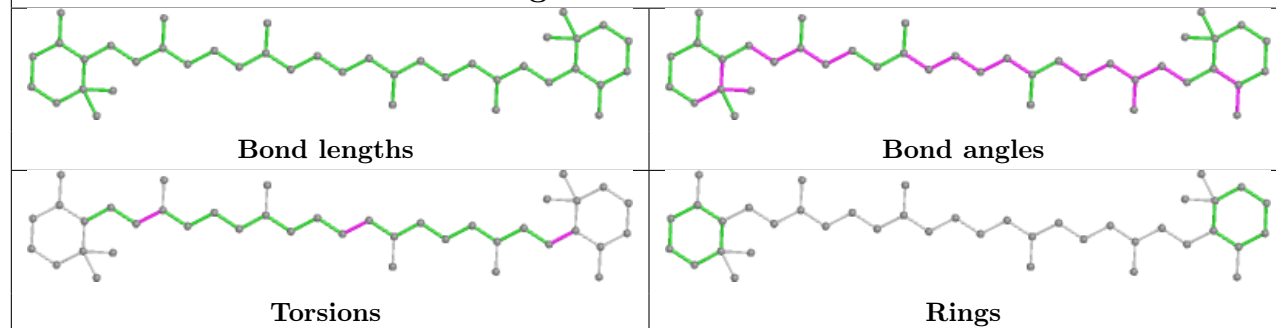




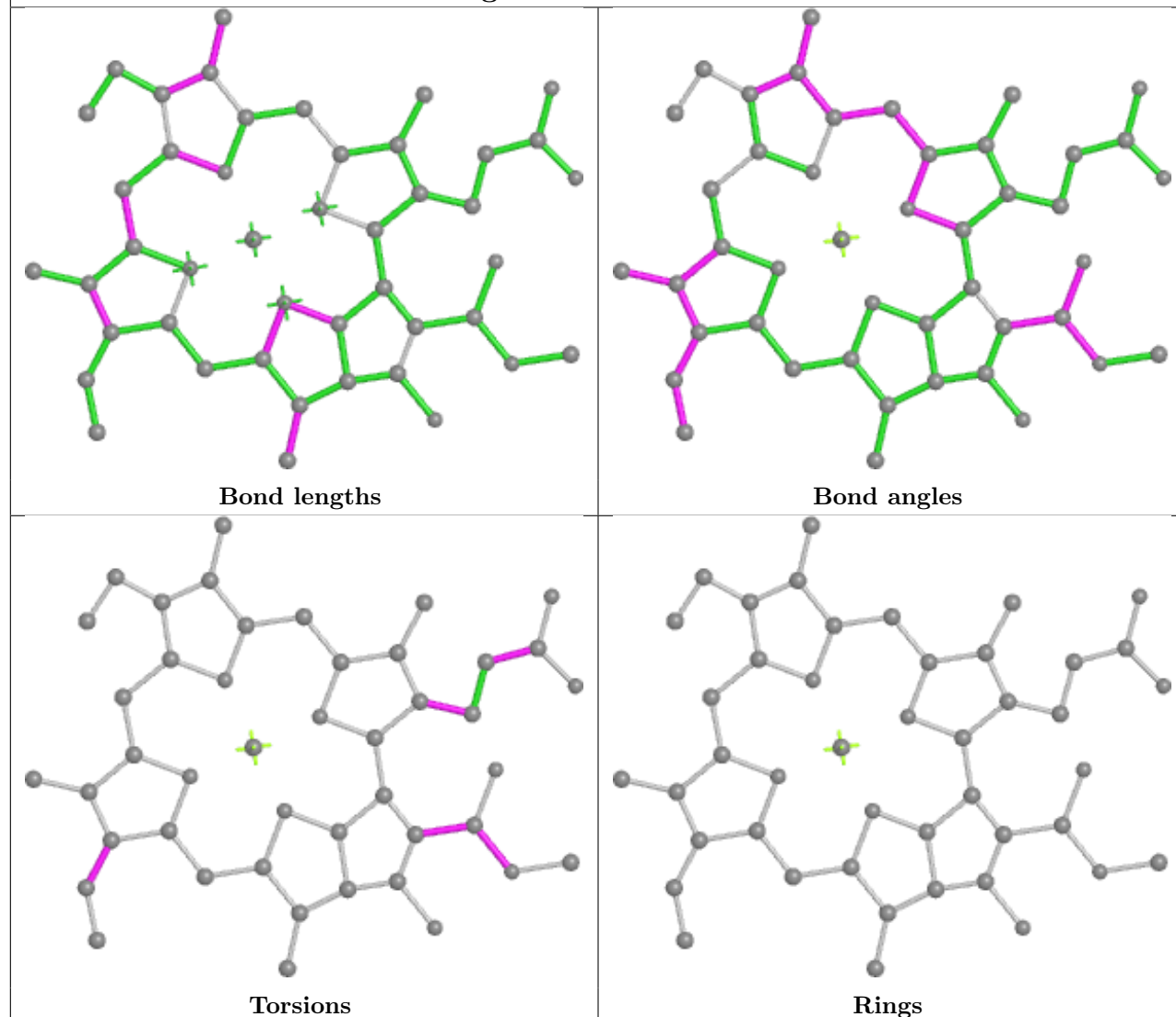
Ligand CLA s 508



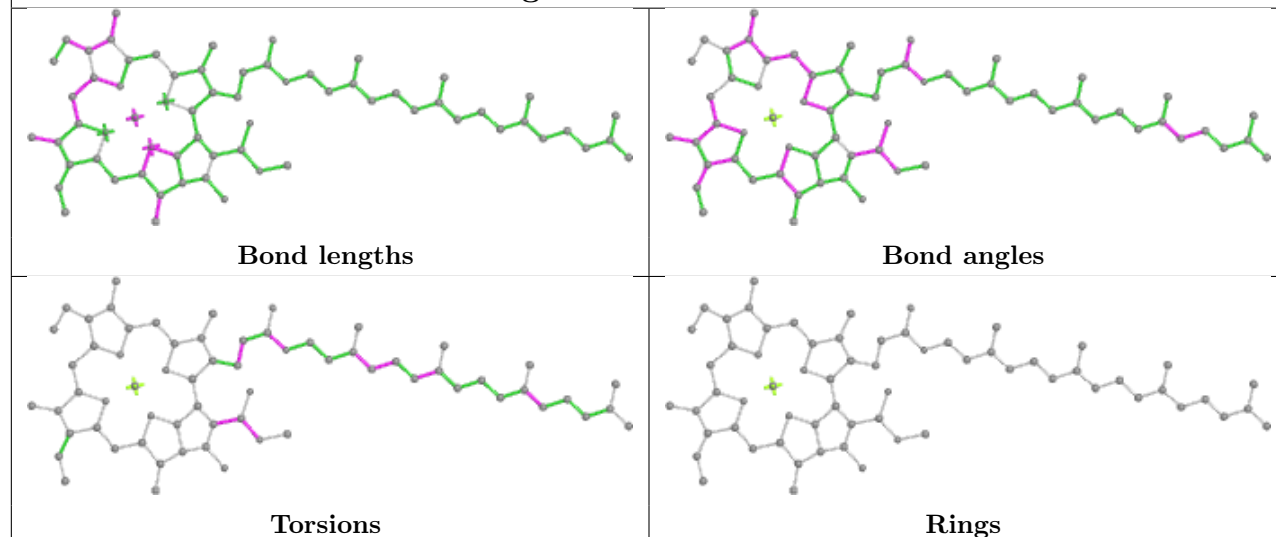
Ligand BCR 1 4015



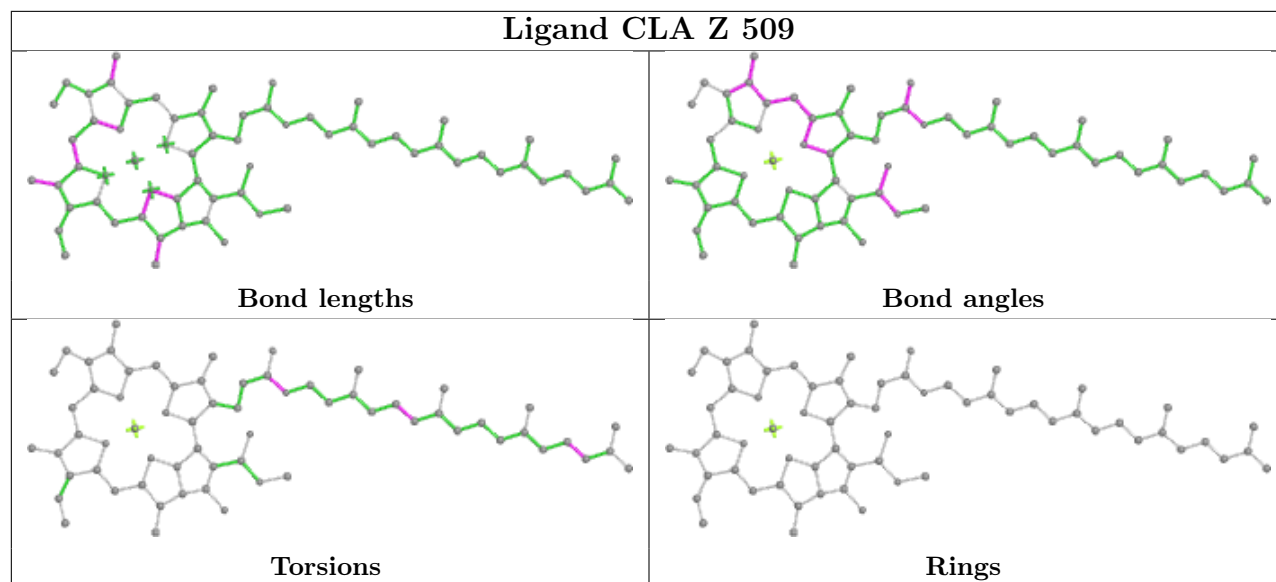
Ligand CLA U 1105



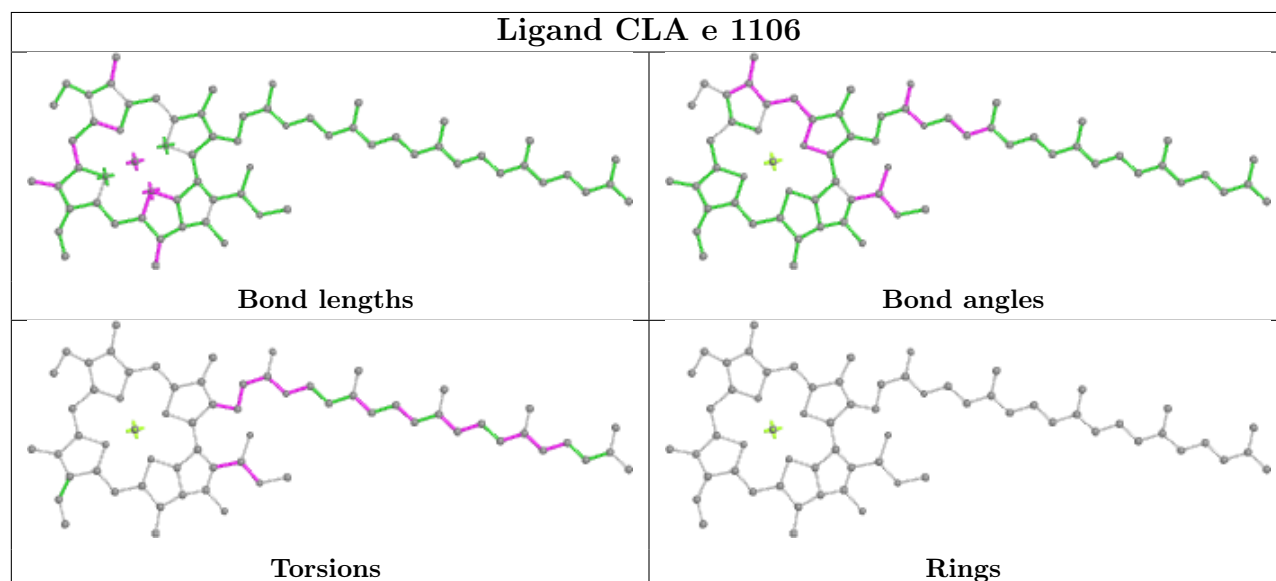
Ligand CLA G 1119



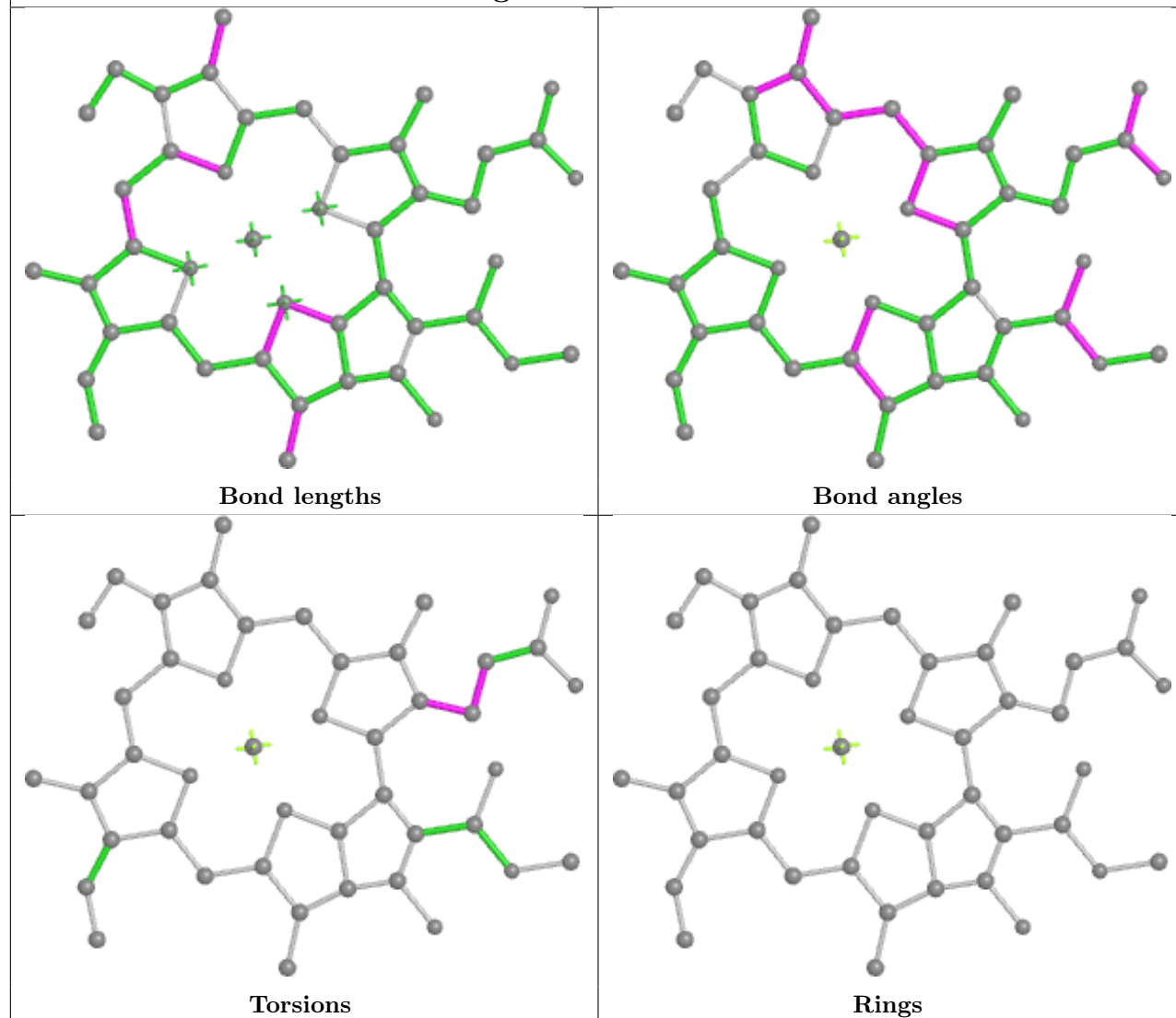
Ligand CLA Z 509



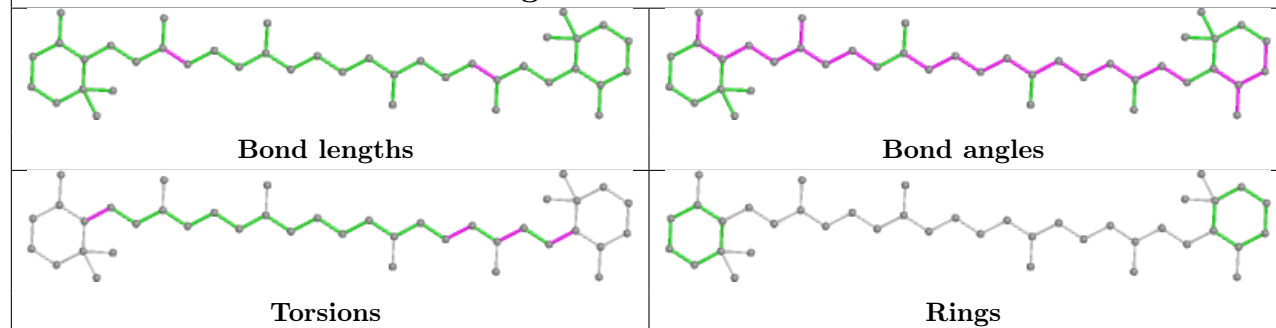
Ligand CLA e 1106

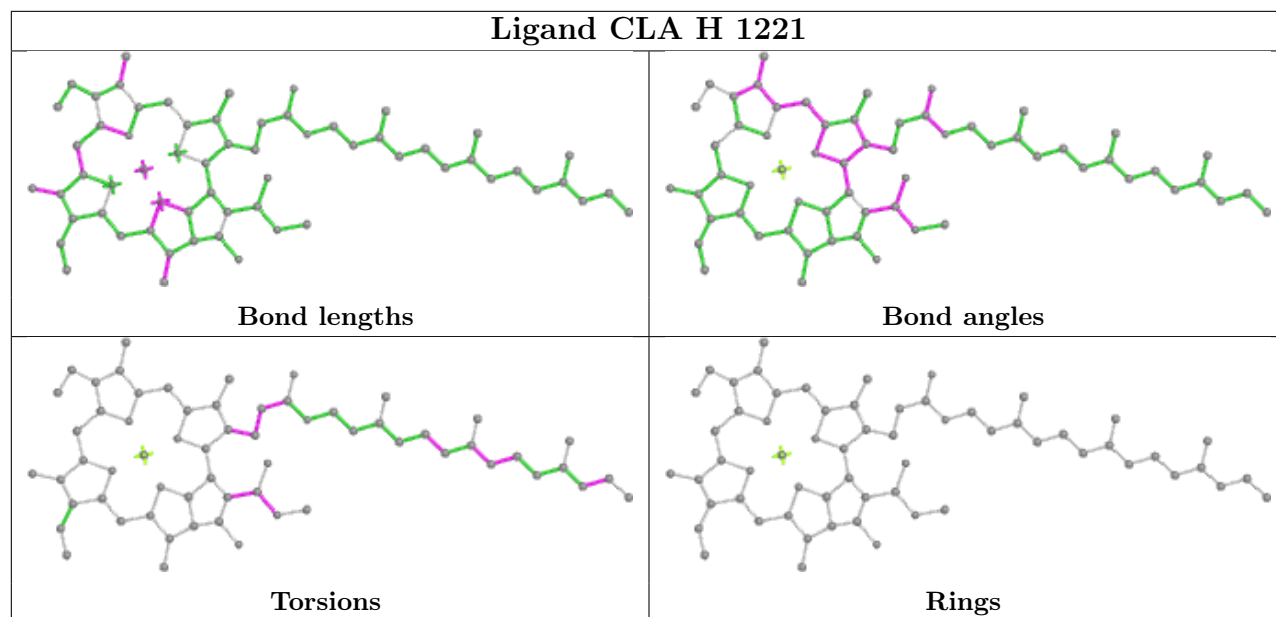
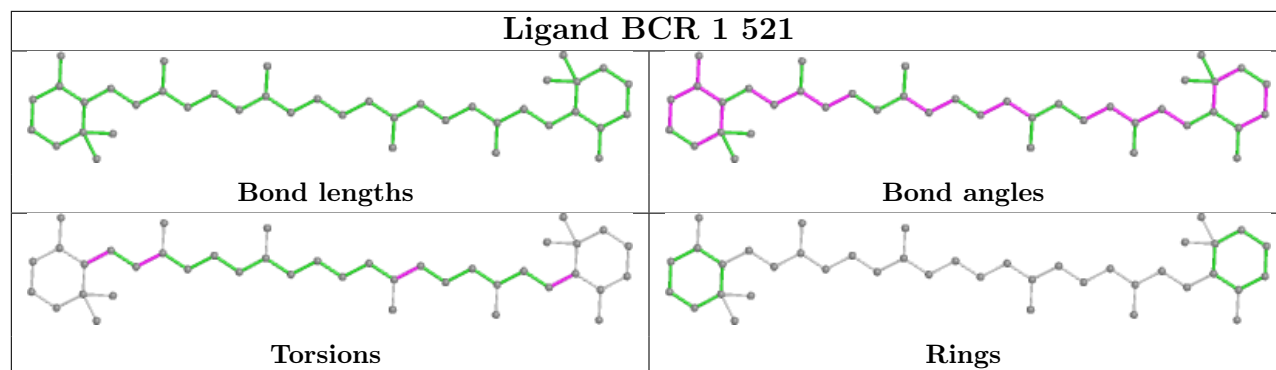


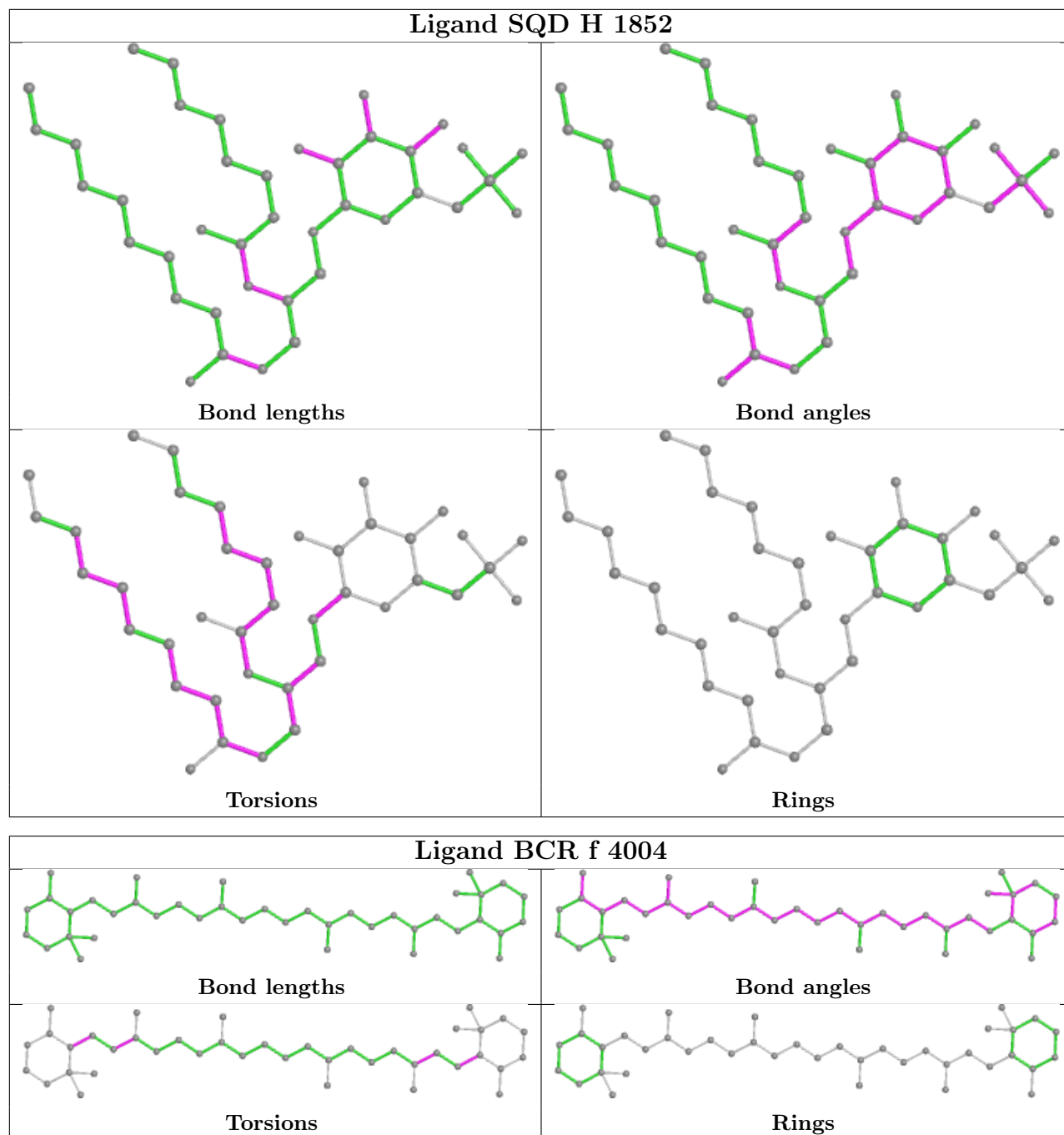
Ligand CLA u 518

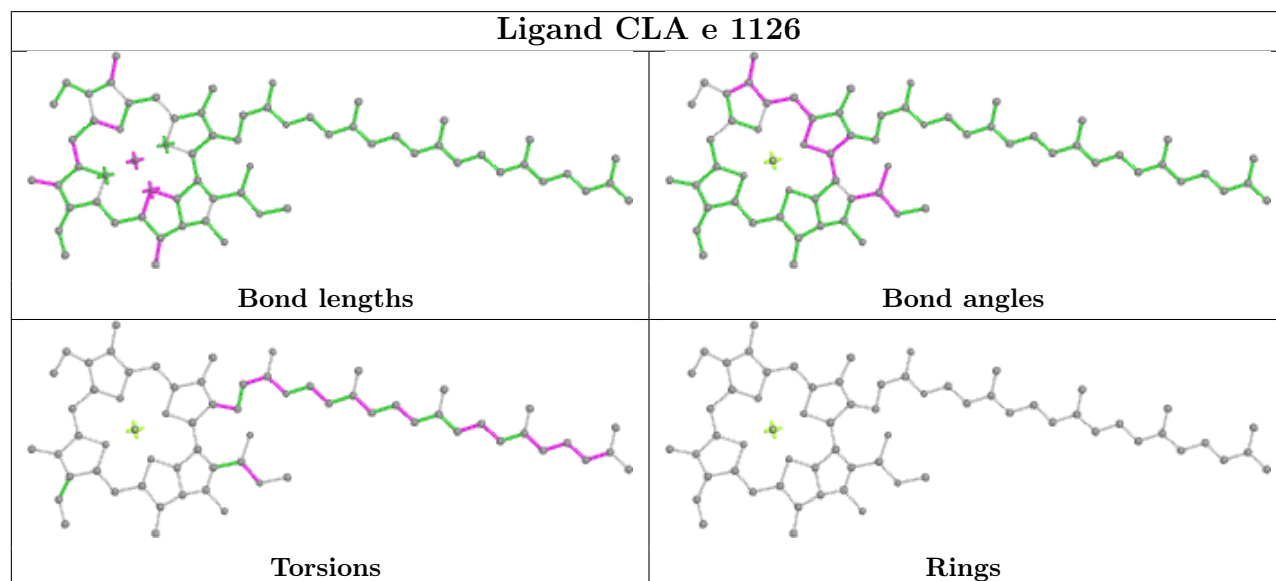
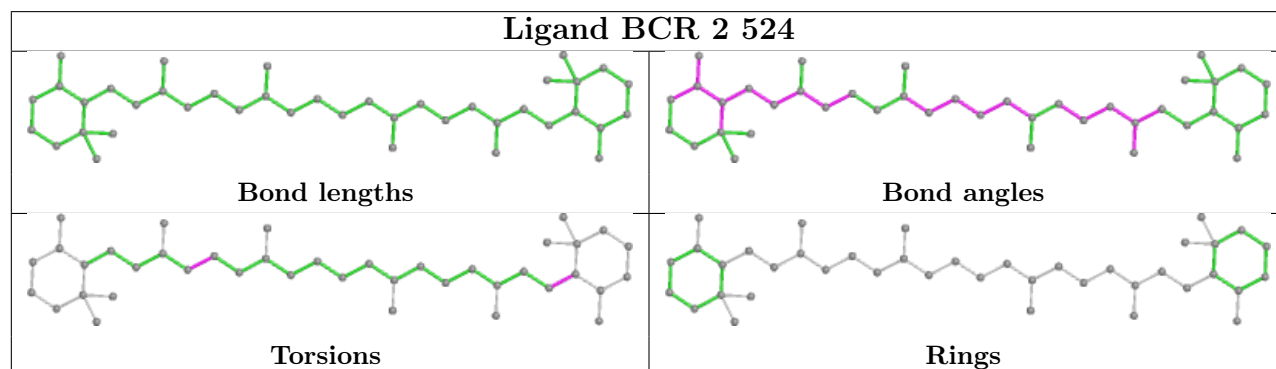
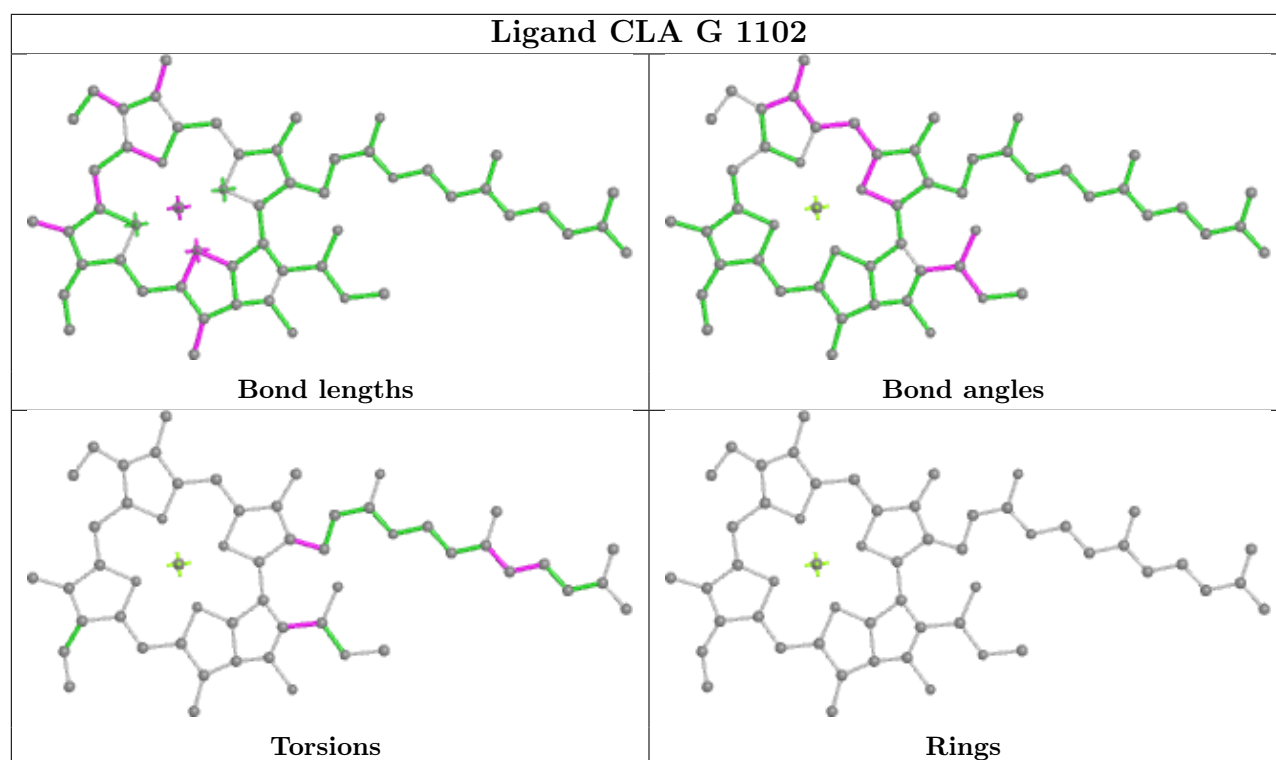


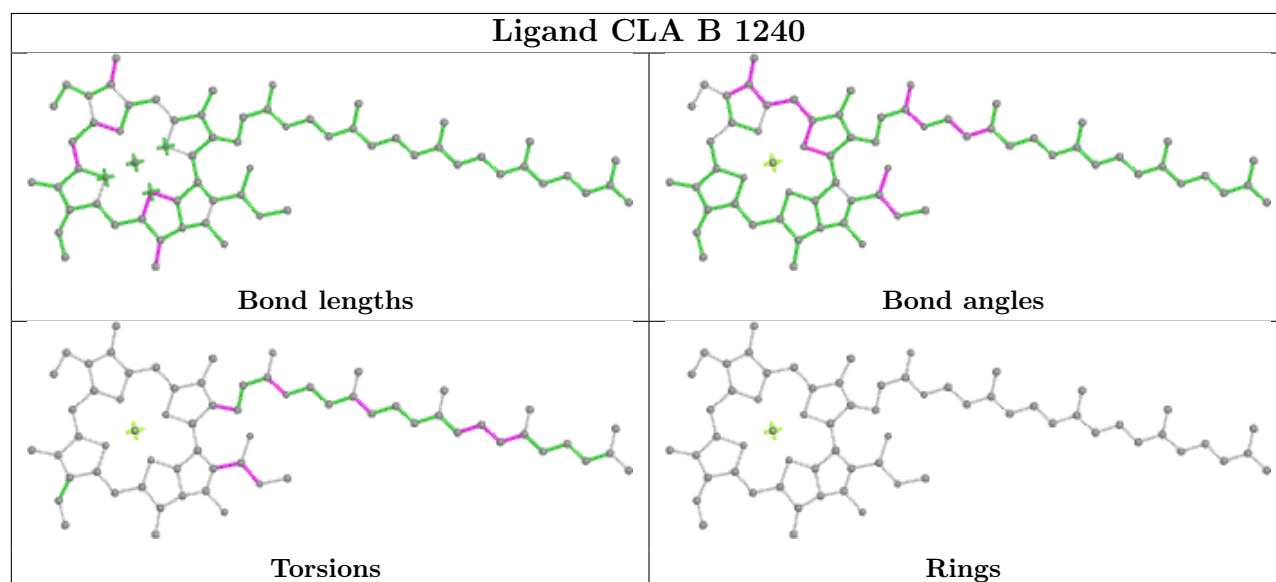
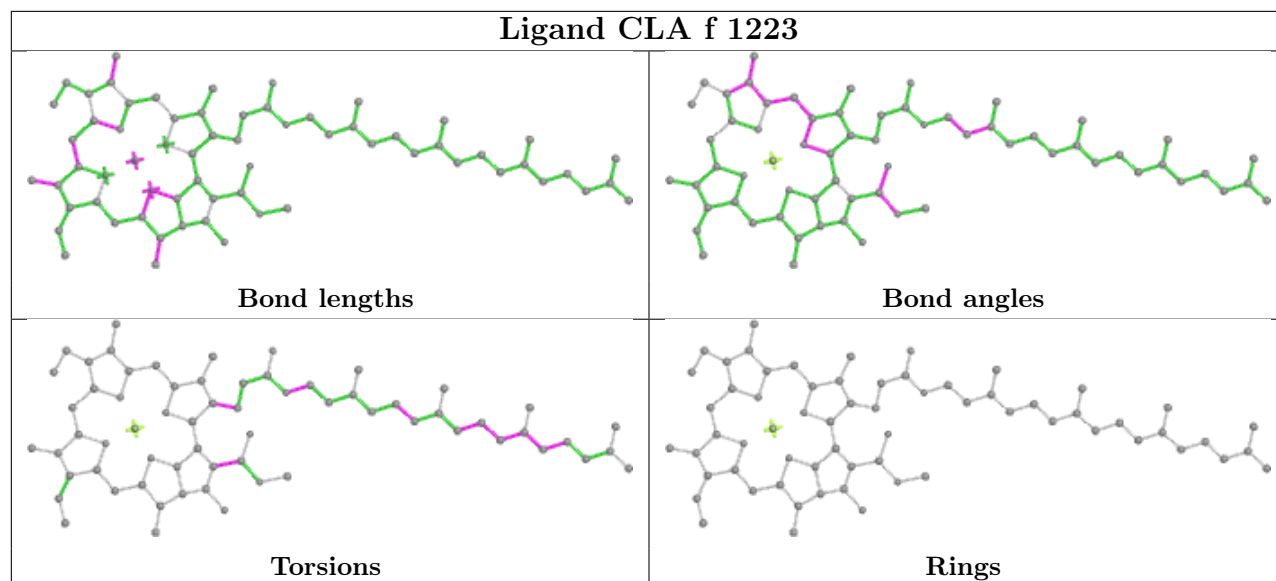
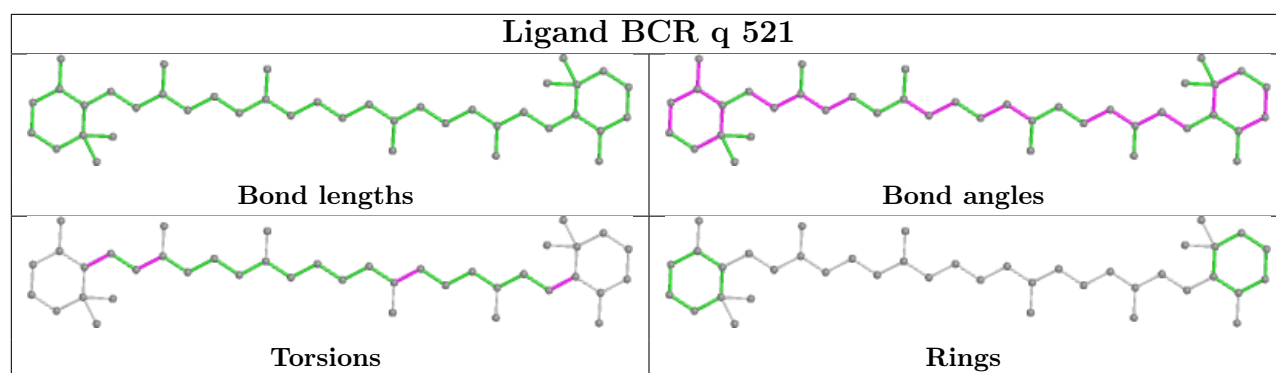
Ligand BCR A 4008



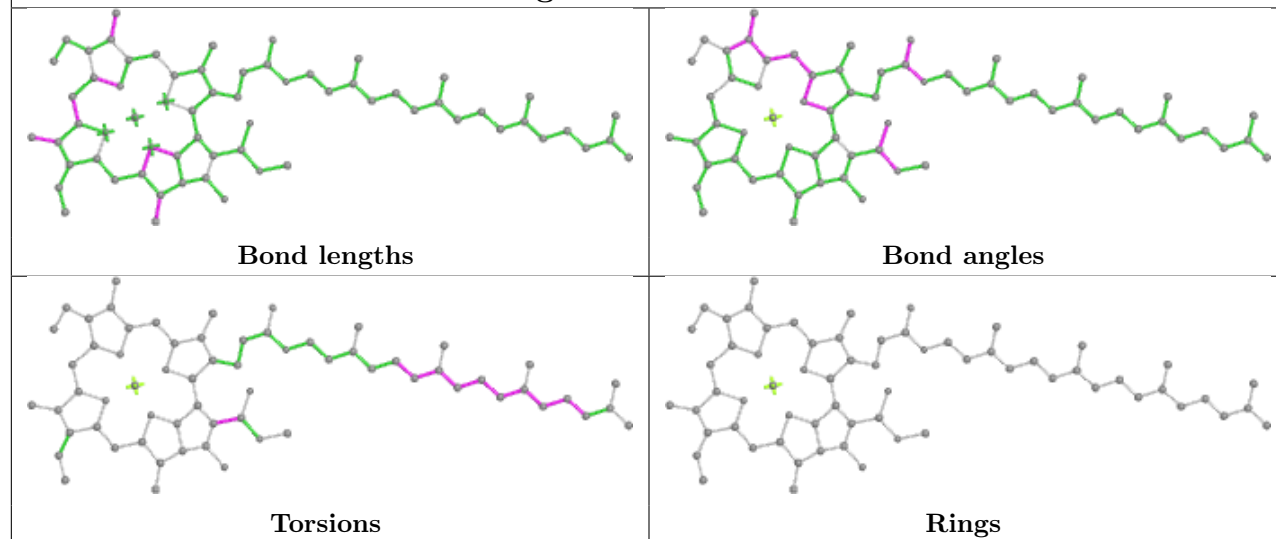




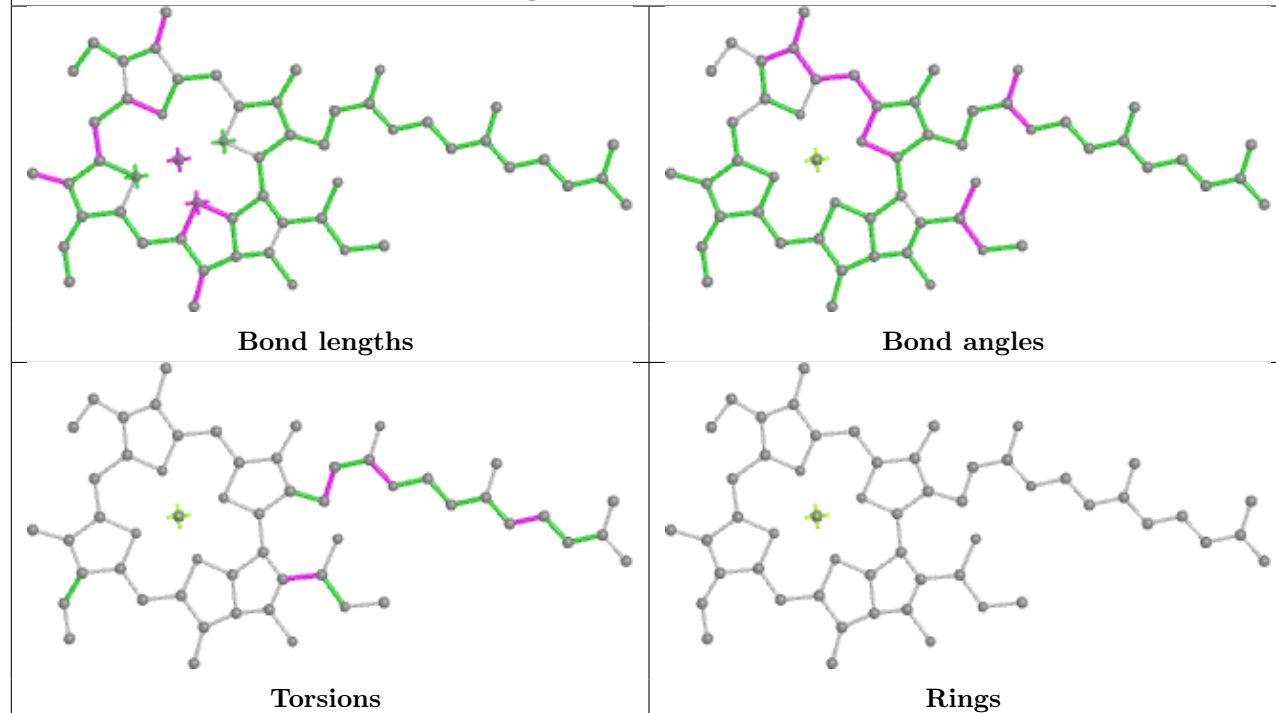




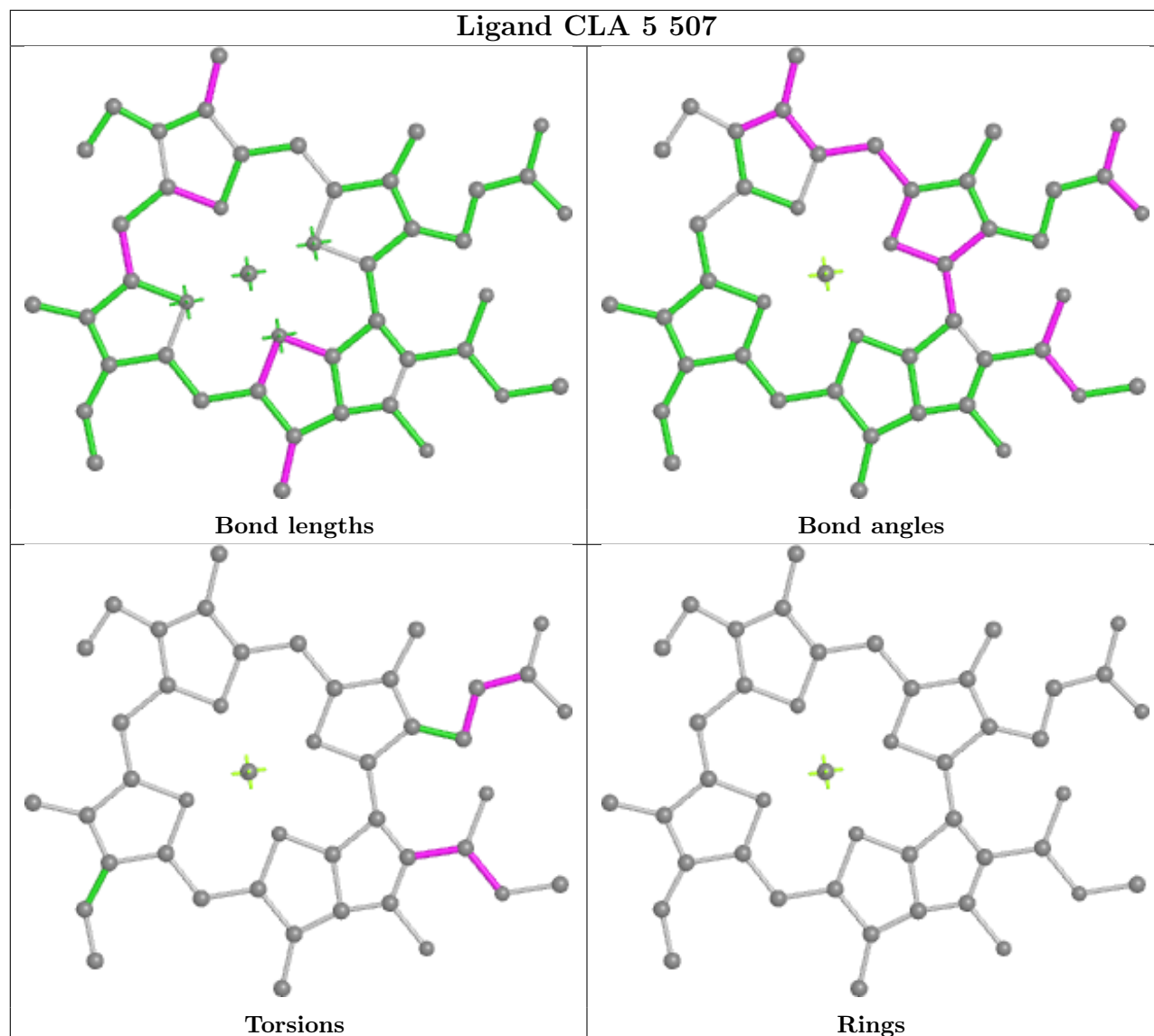
Ligand CLA 5 509



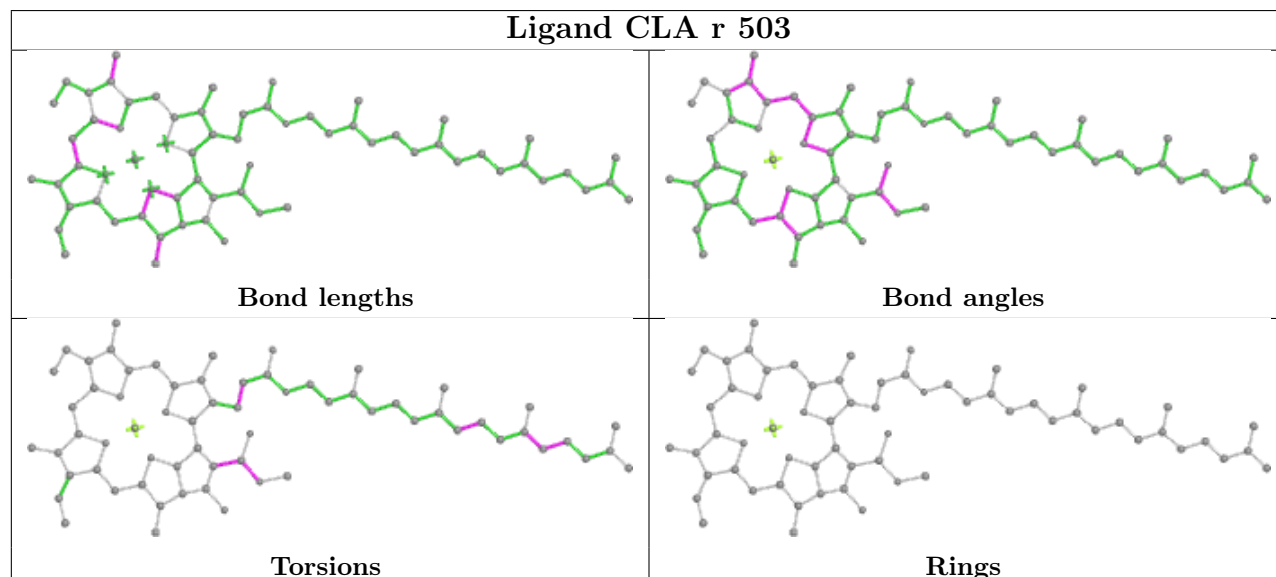
Ligand CLA B 1232

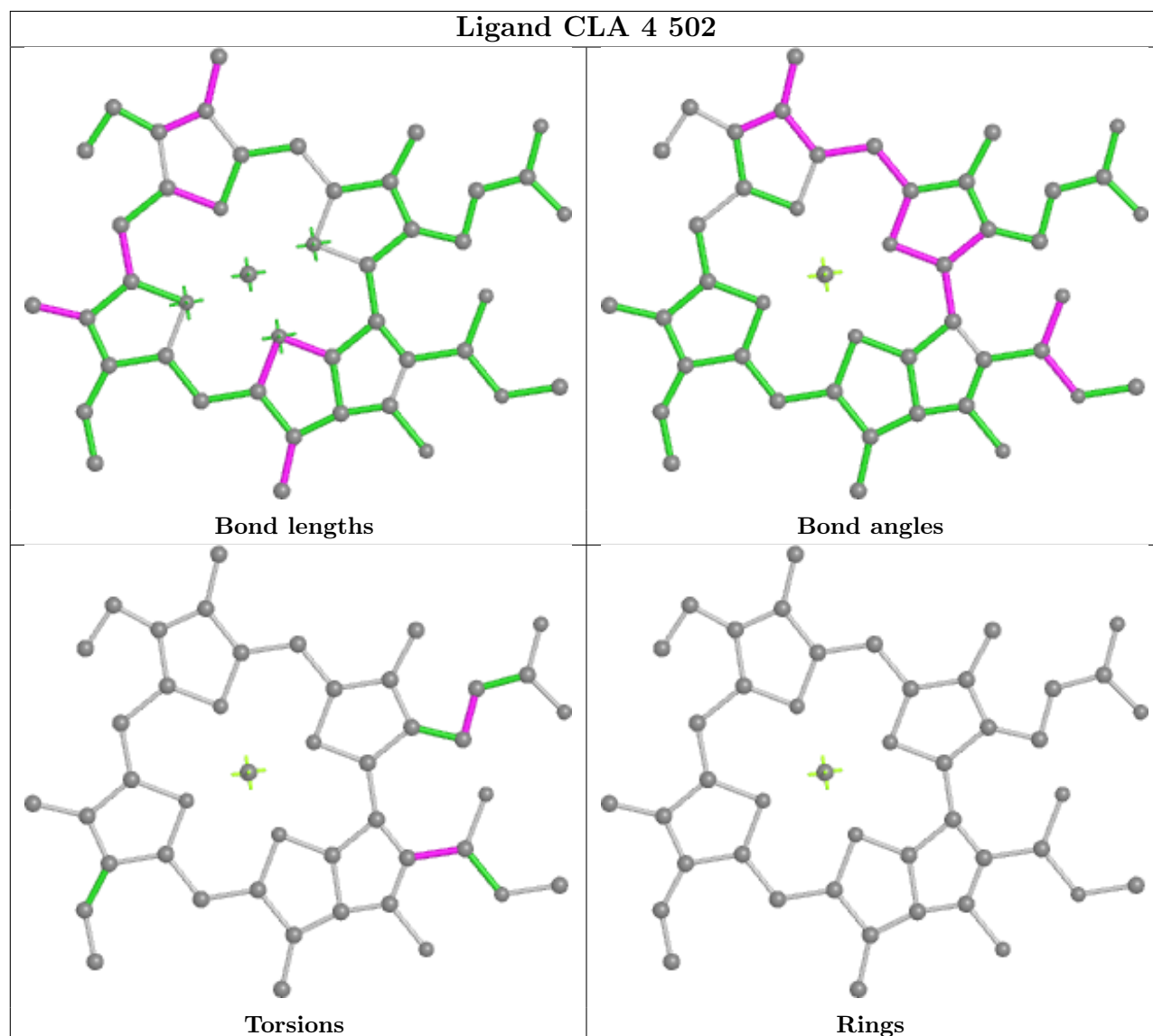
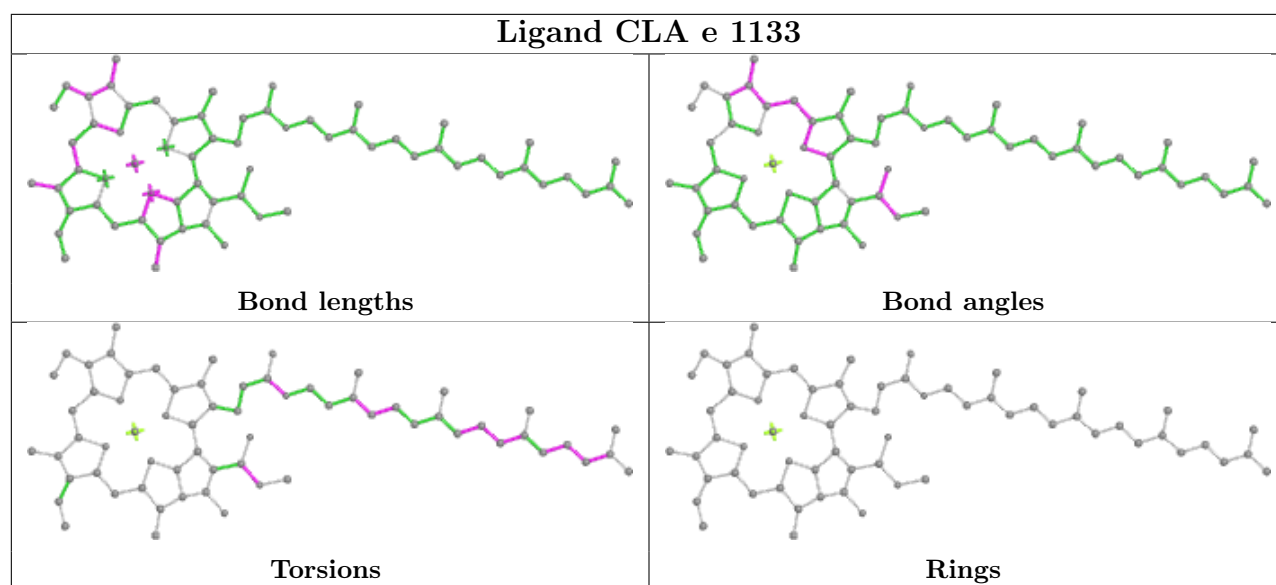


Ligand CLA 5 507

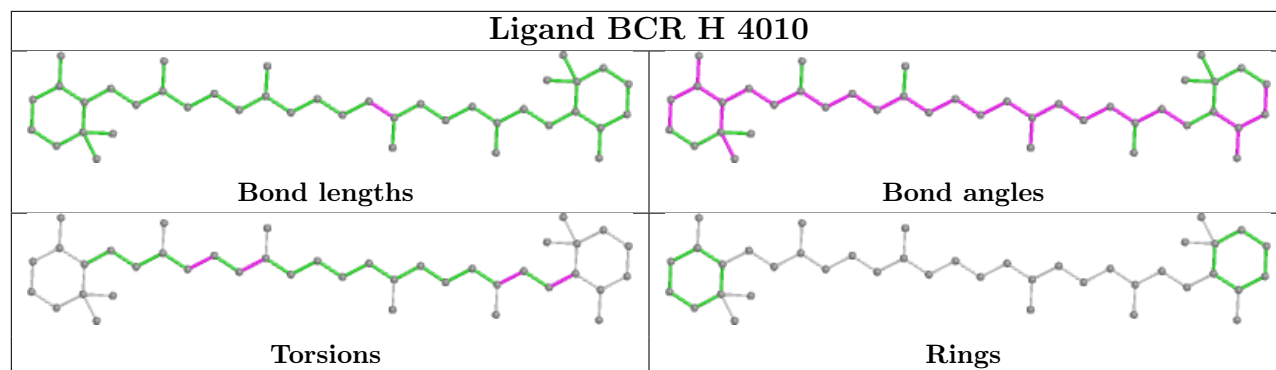


Ligand CLA r 503

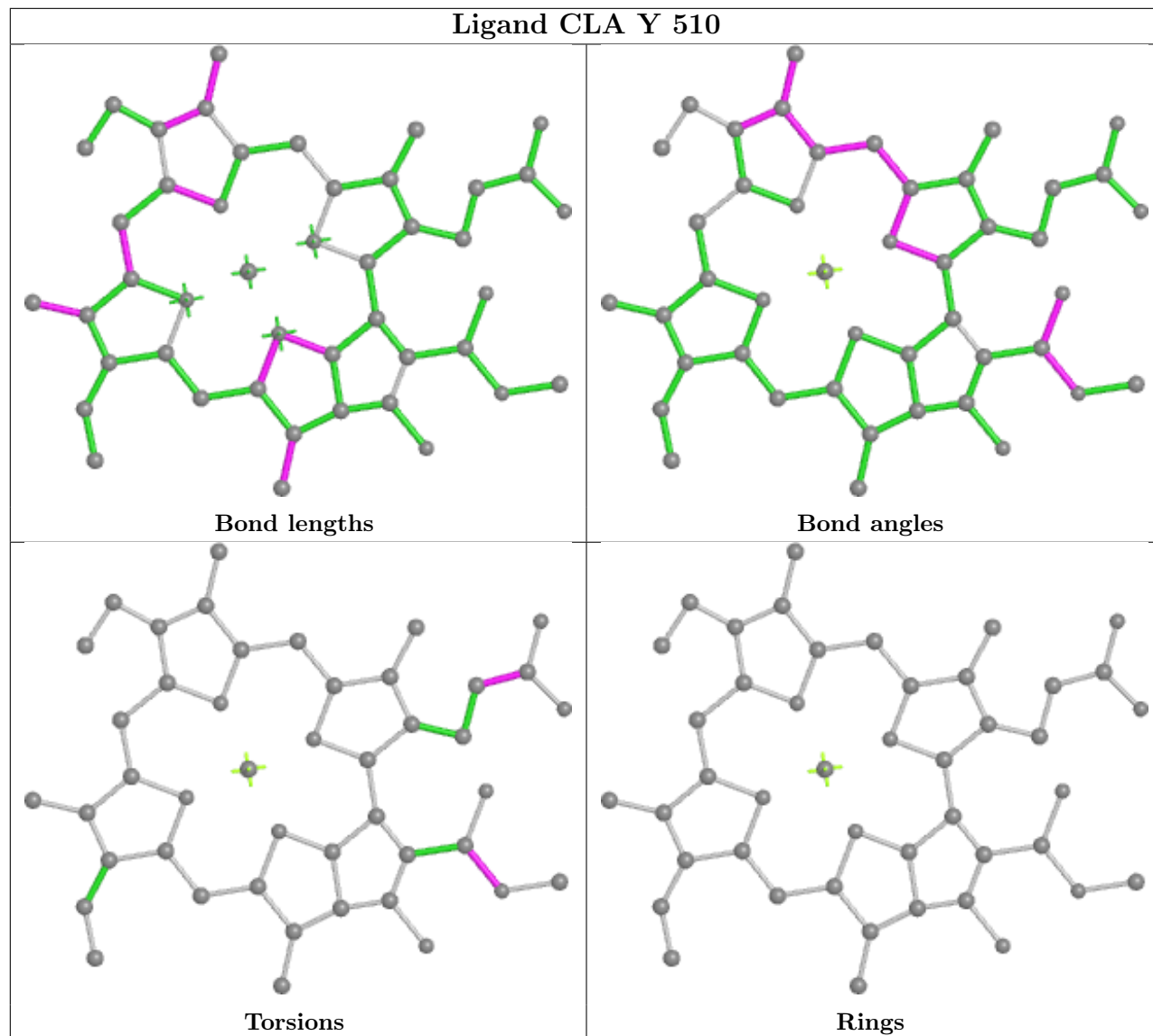




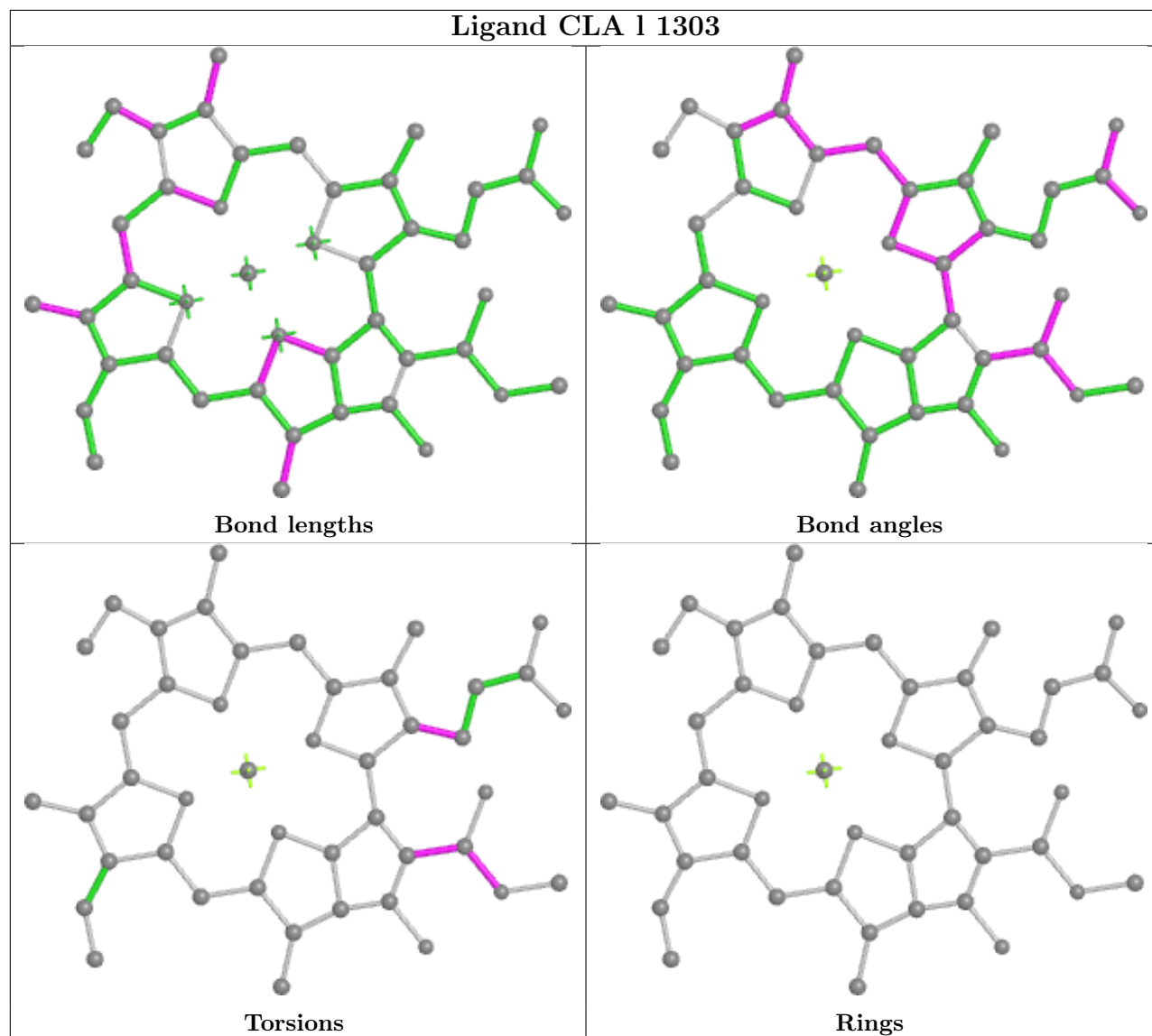
Ligand BCR H 4010



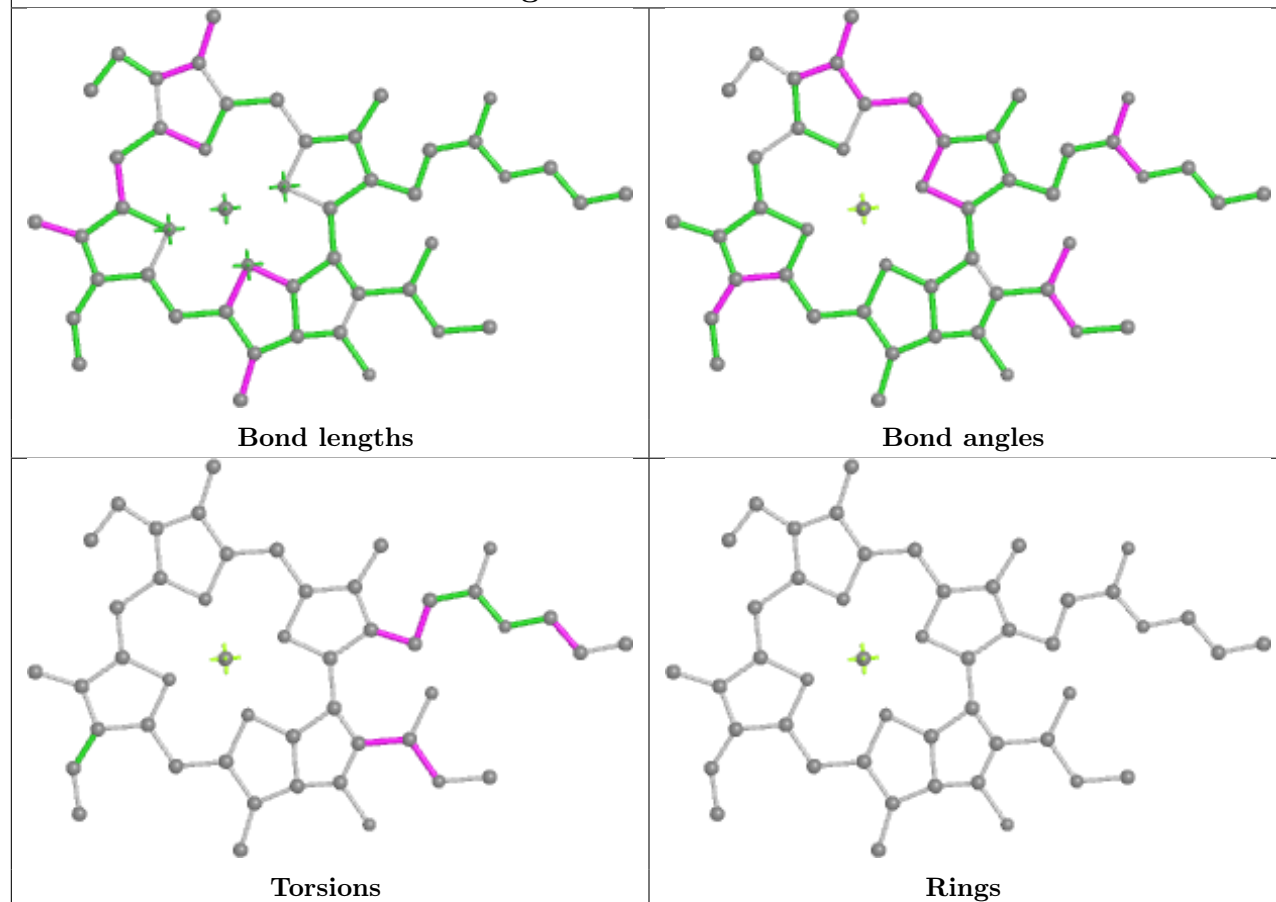
Ligand CLA Y 510



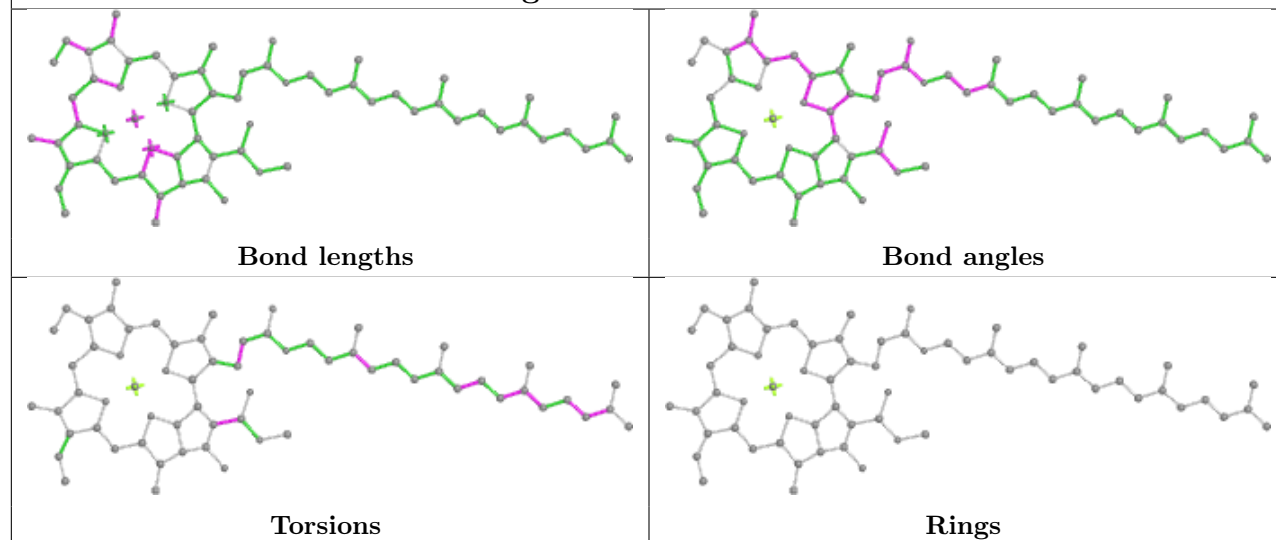
Ligand CLA 1 1303

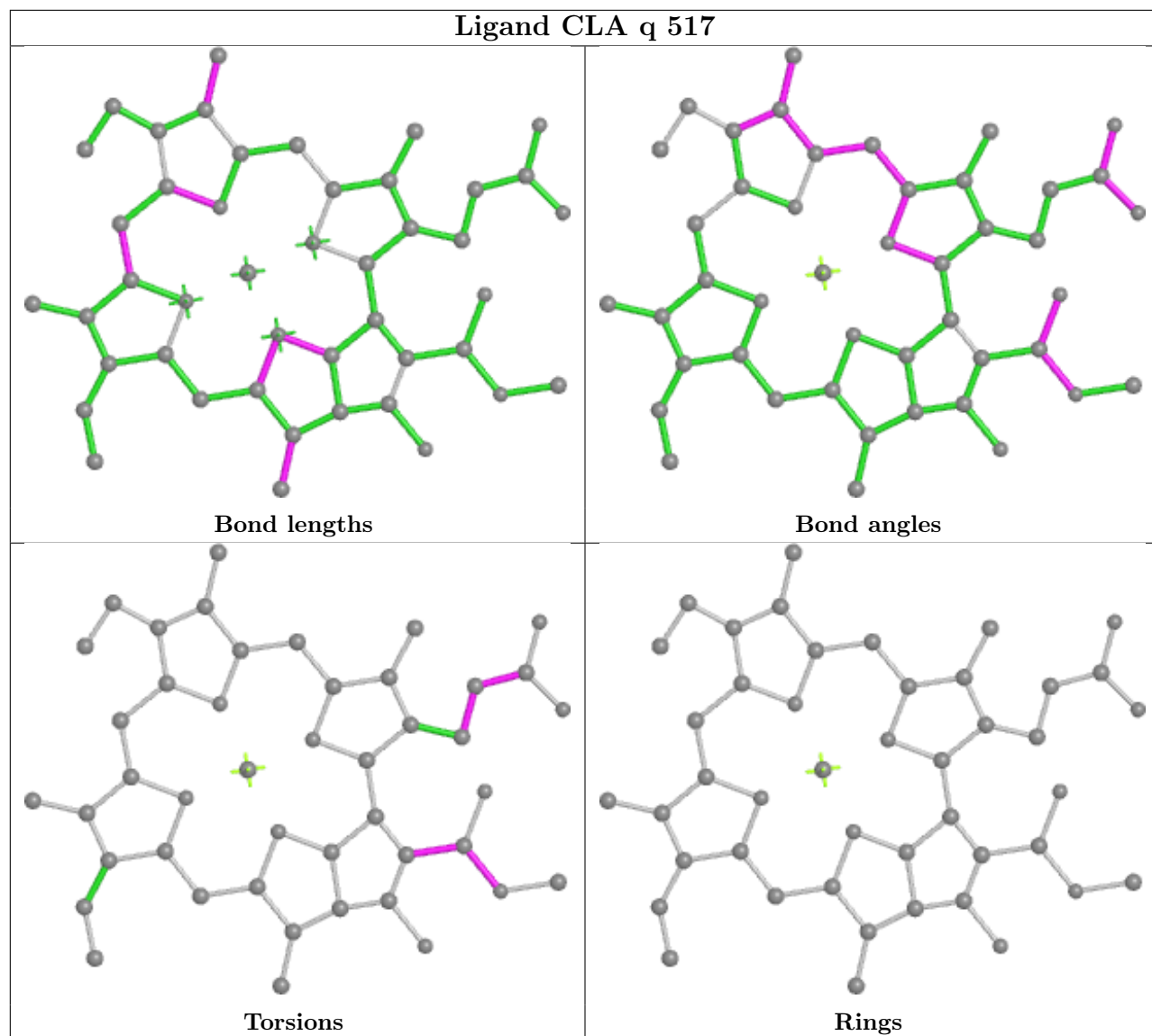
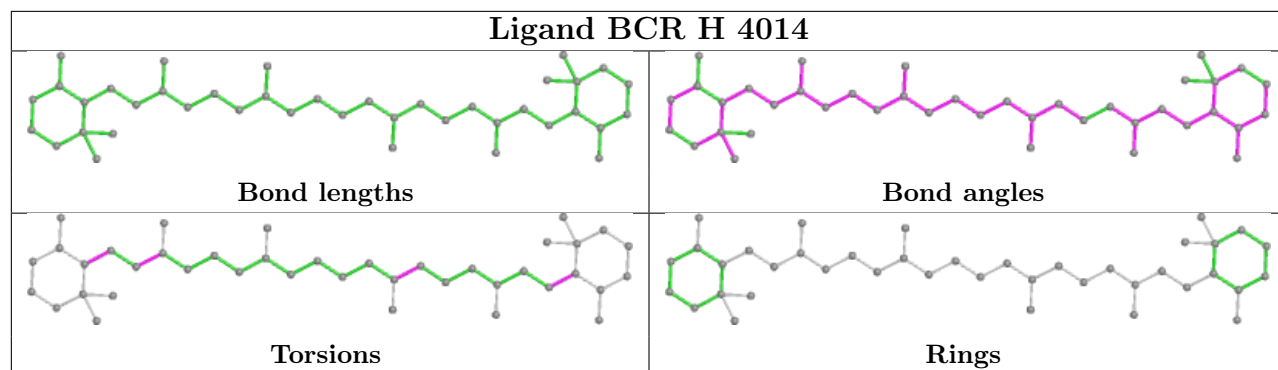


Ligand CLA m 1103

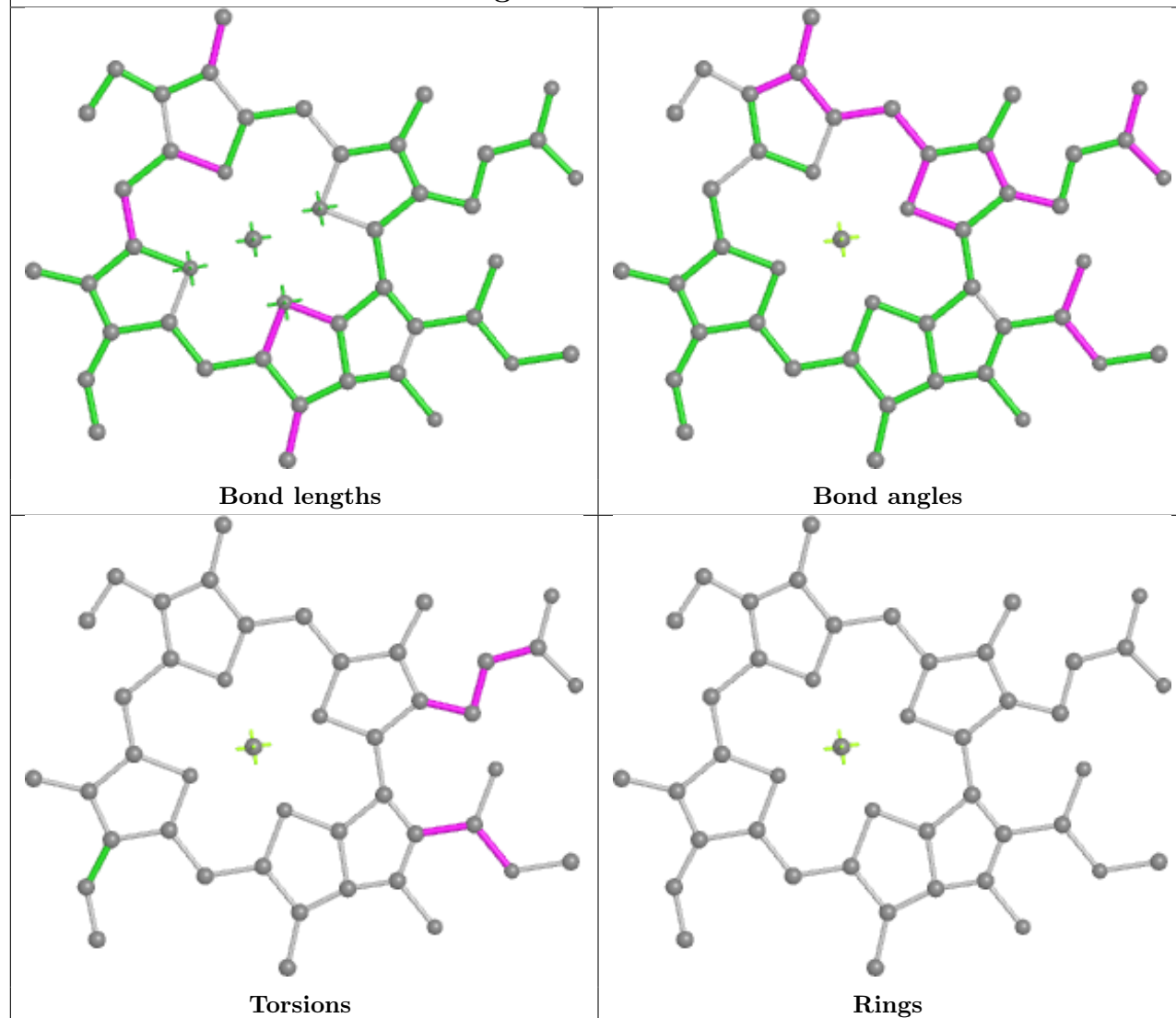


Ligand CLA G 1127

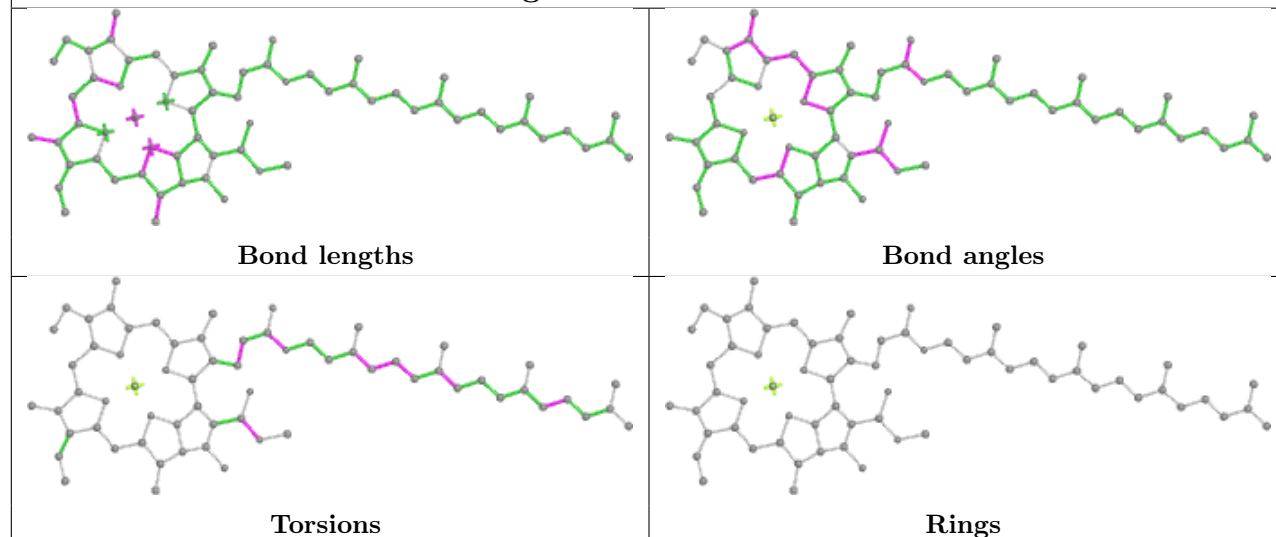




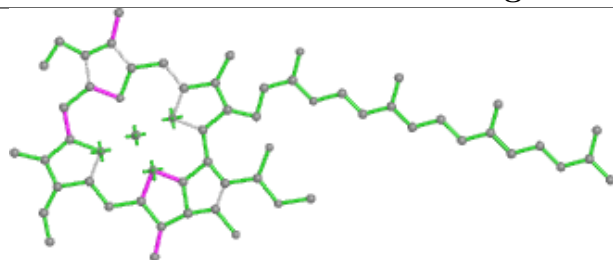
Ligand CLA 6 516



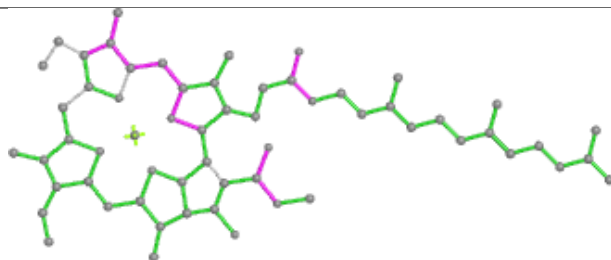
Ligand CLA H 1204



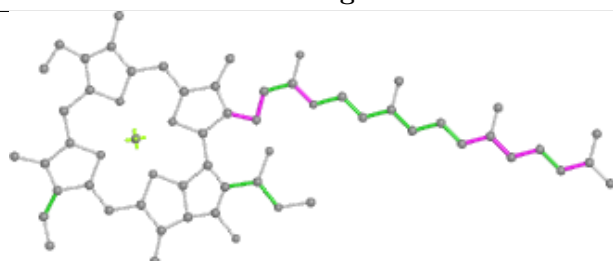
Ligand CLA H 1217



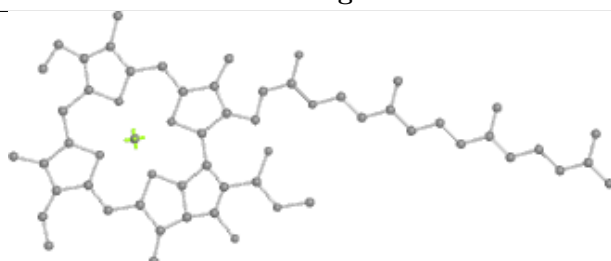
Bond lengths



Bond angles

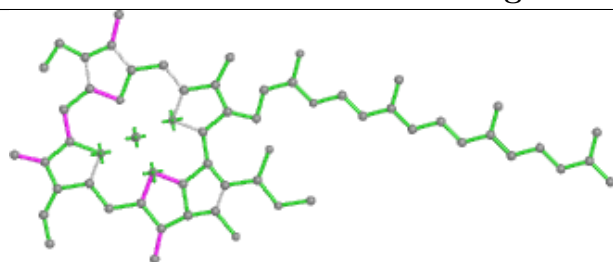


Torsions

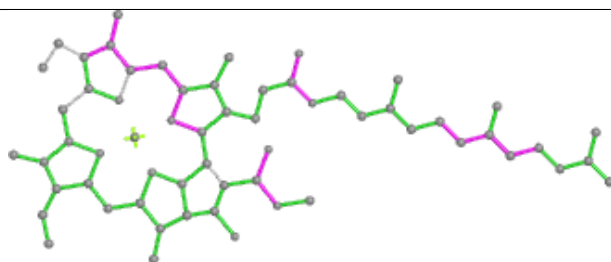


Rings

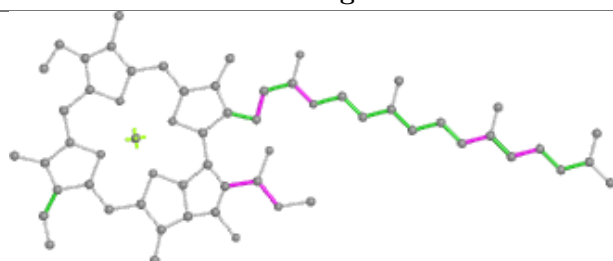
Ligand CLA H 1201



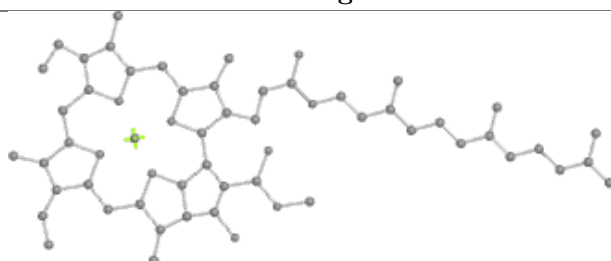
Bond lengths



Bond angles

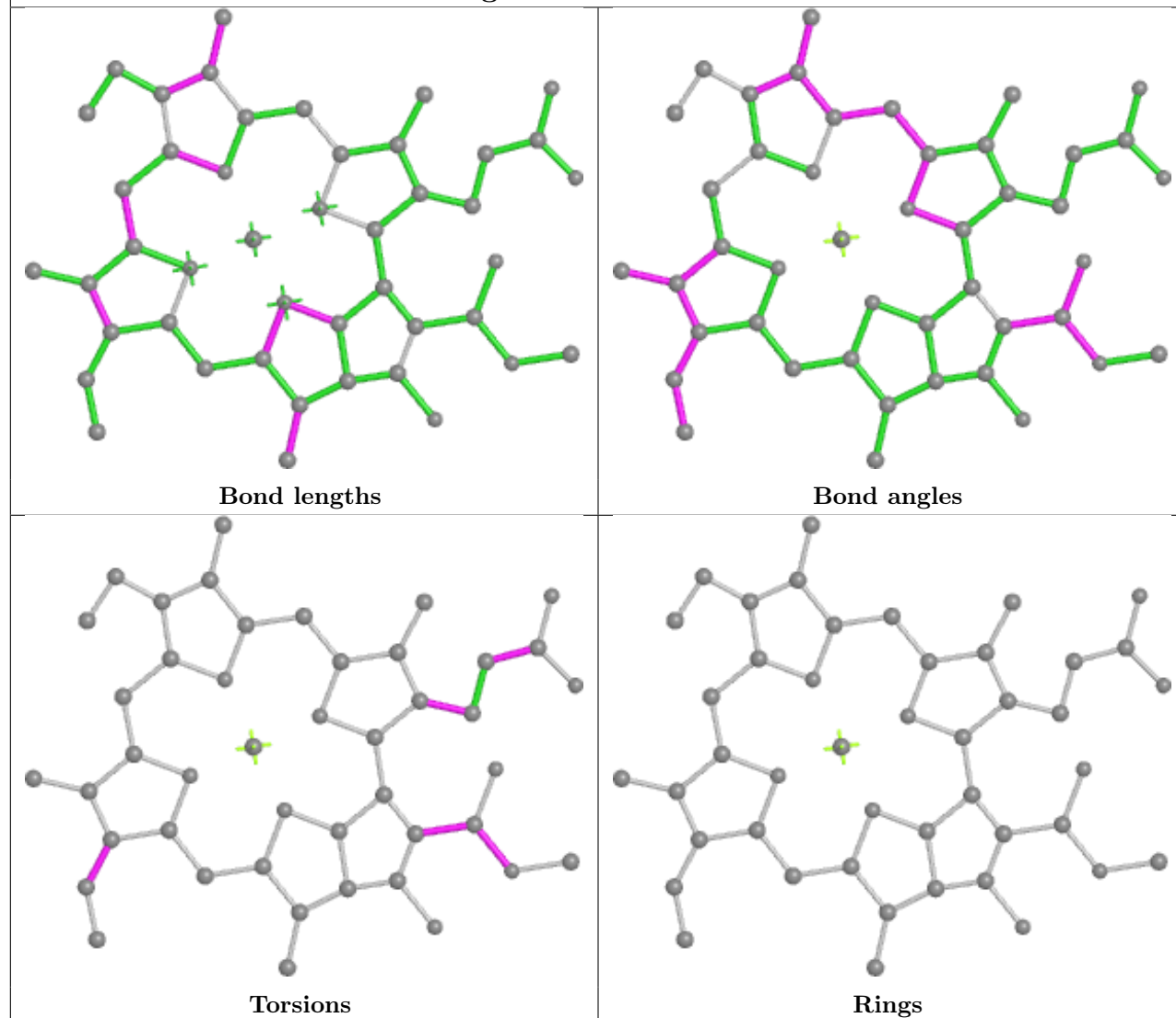


Torsions

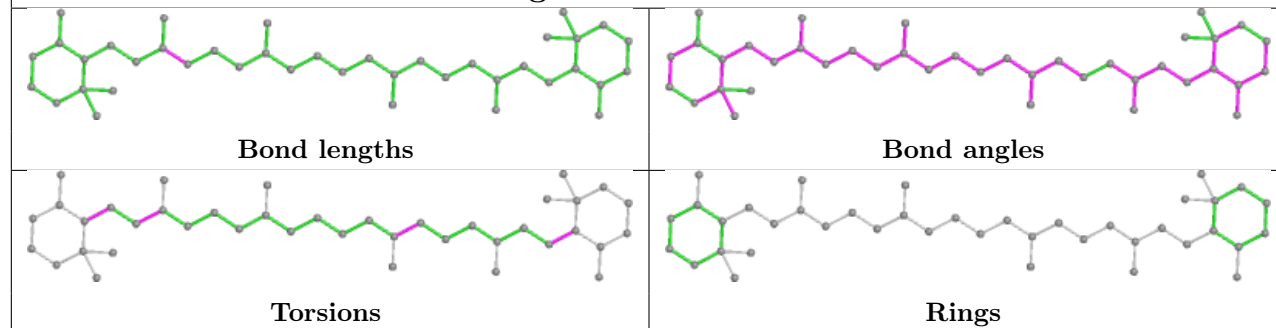


Rings

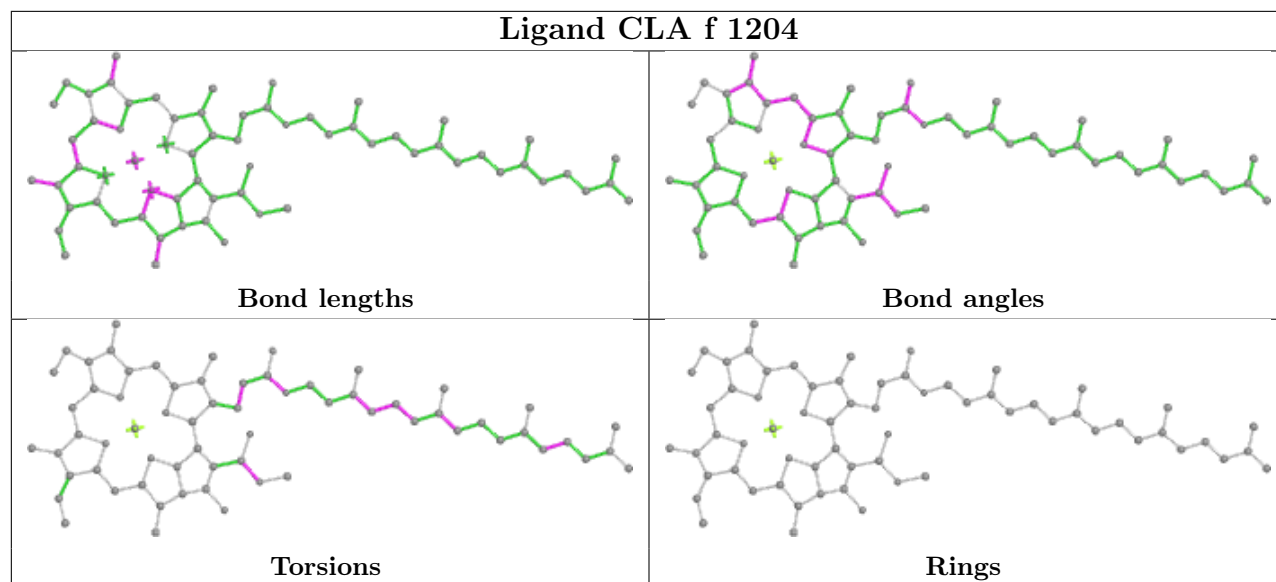
Ligand CLA K 1105



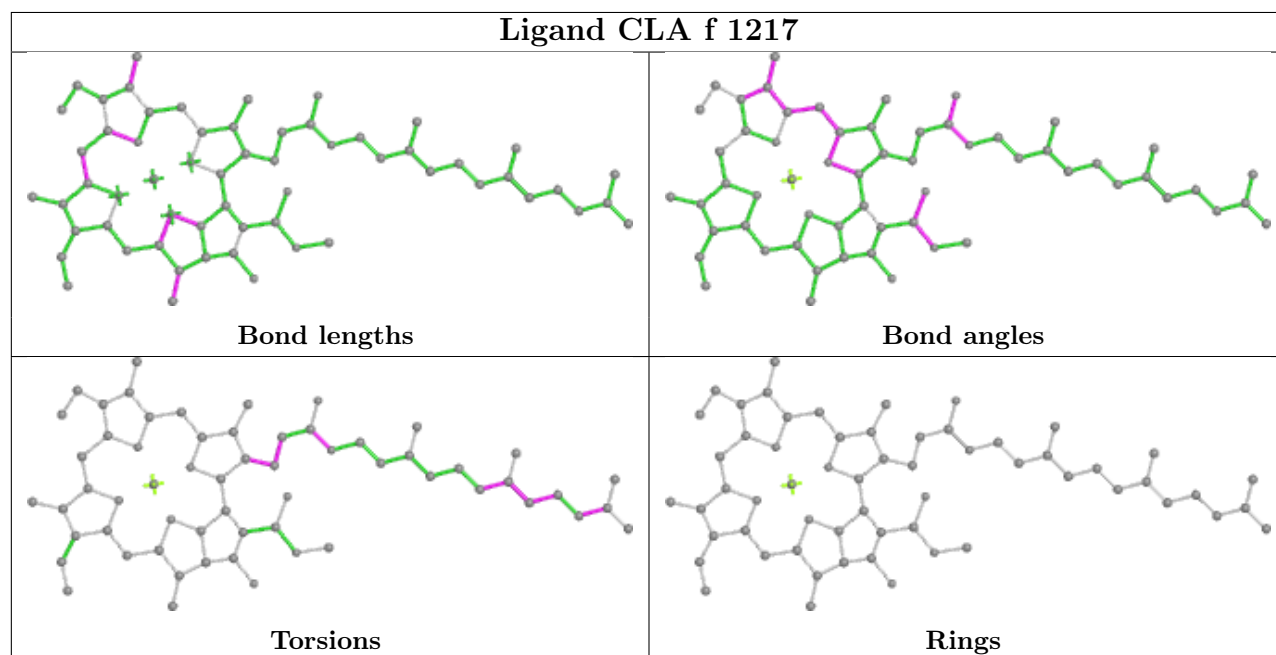
Ligand BCR f 4014



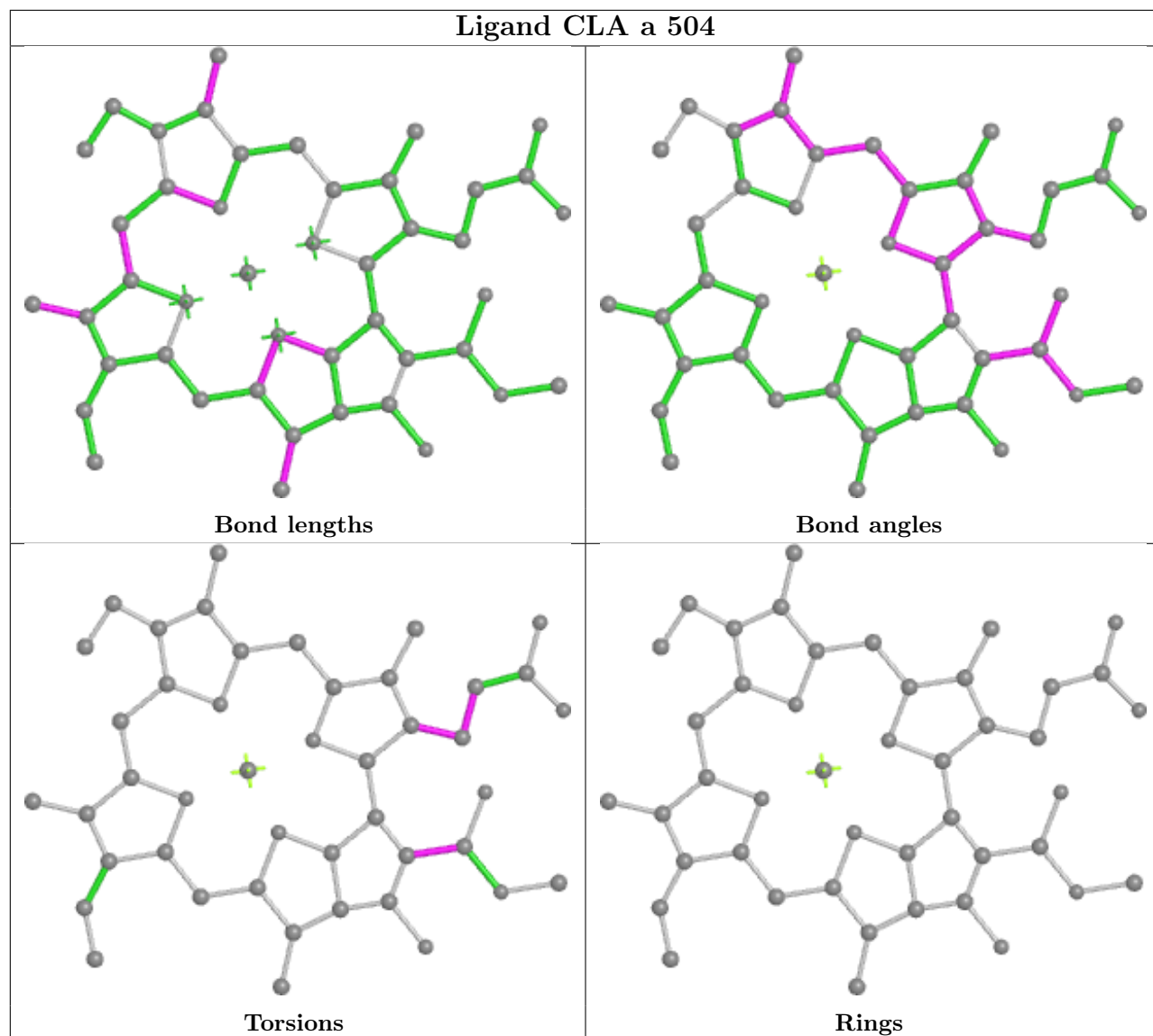
Ligand CLA f 1204



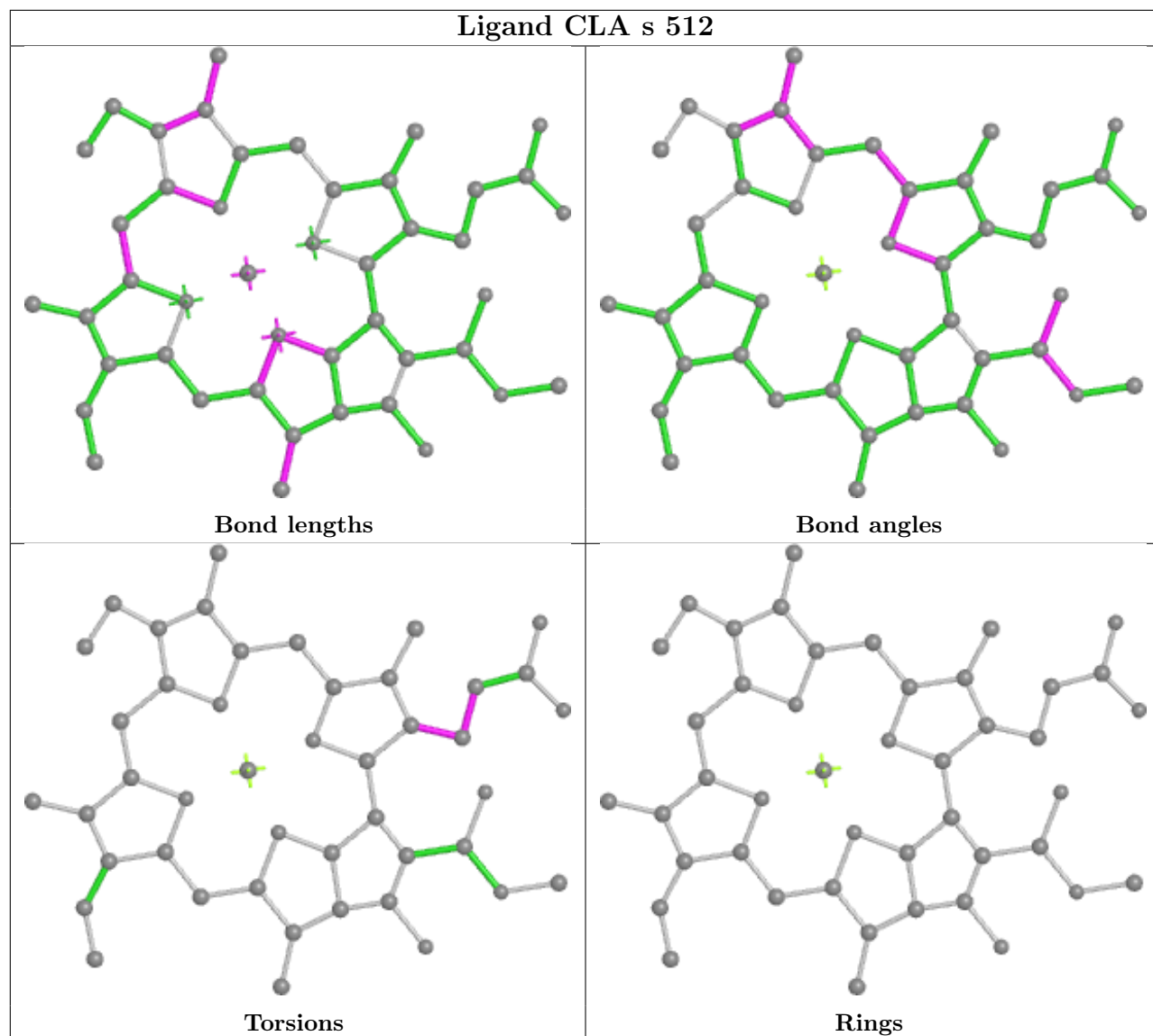
Ligand CLA f 1217



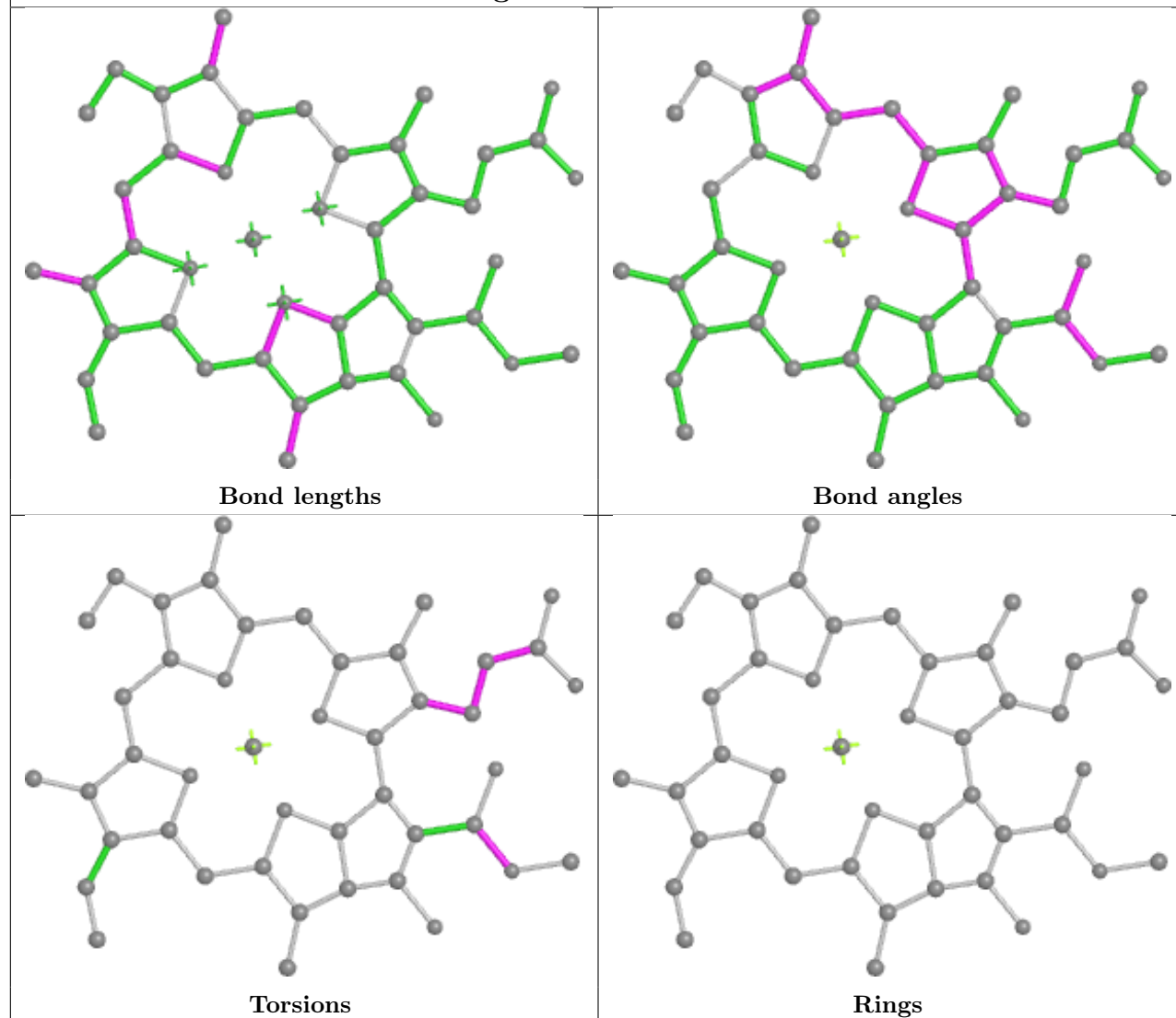
Ligand CLA a 504



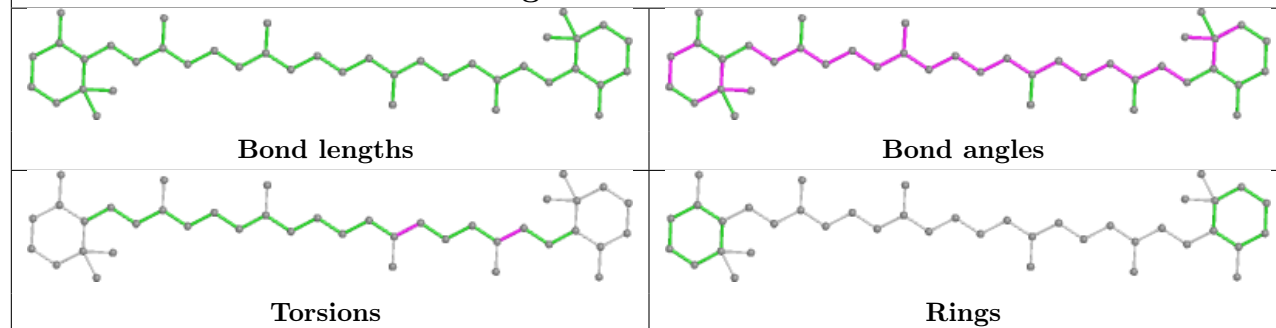
Ligand CLA s 512

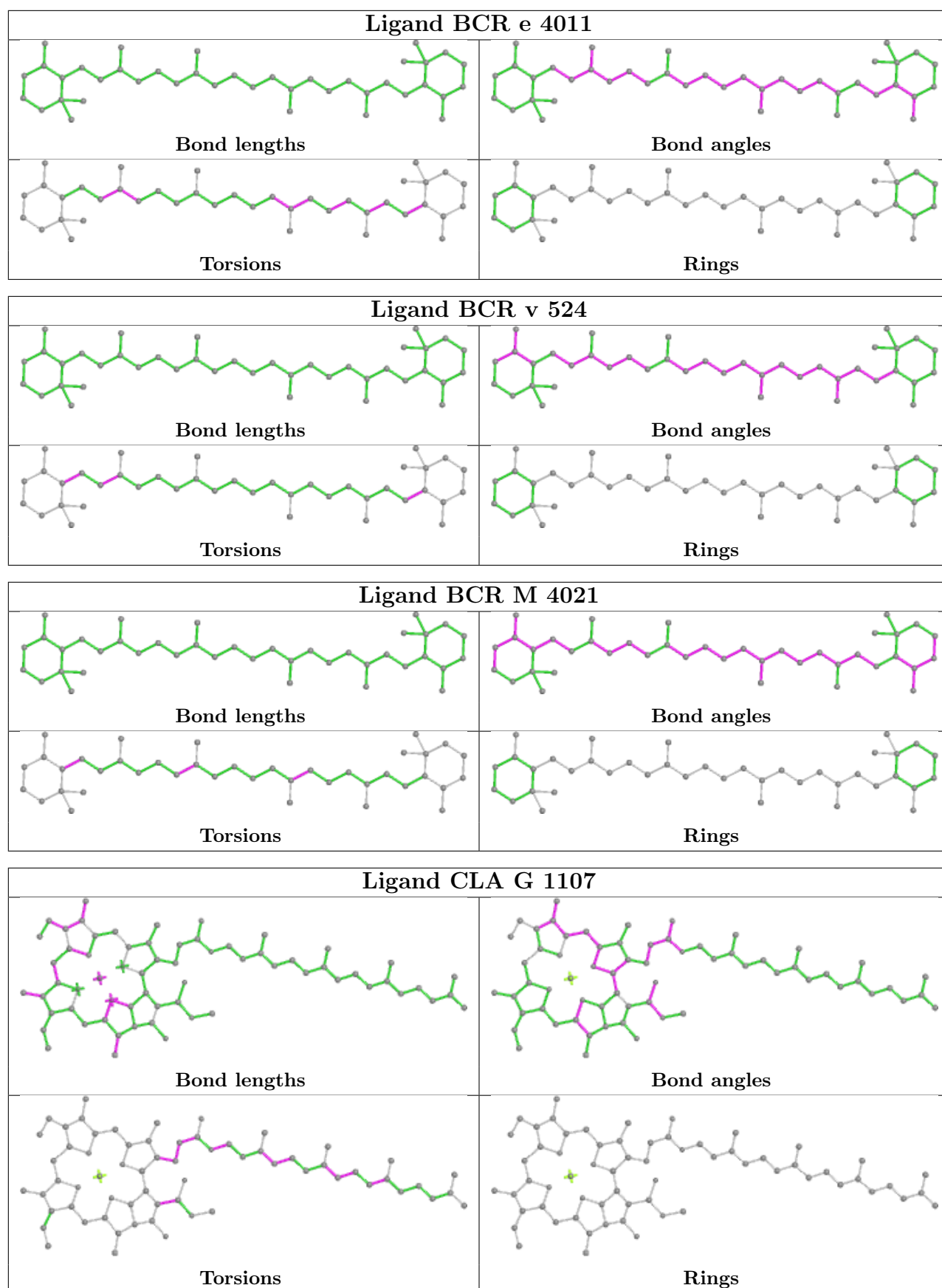


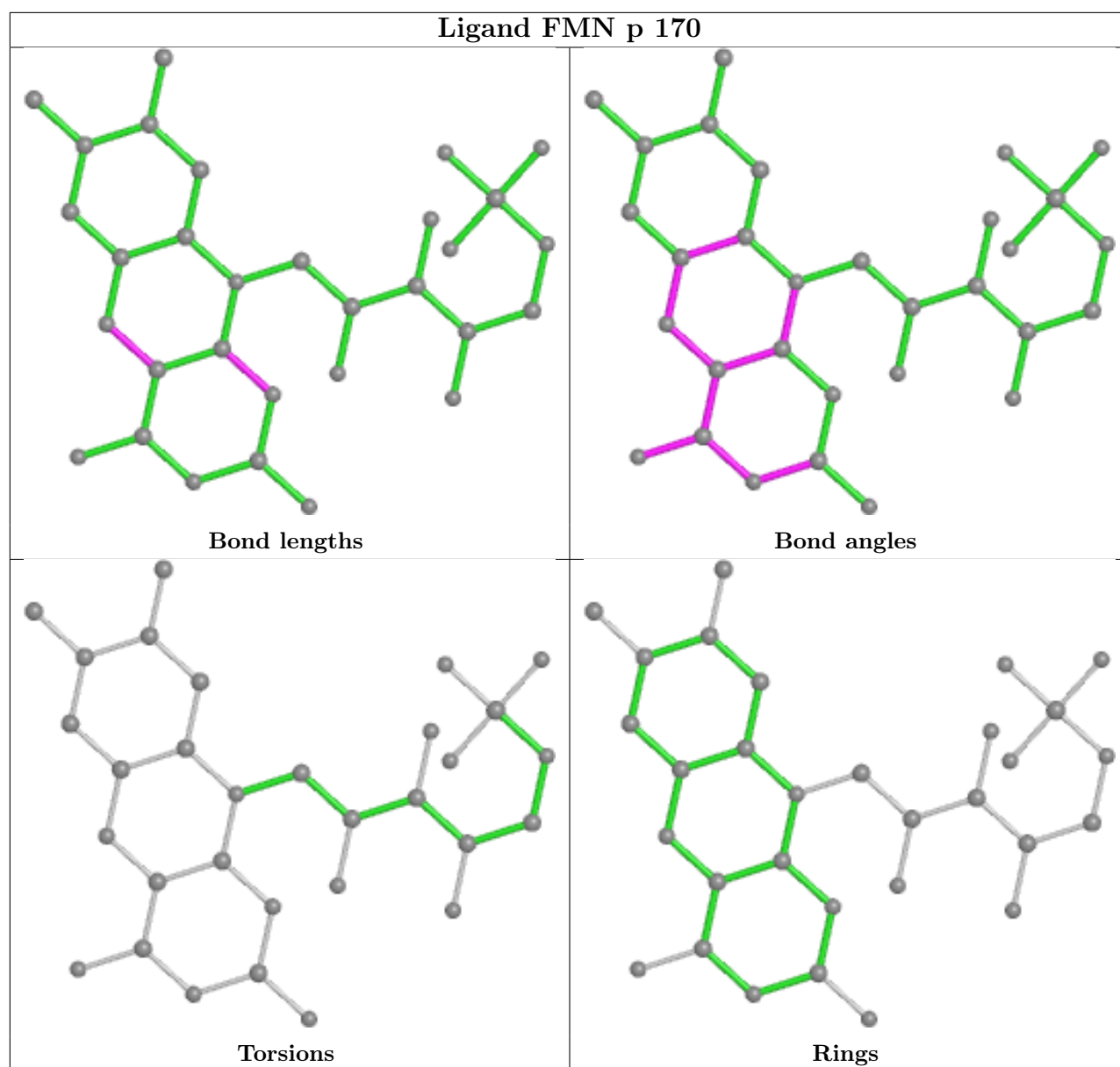
Ligand CLA u 501



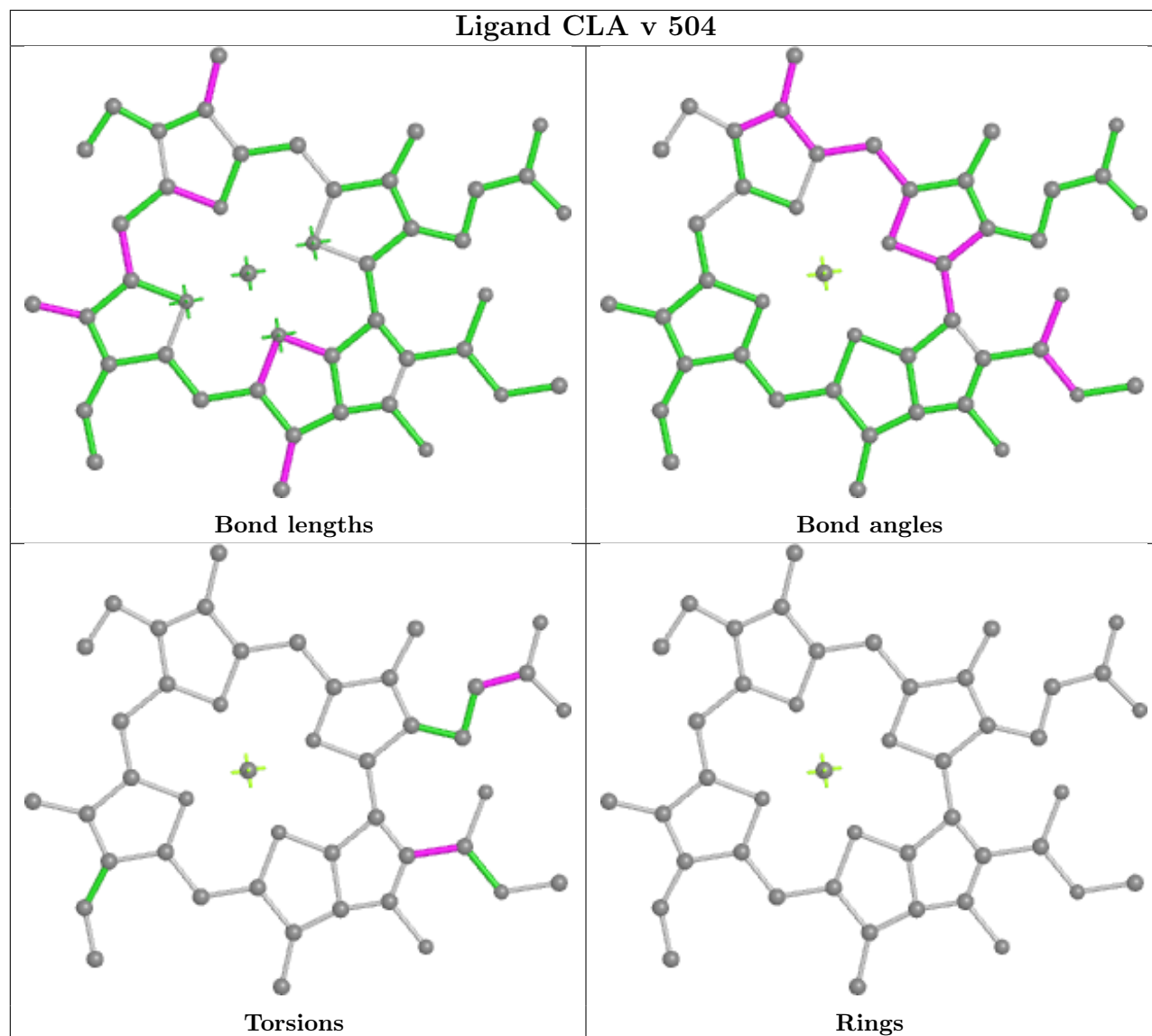
Ligand BCR T 4013



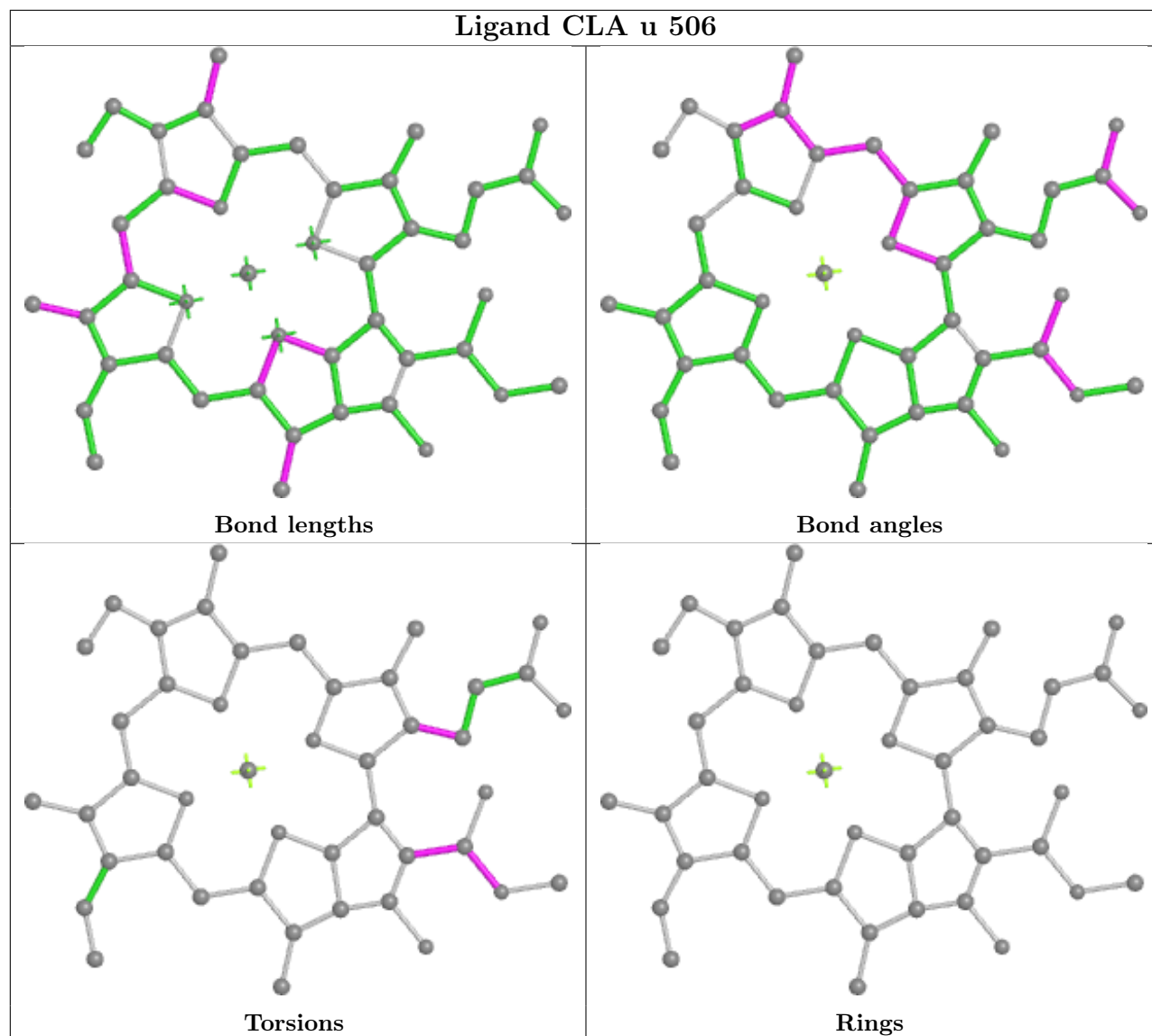


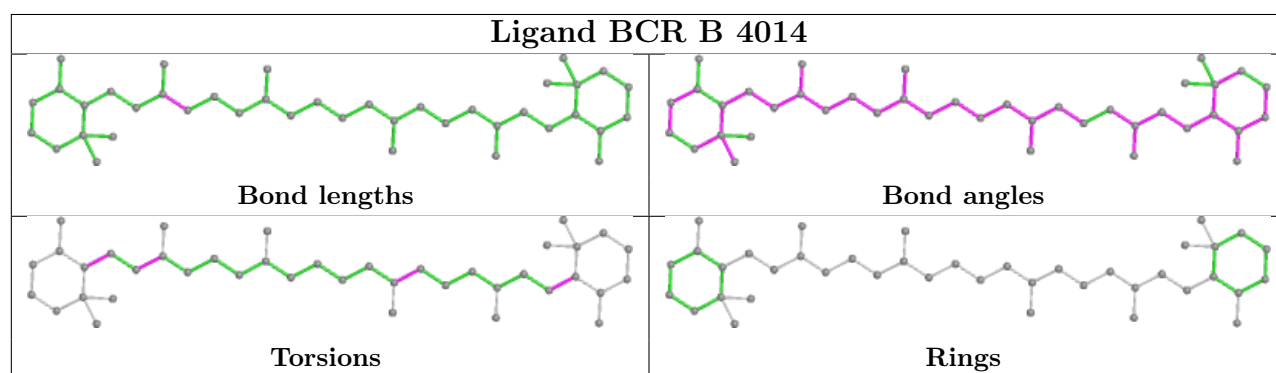
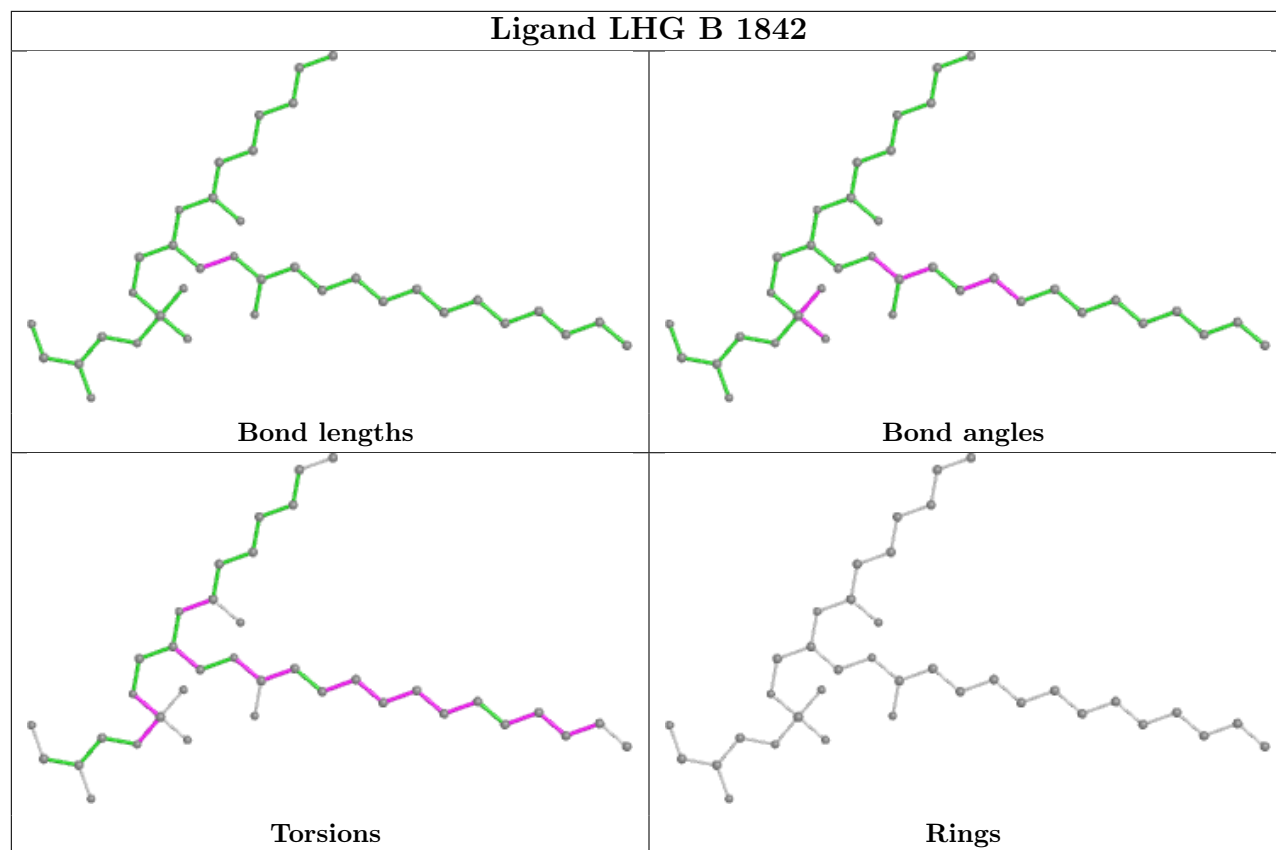


Ligand CLA v 504

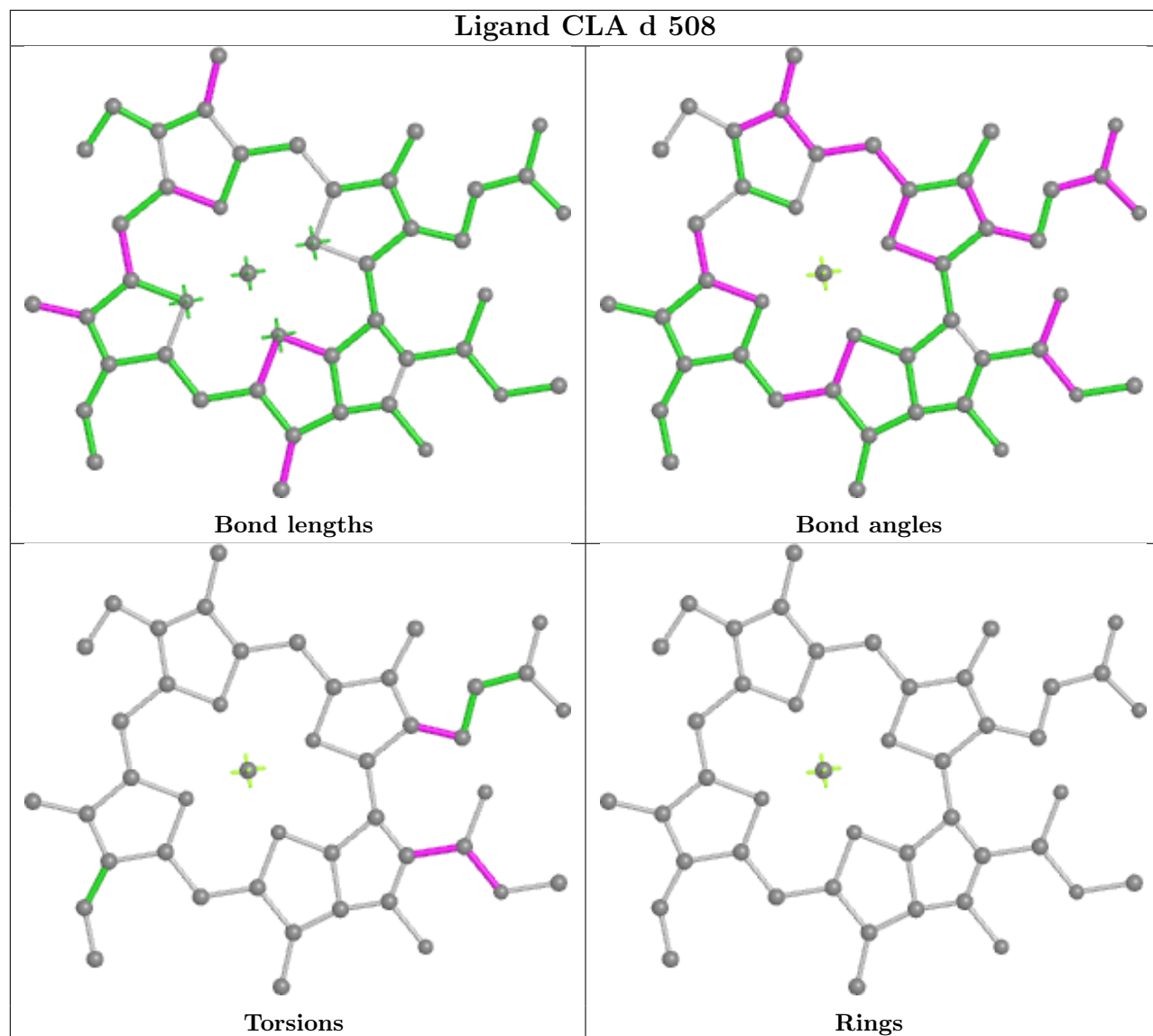


Ligand CLA u 506

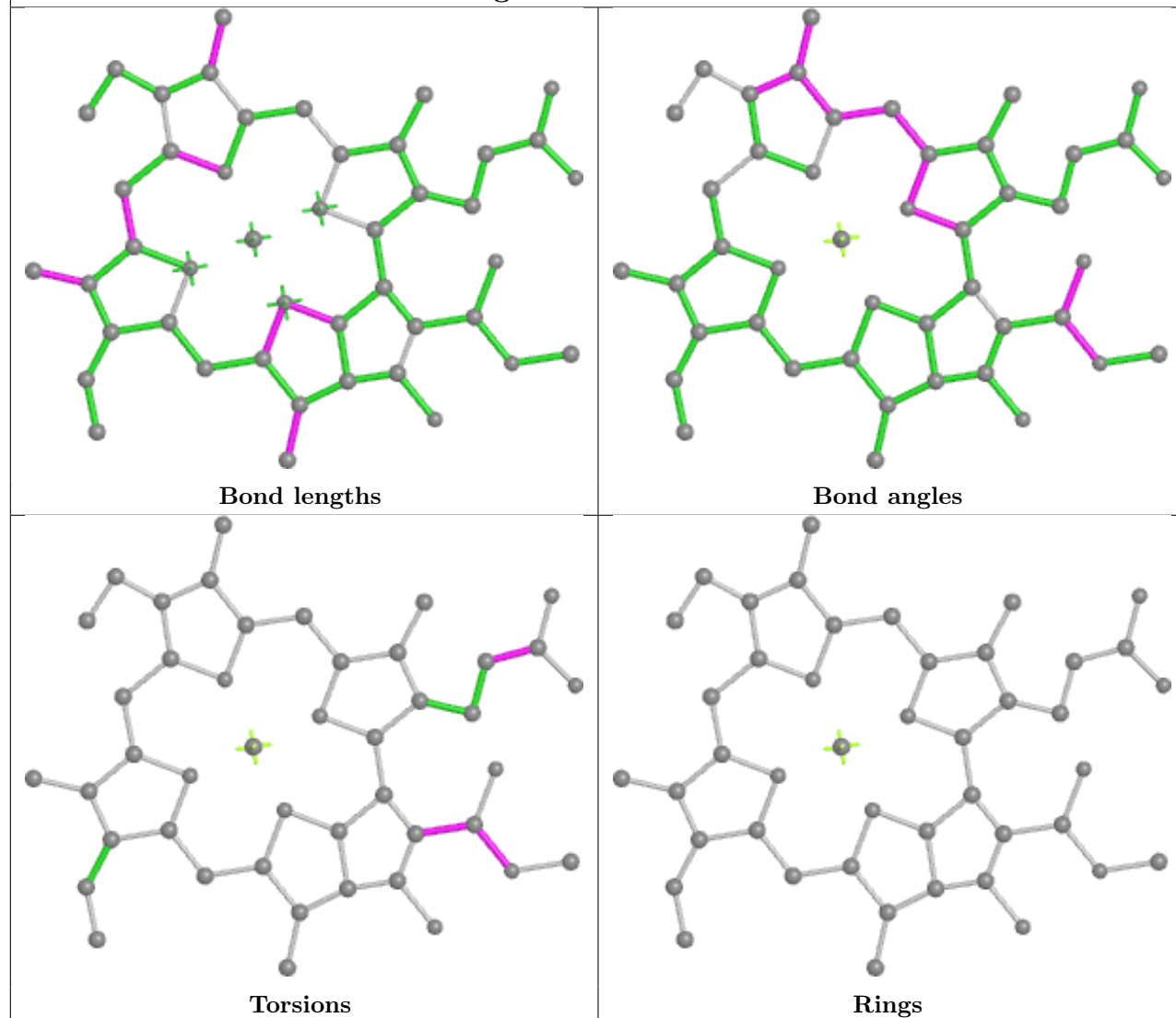




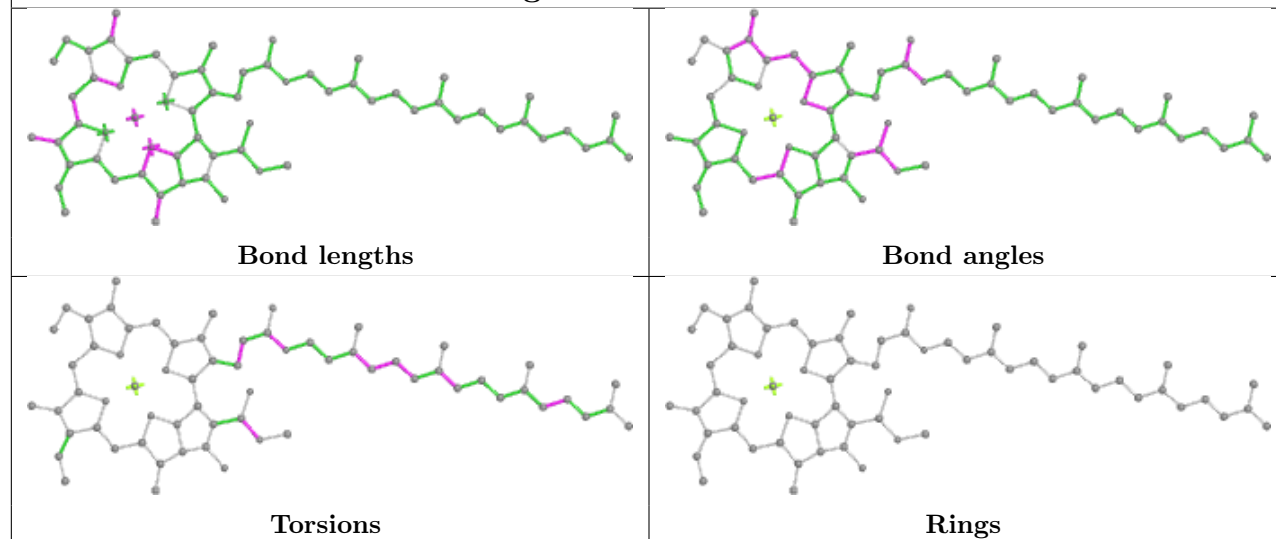
Ligand CLA d 508

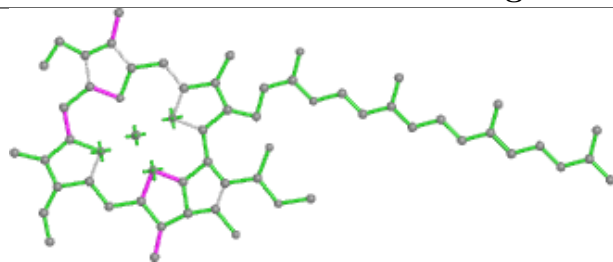


Ligand CLA v 510

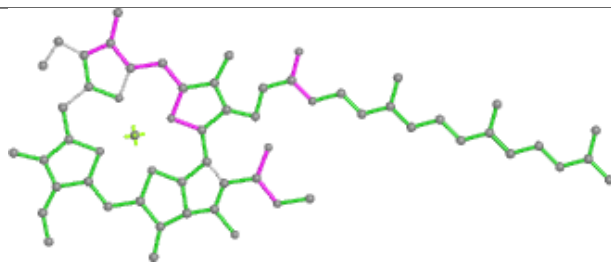


Ligand CLA B 1204

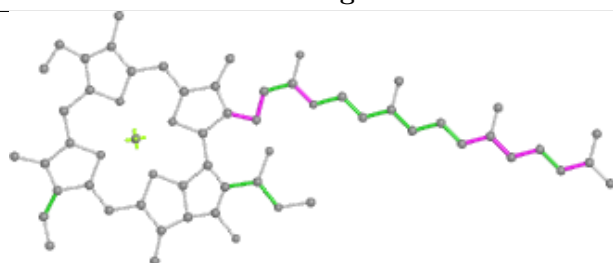


Ligand CLA B 1217

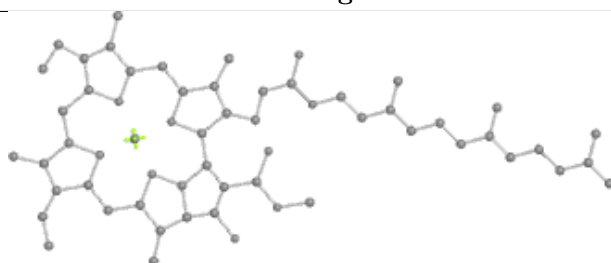
Bond lengths



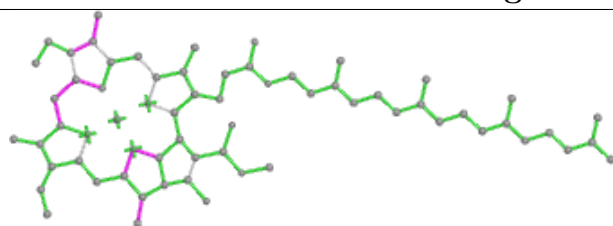
Bond angles



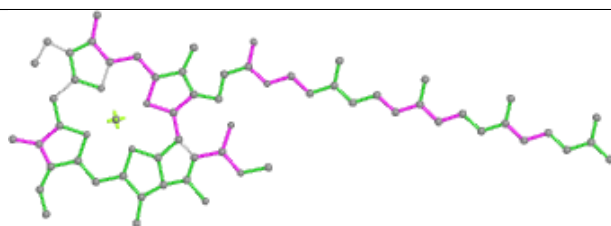
Torsions



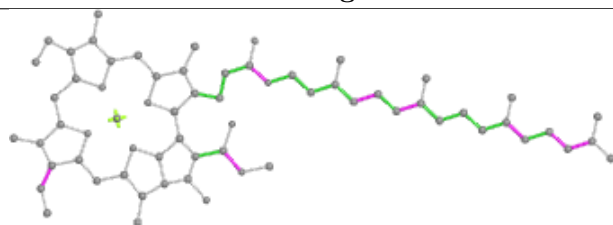
Rings

Ligand CLA H 1239

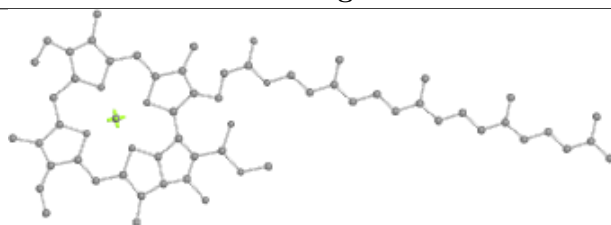
Bond lengths



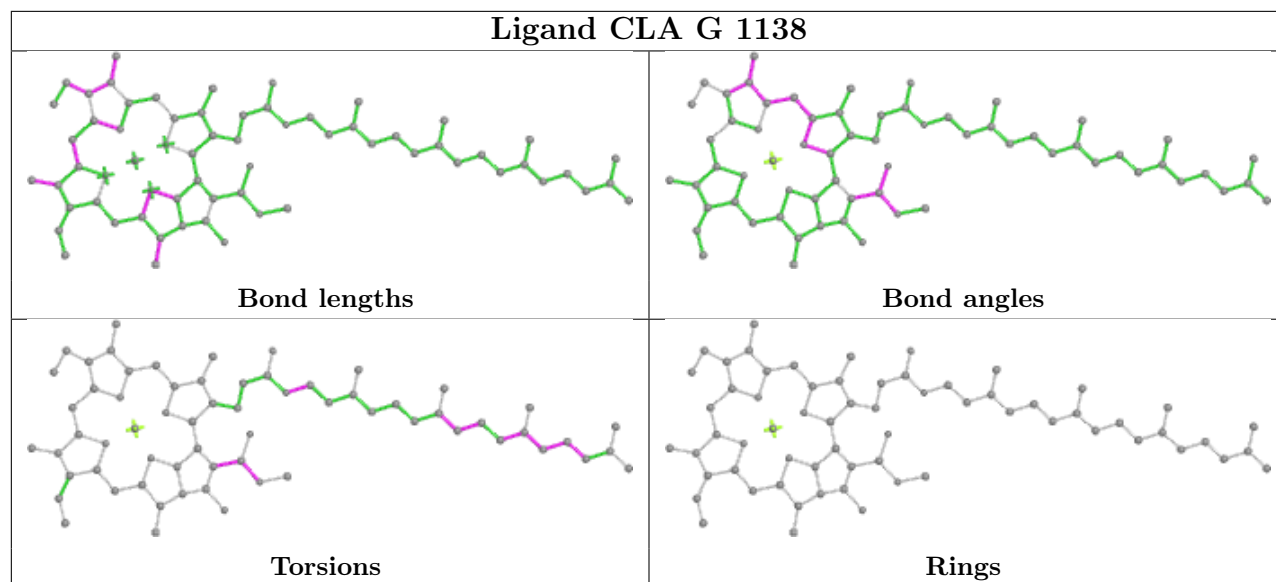
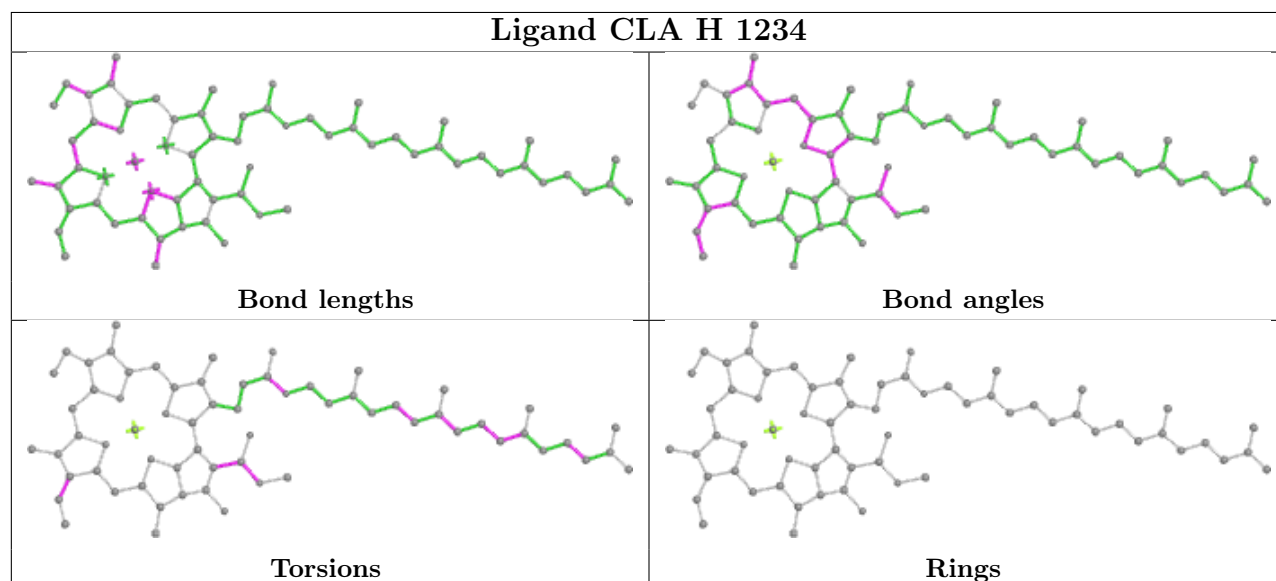
Bond angles



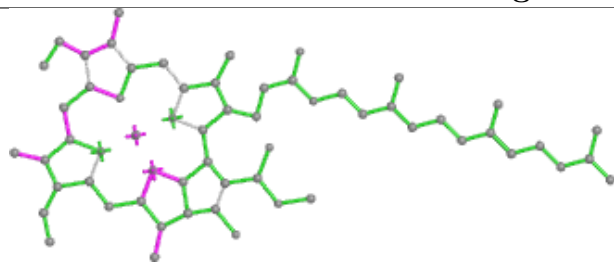
Torsions



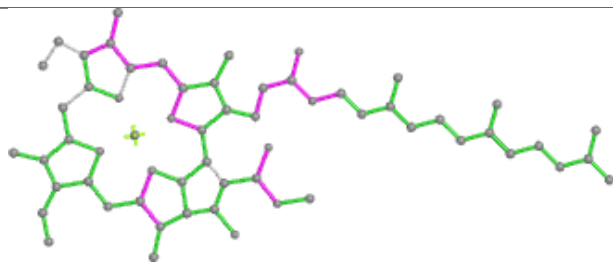
Rings

Ligand CLA G 1138**Ligand CLA H 1234**

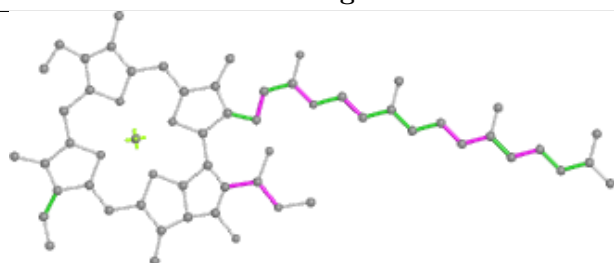
Ligand CLA f 1216



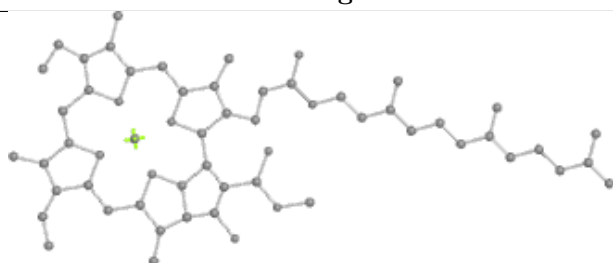
Bond lengths



Bond angles

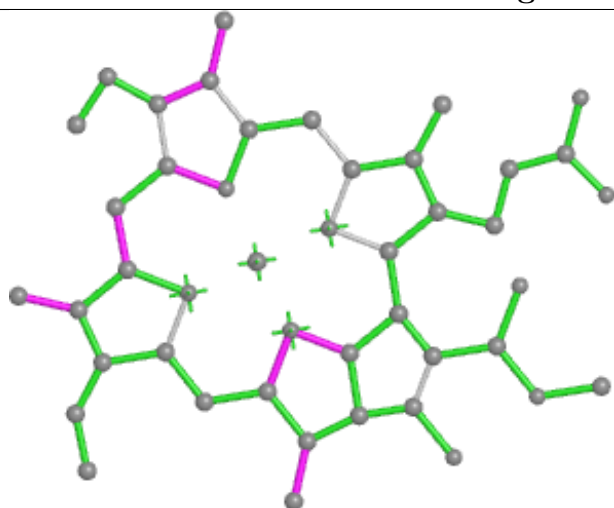


Torsions

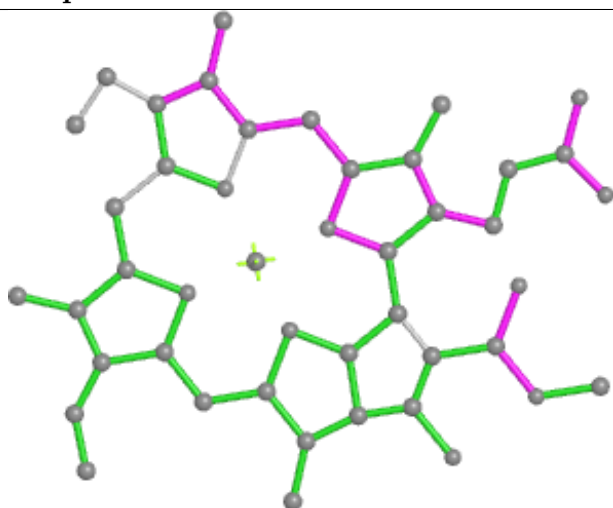


Rings

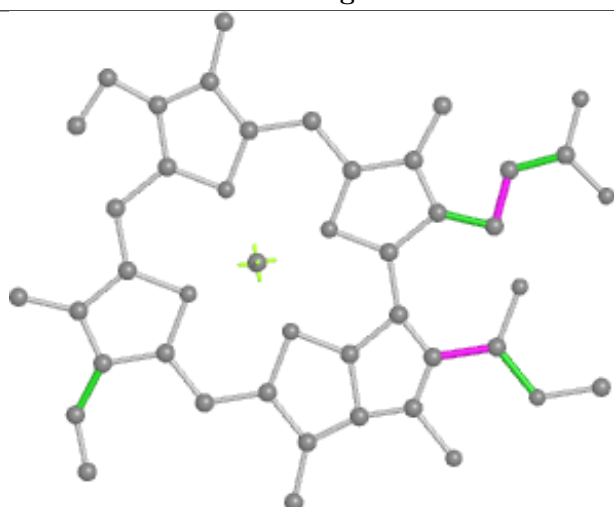
Ligand CLA q 502



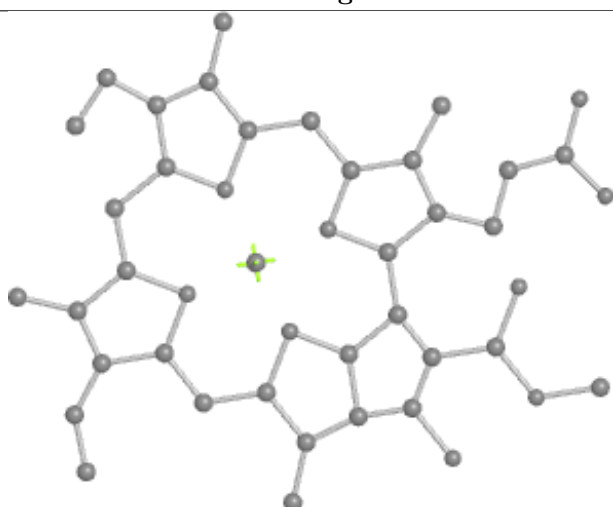
Bond lengths



Bond angles

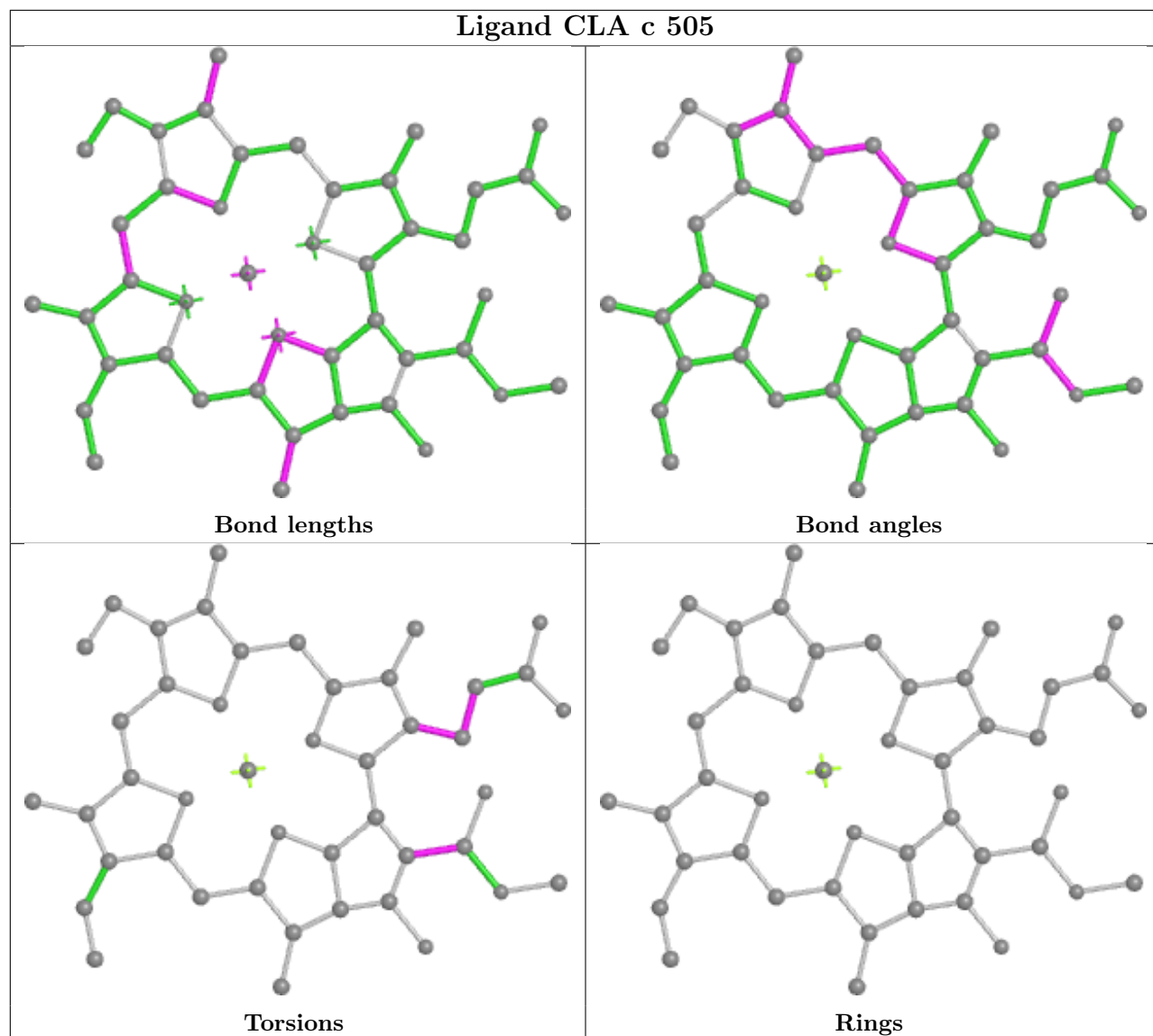


Torsions

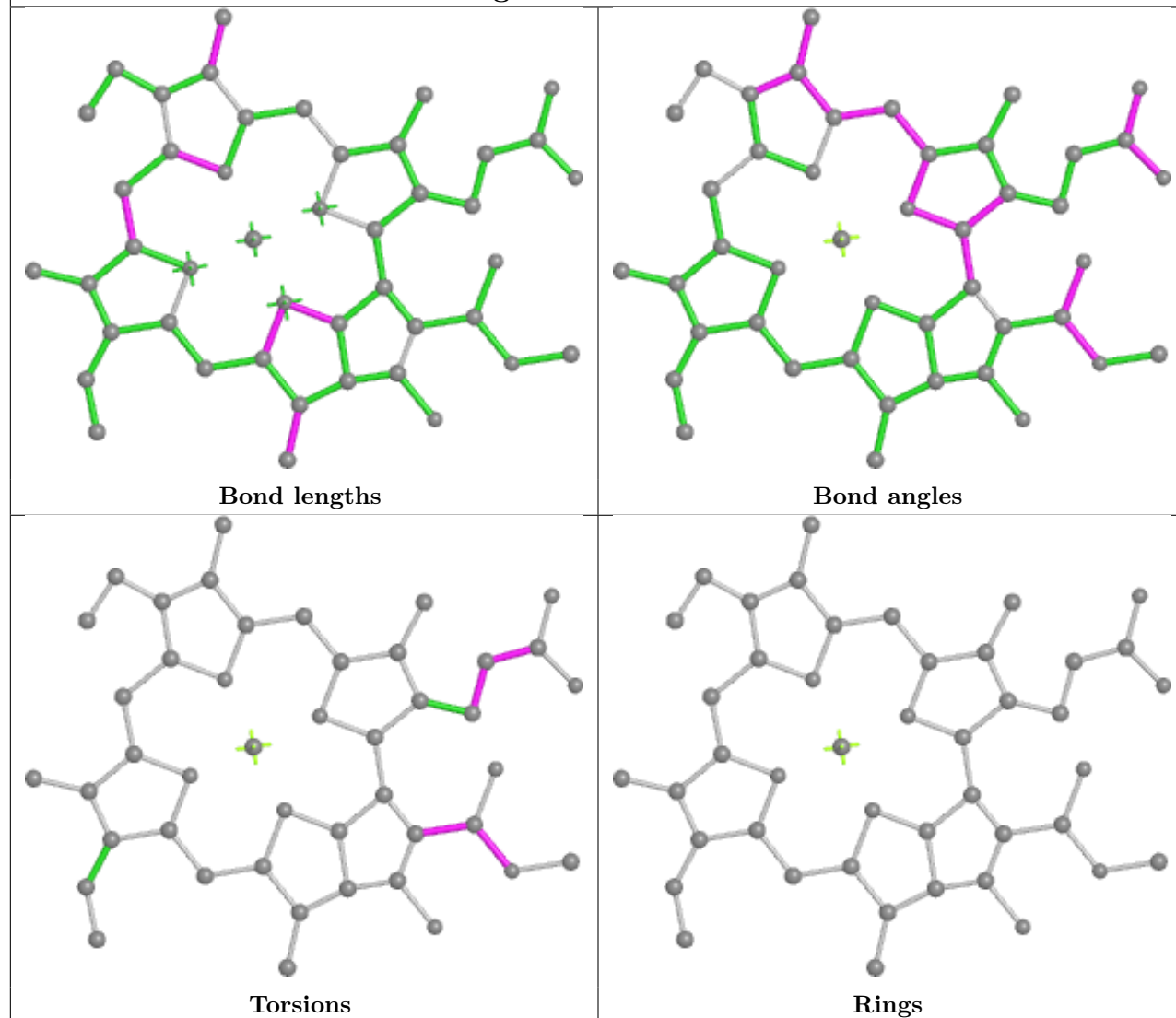


Rings

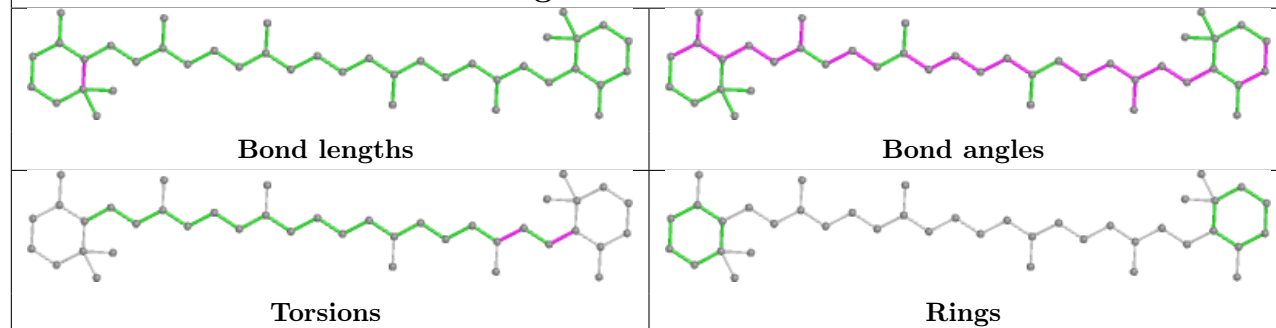
Ligand CLA c 505

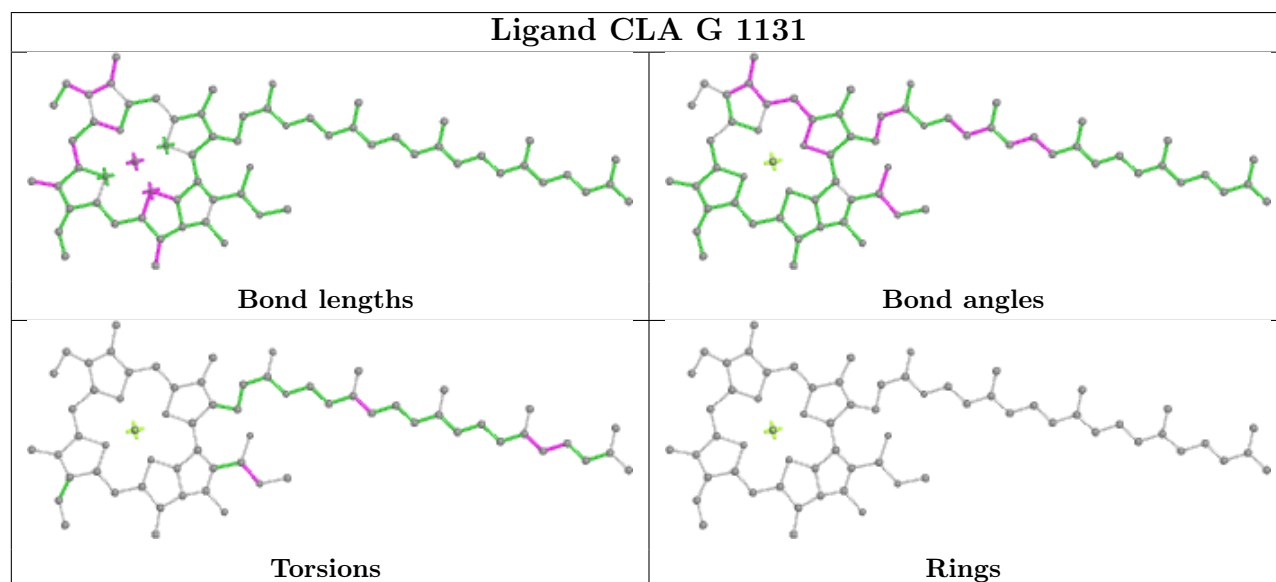
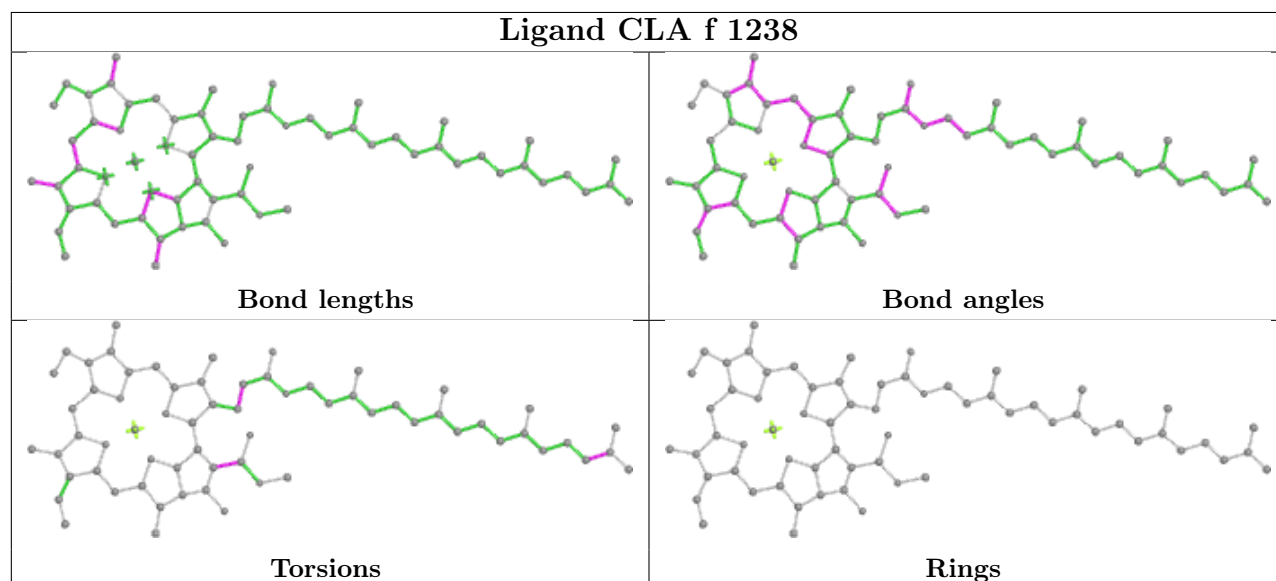
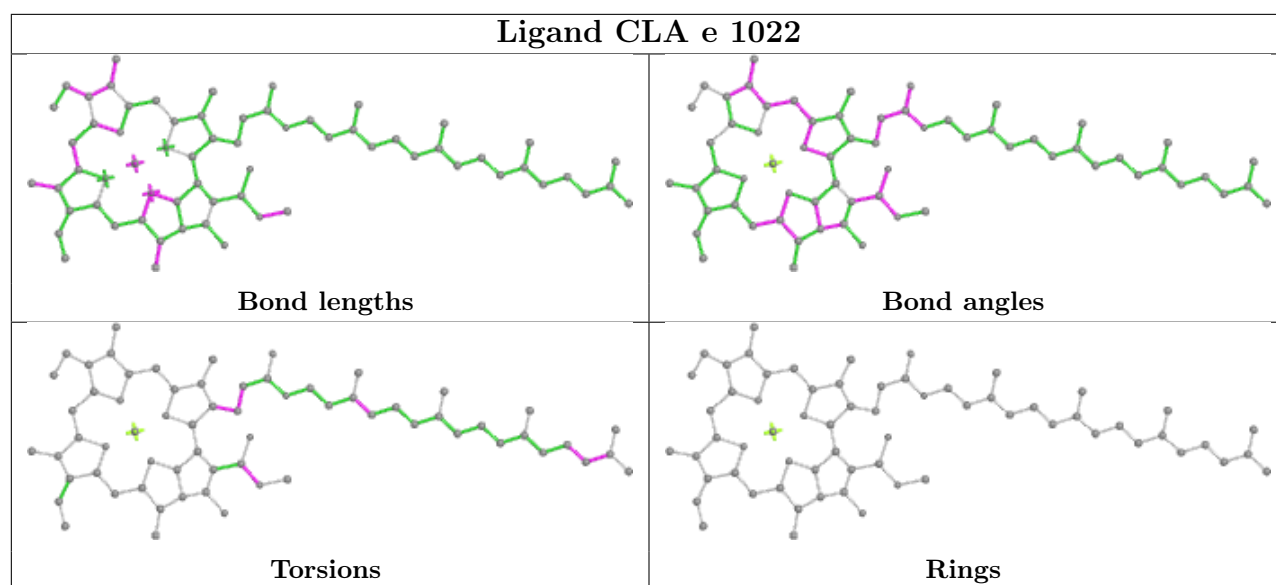


Ligand CLA u 507

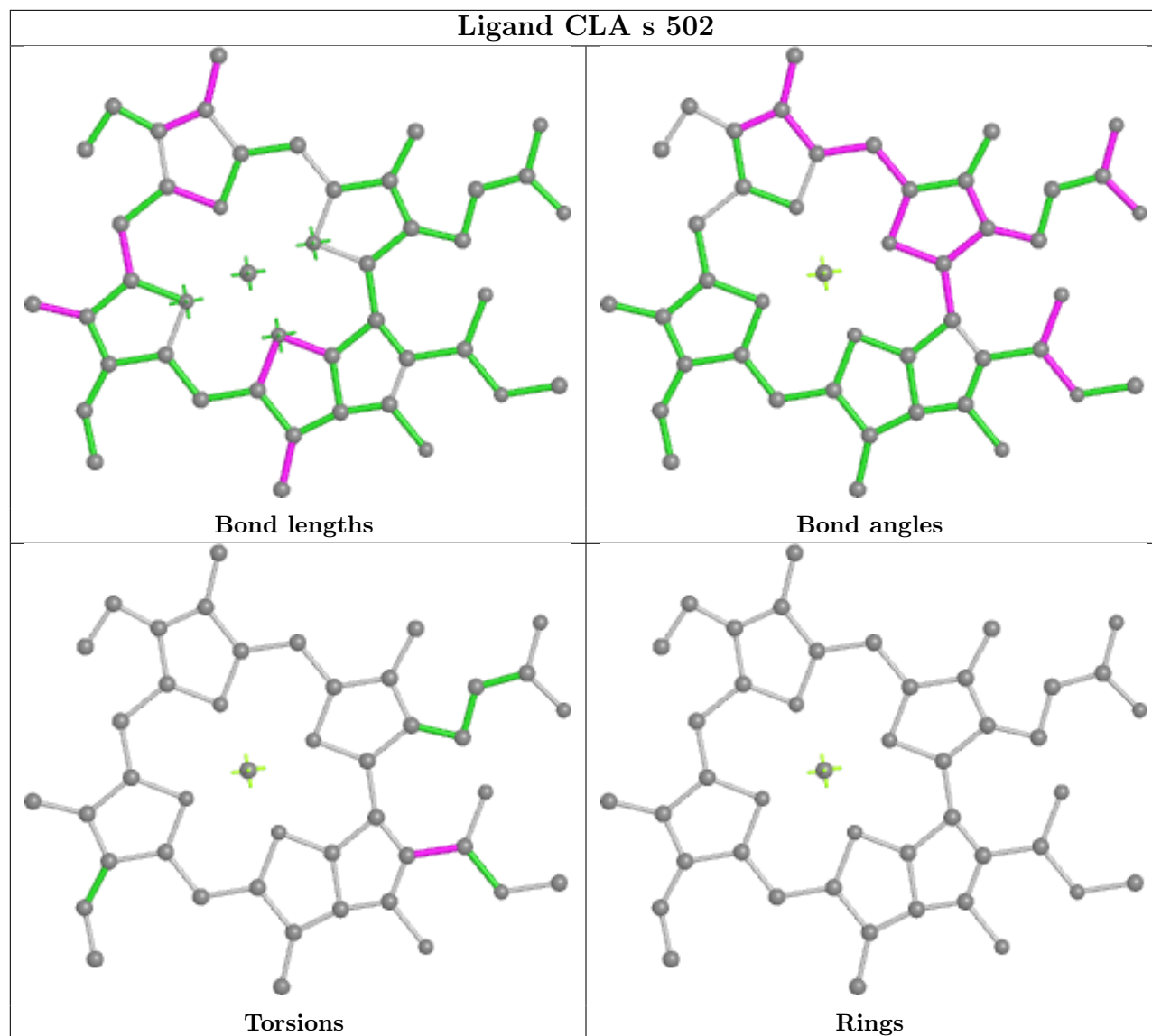


Ligand BCR 5 523

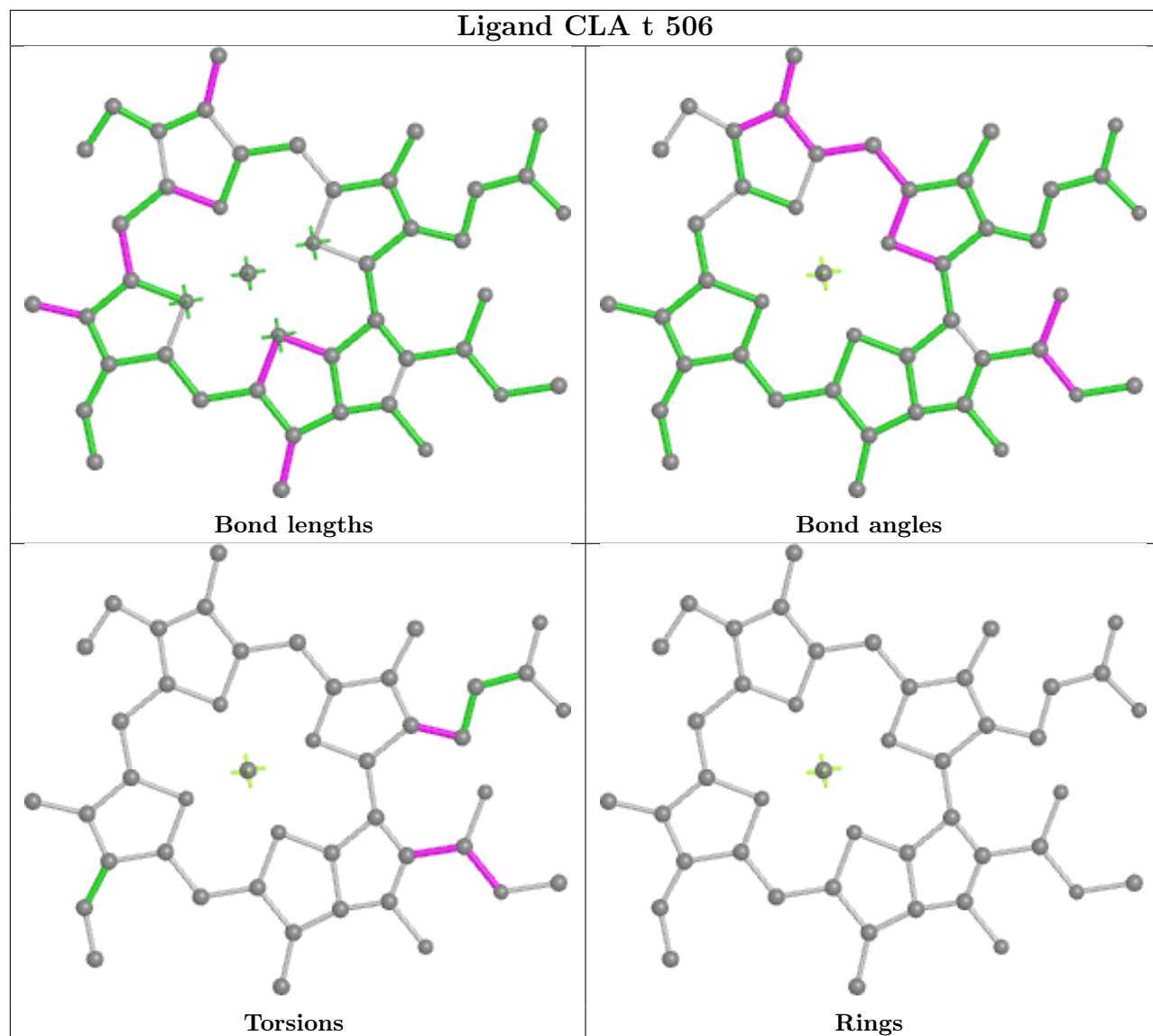


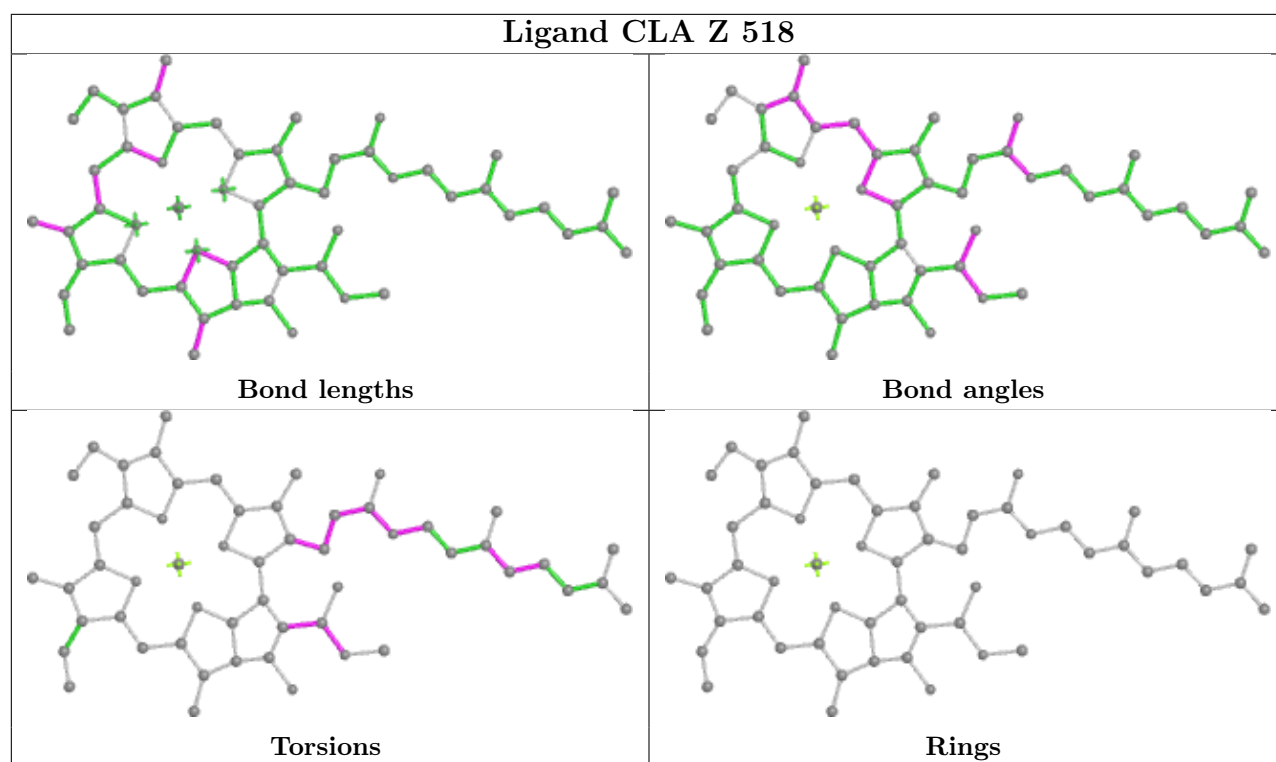


Ligand CLA s 502

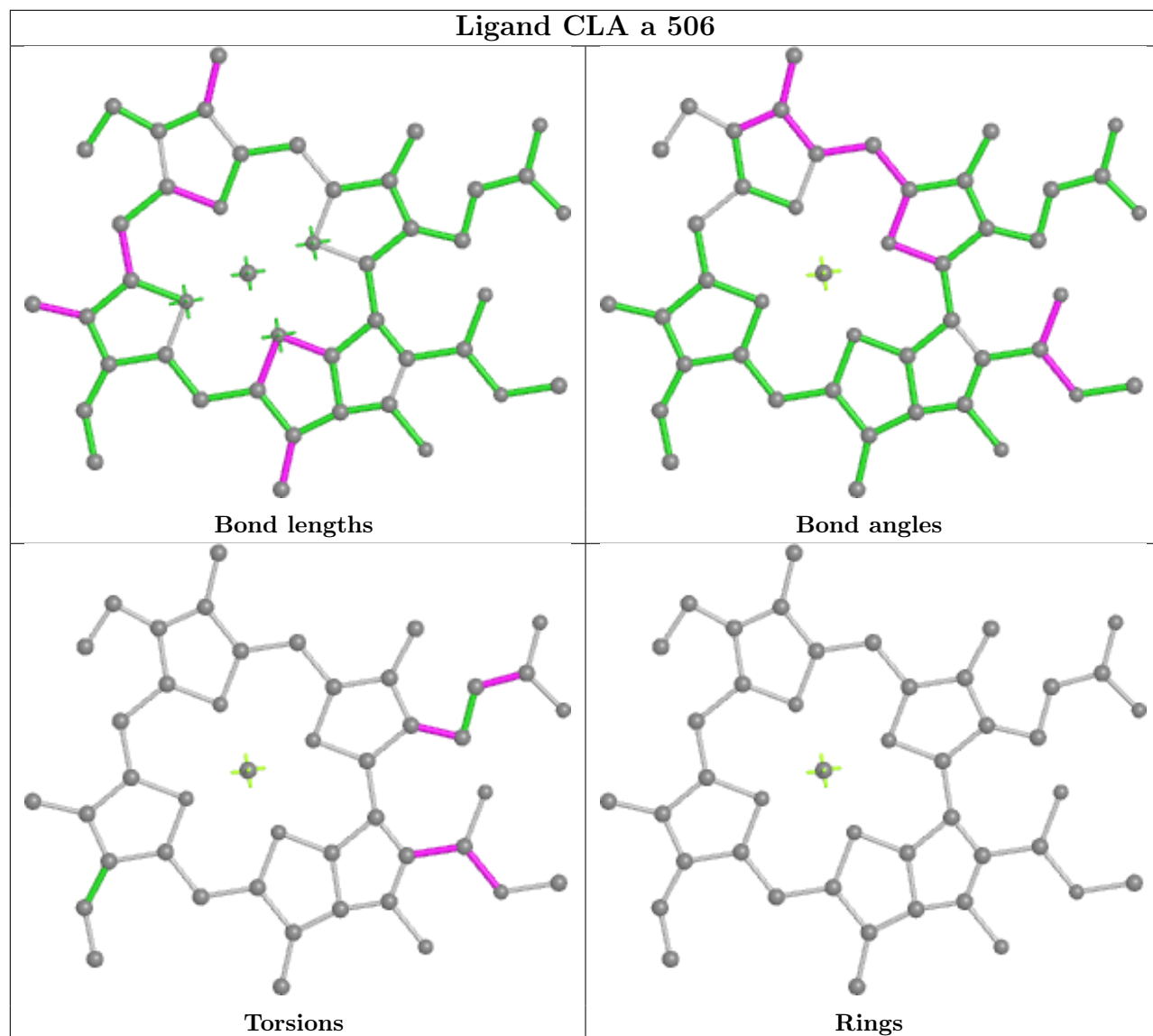


Ligand CLA t 506

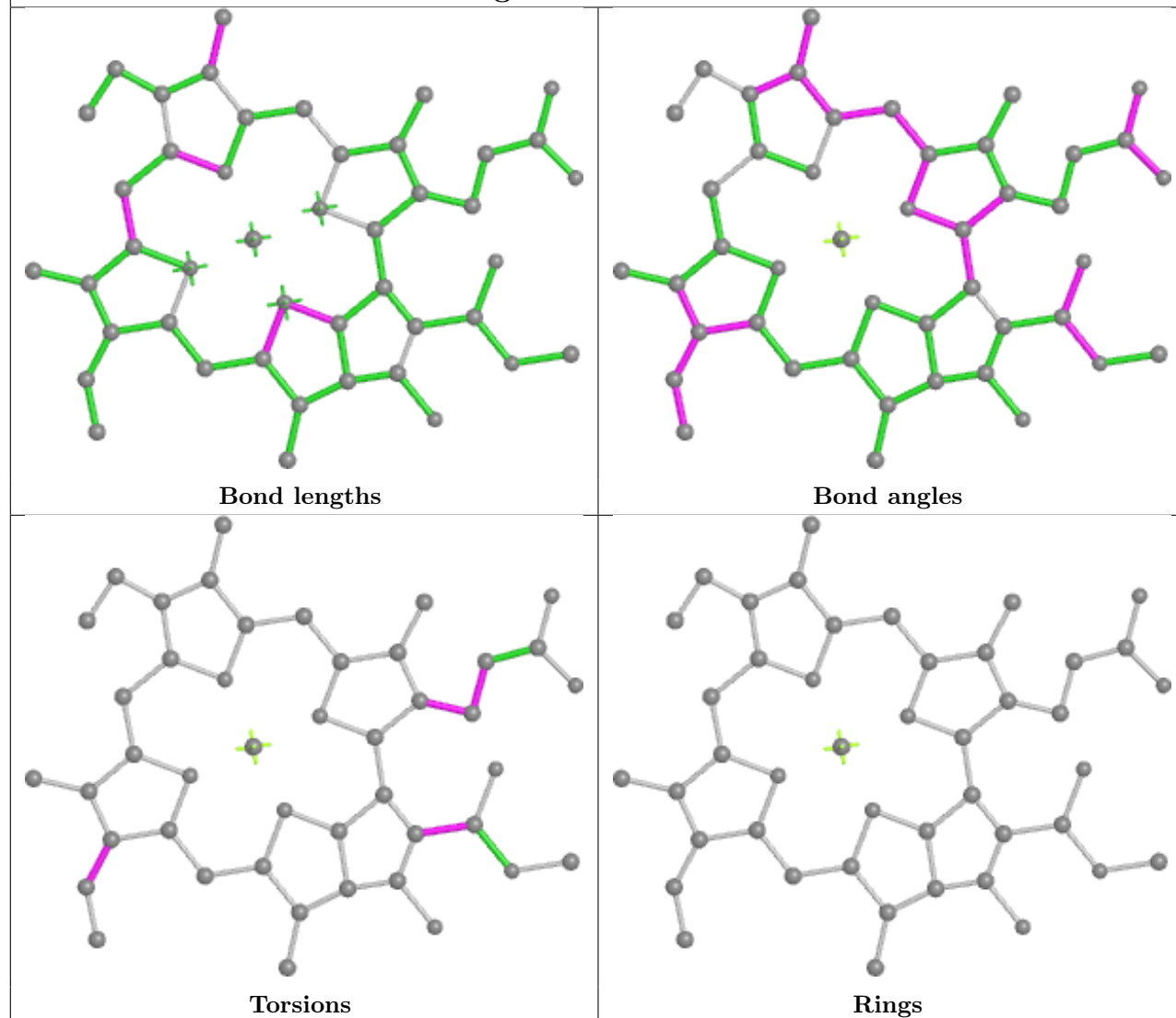




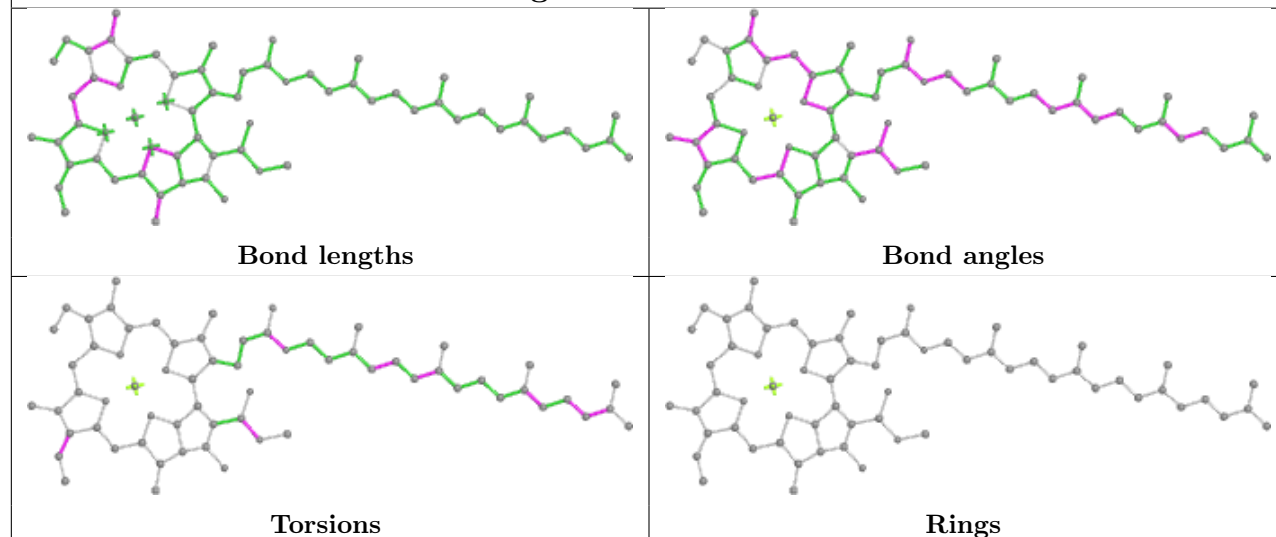
Ligand CLA a 506



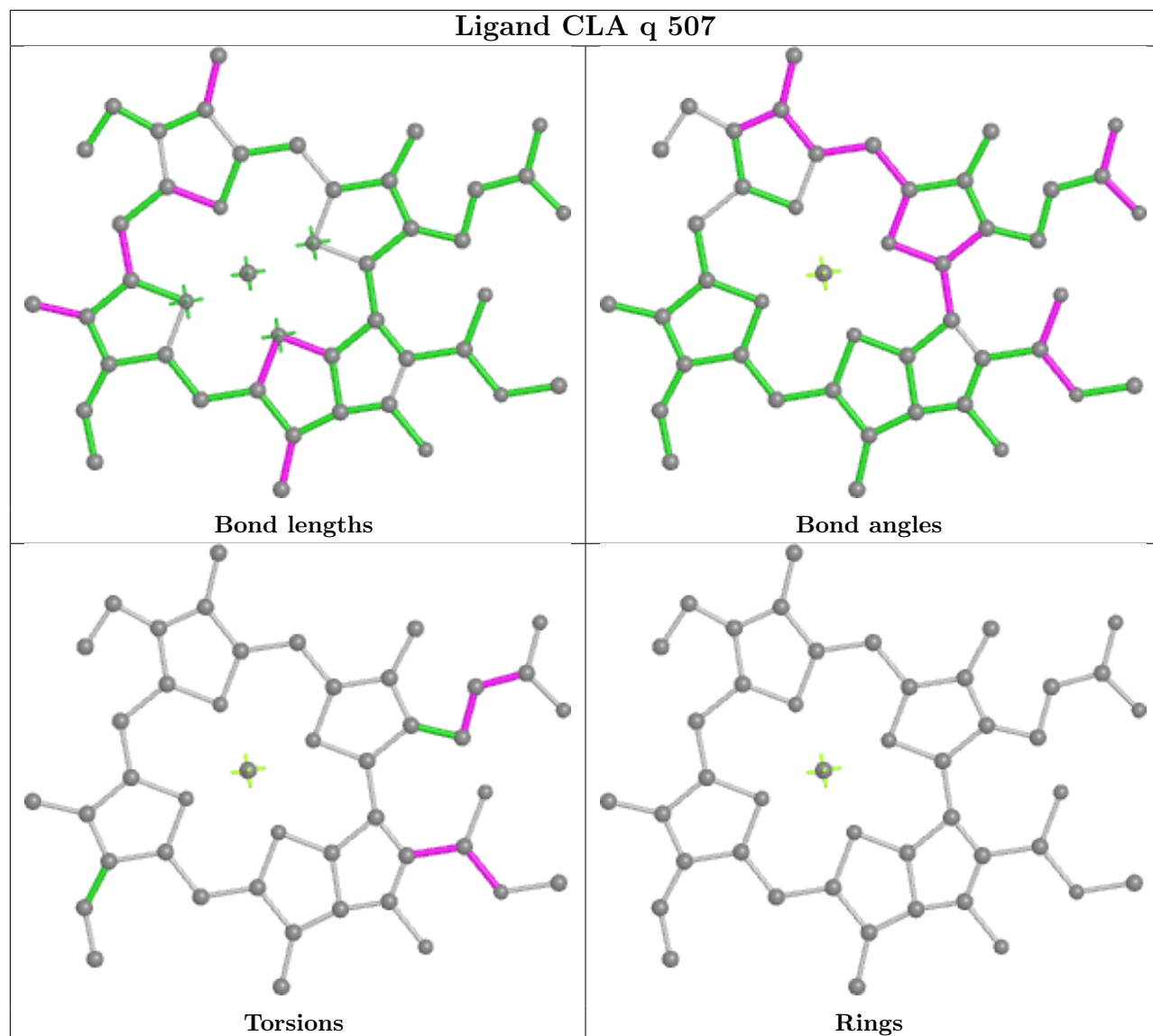
Ligand CLA a 516



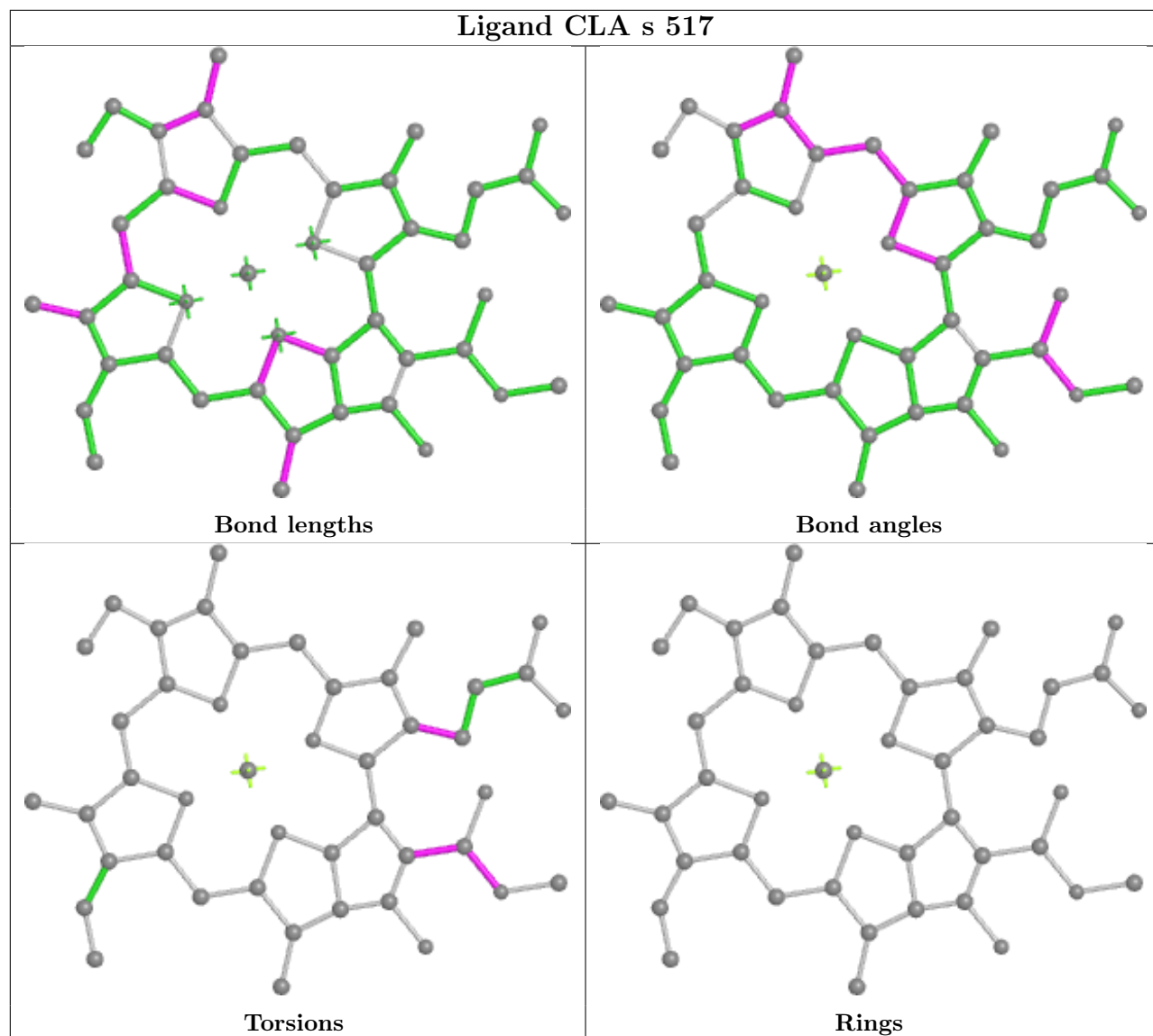
Ligand CLA f 1239



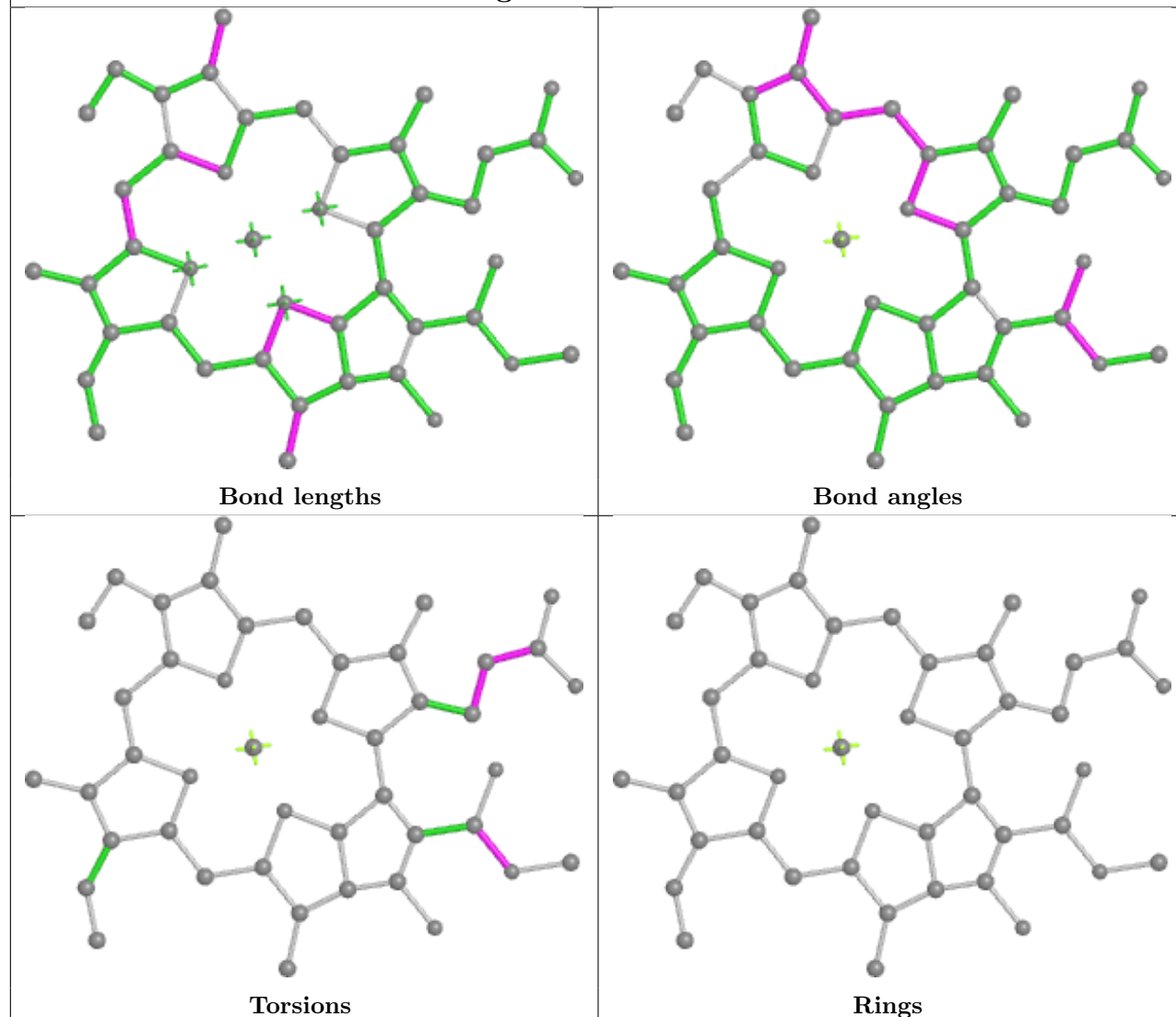
Ligand CLA q 507



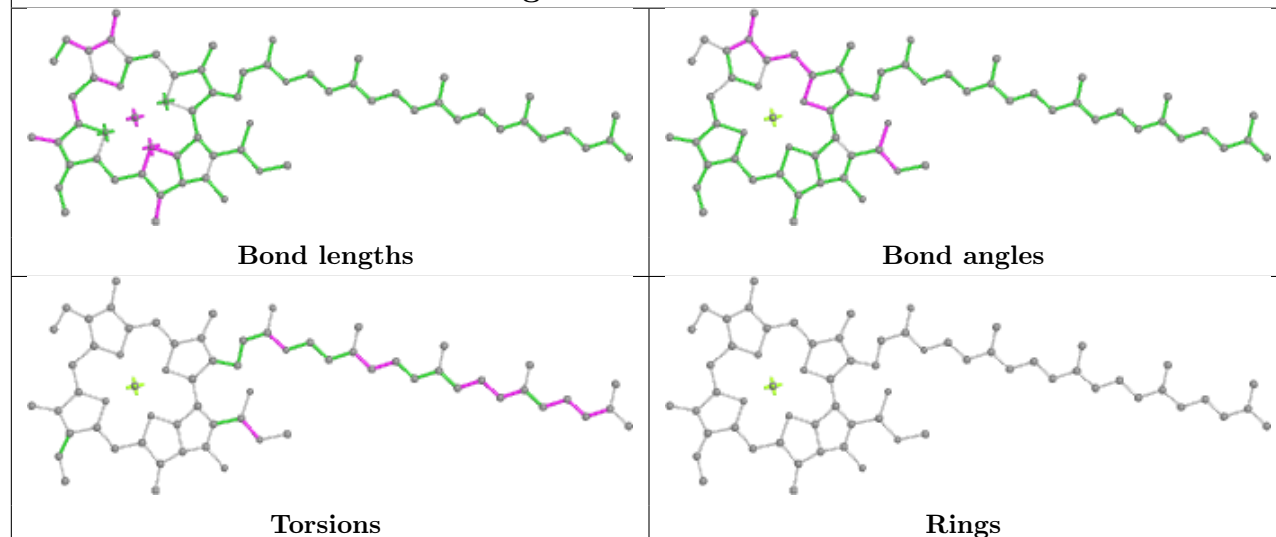
Ligand CLA s 517



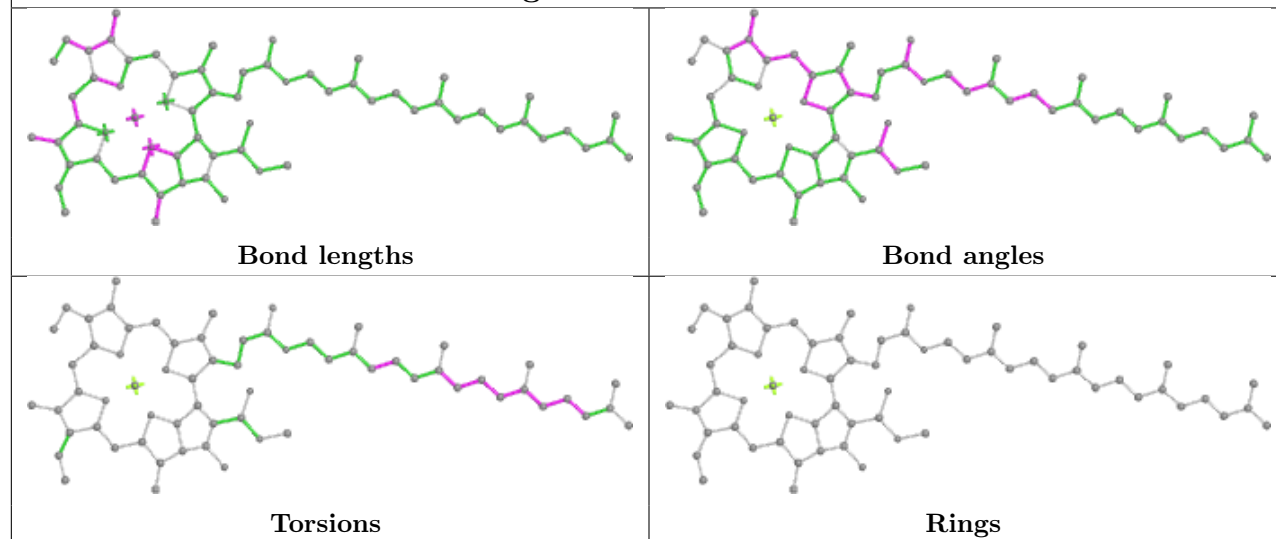
Ligand CLA t 513



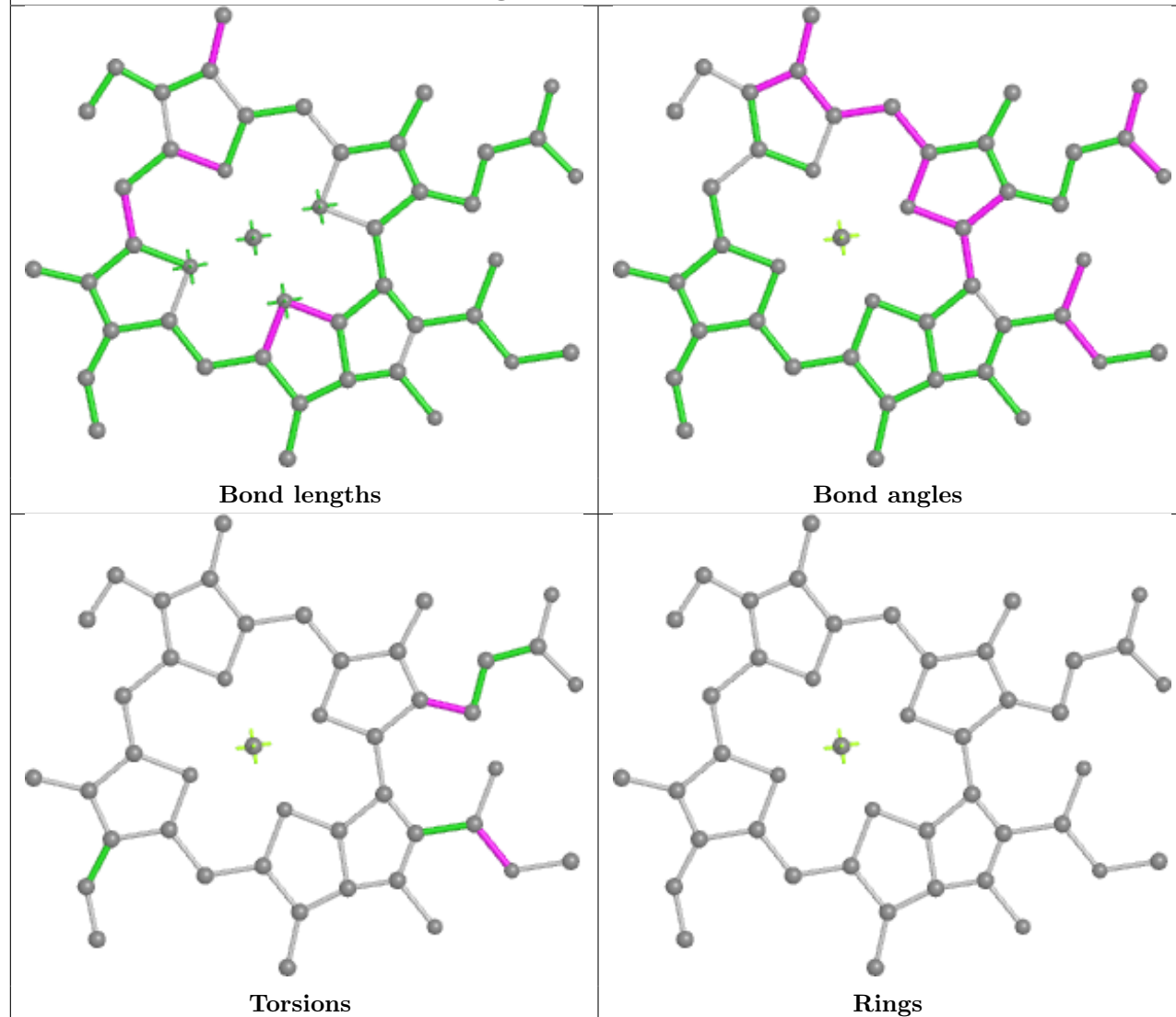
Ligand CLA A 1133

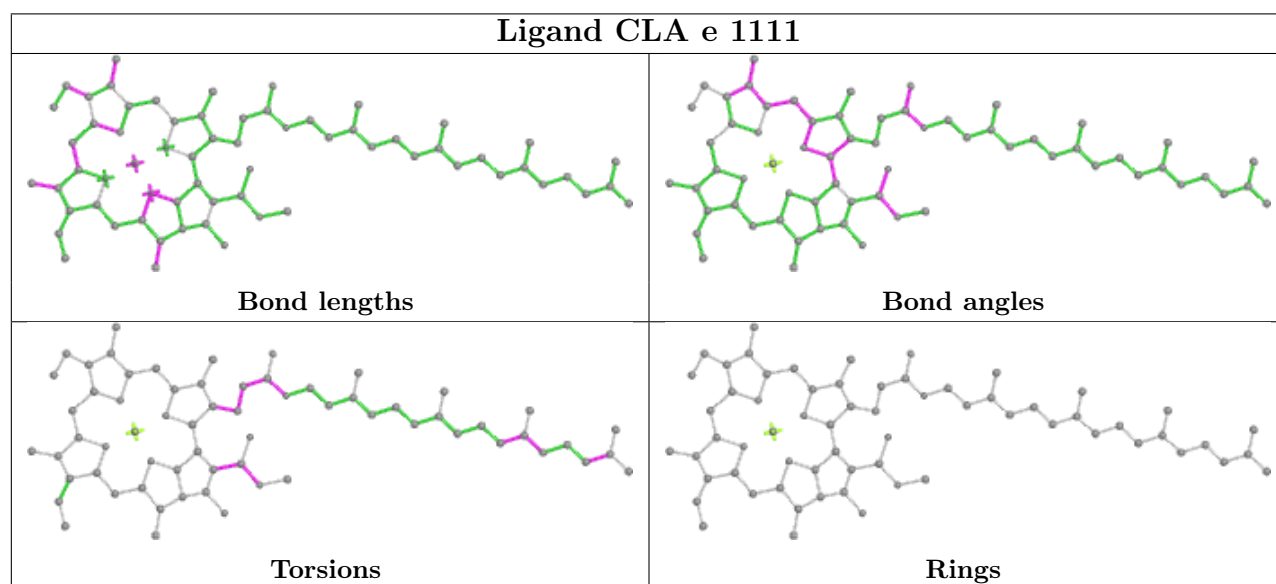
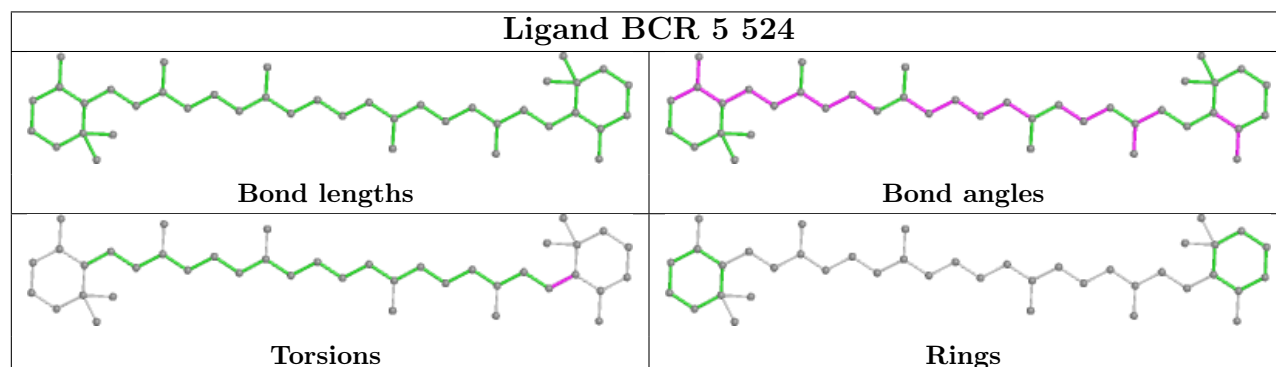
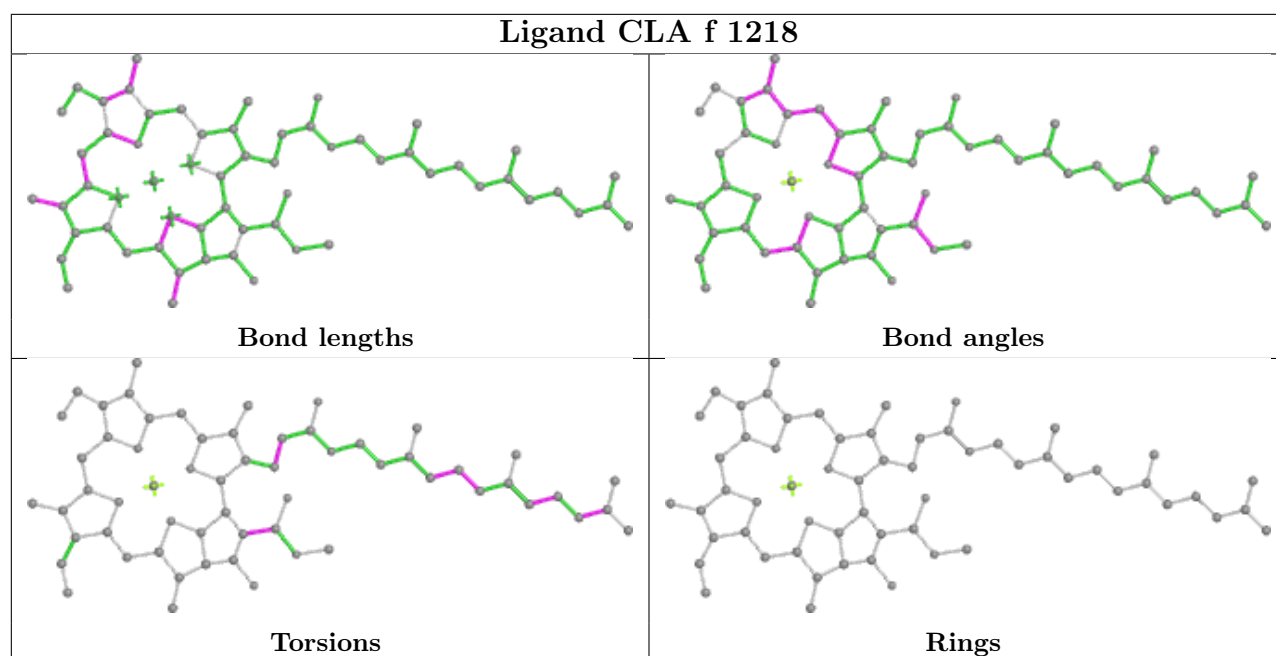


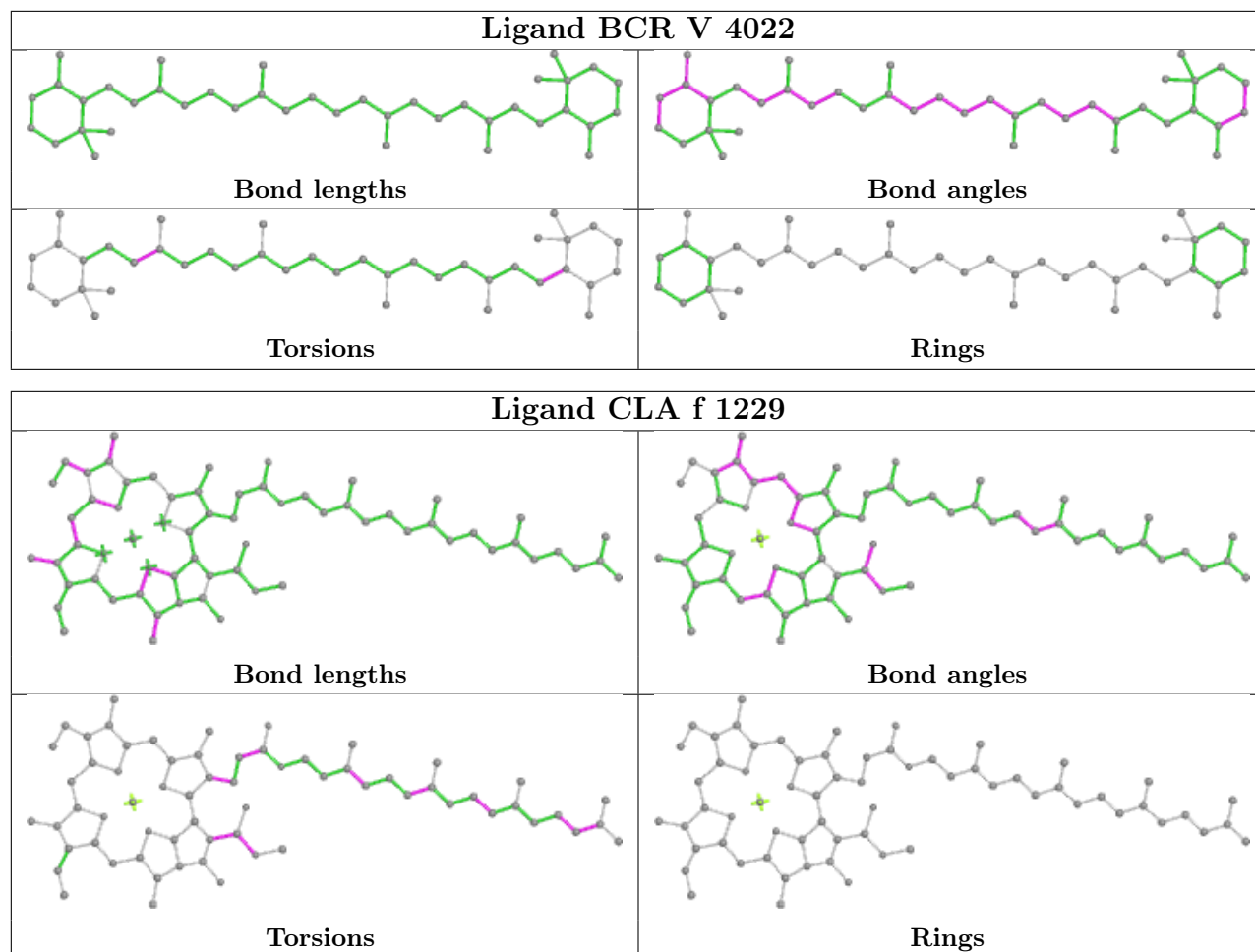
Ligand CLA A 1136



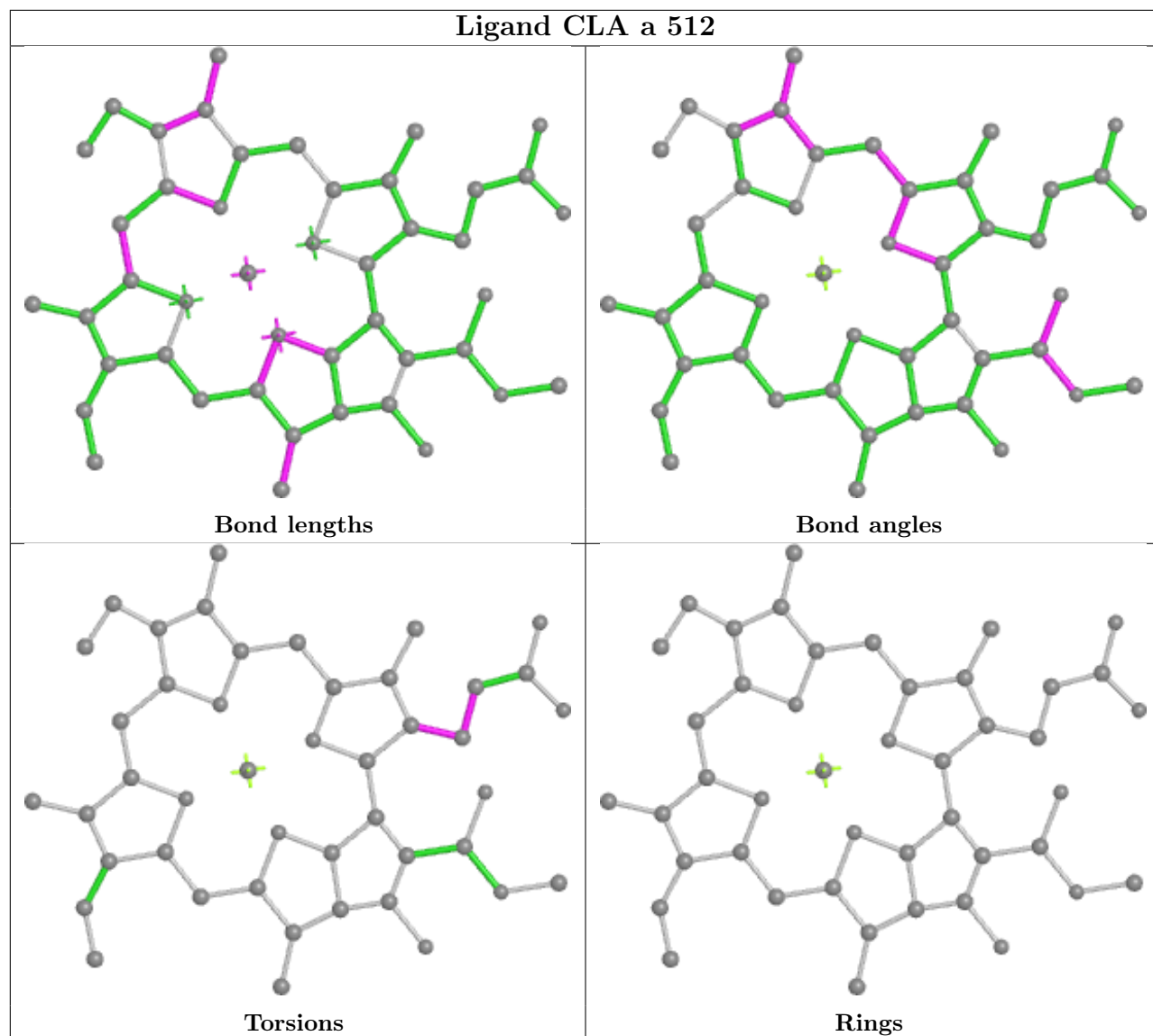
Ligand CLA u 511



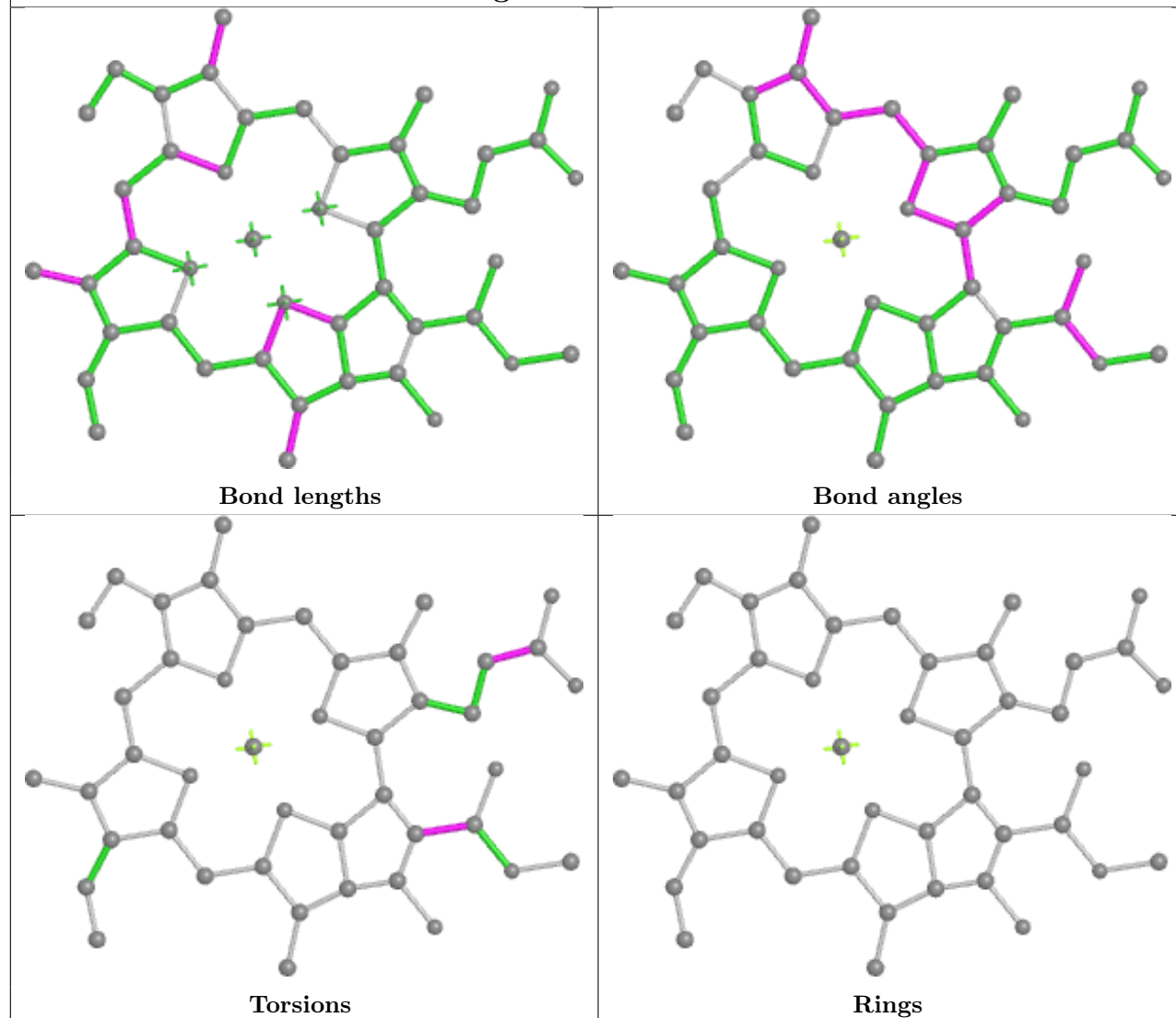




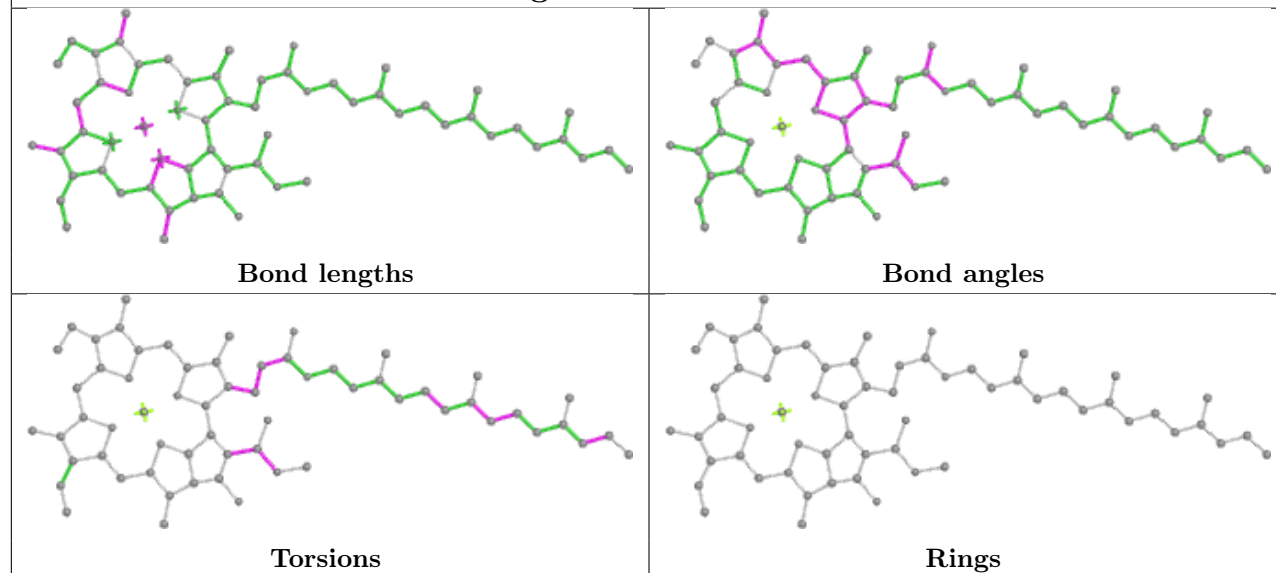
Ligand CLA a 512

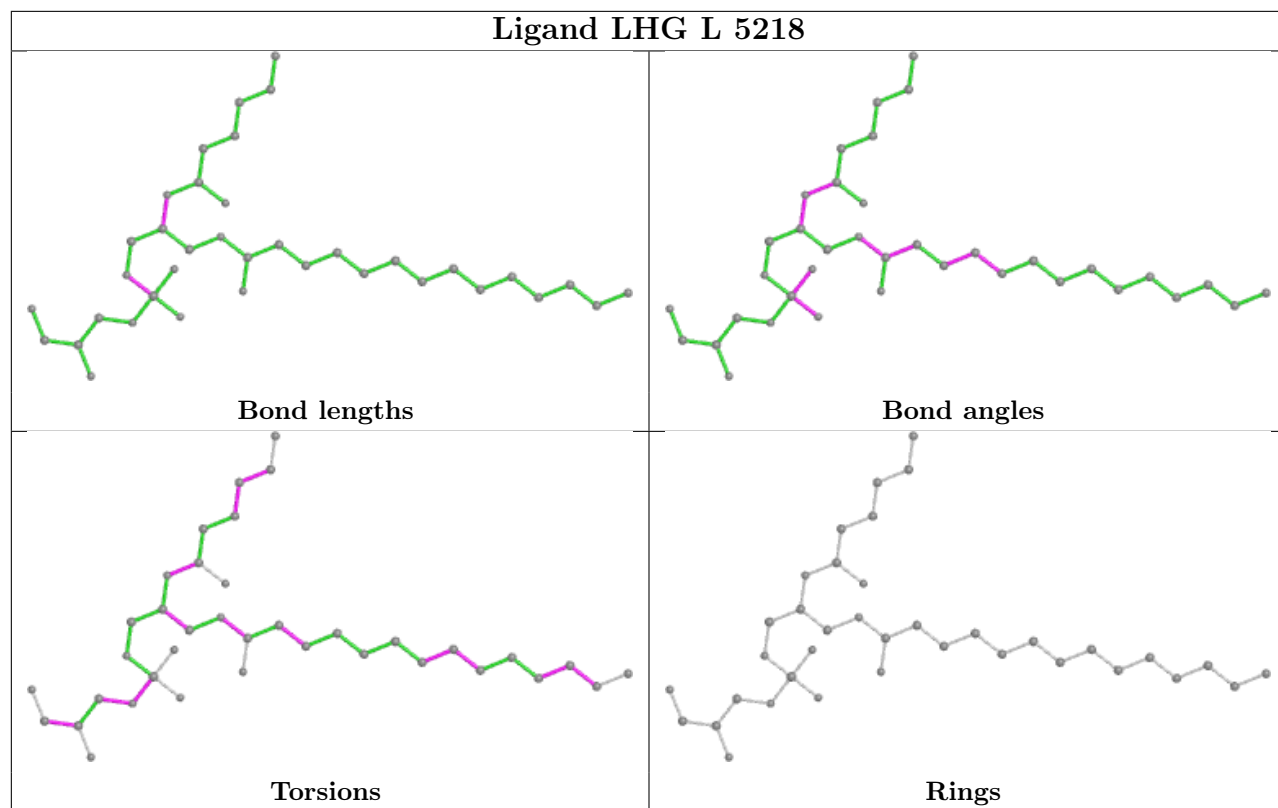


Ligand CLA d 504

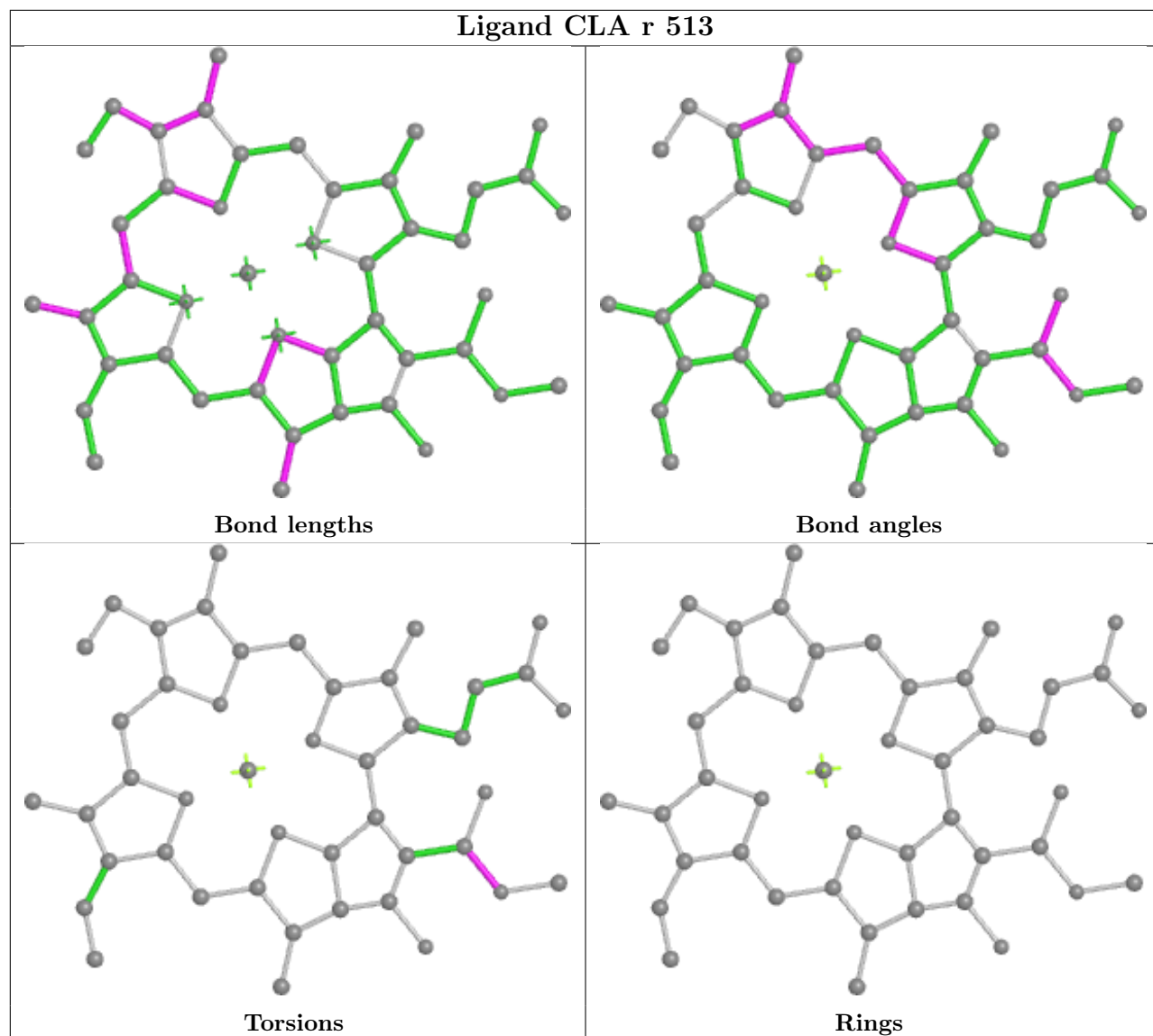


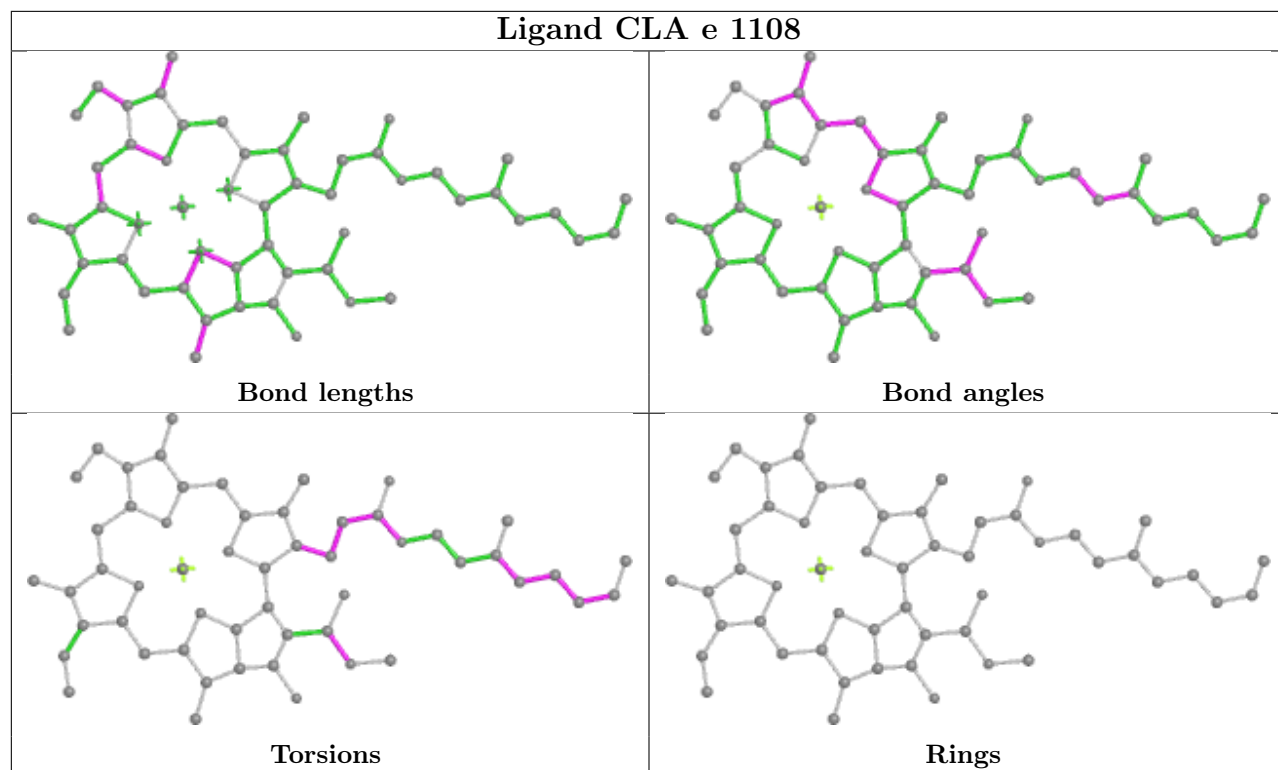
Ligand CLA f 1221



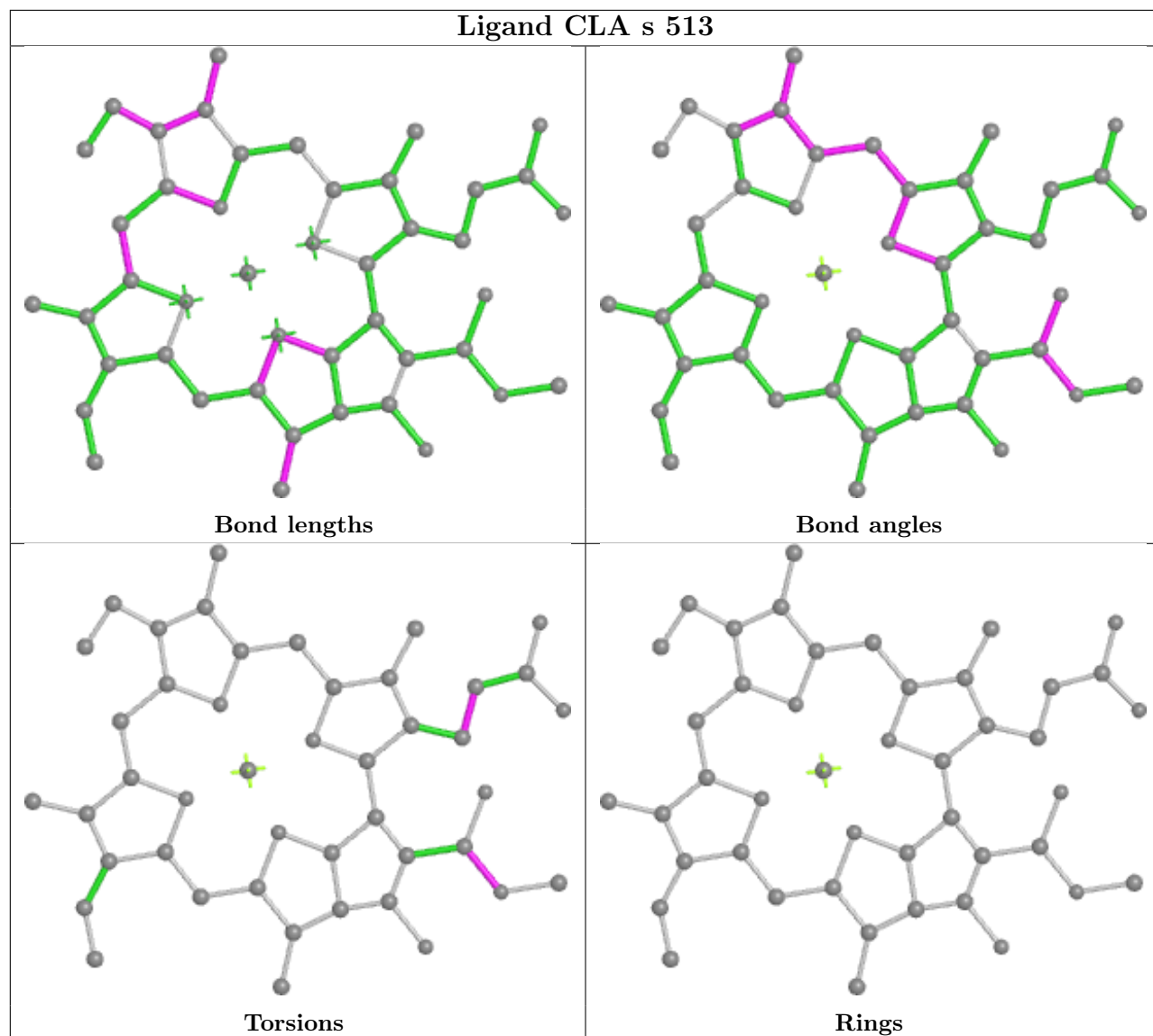


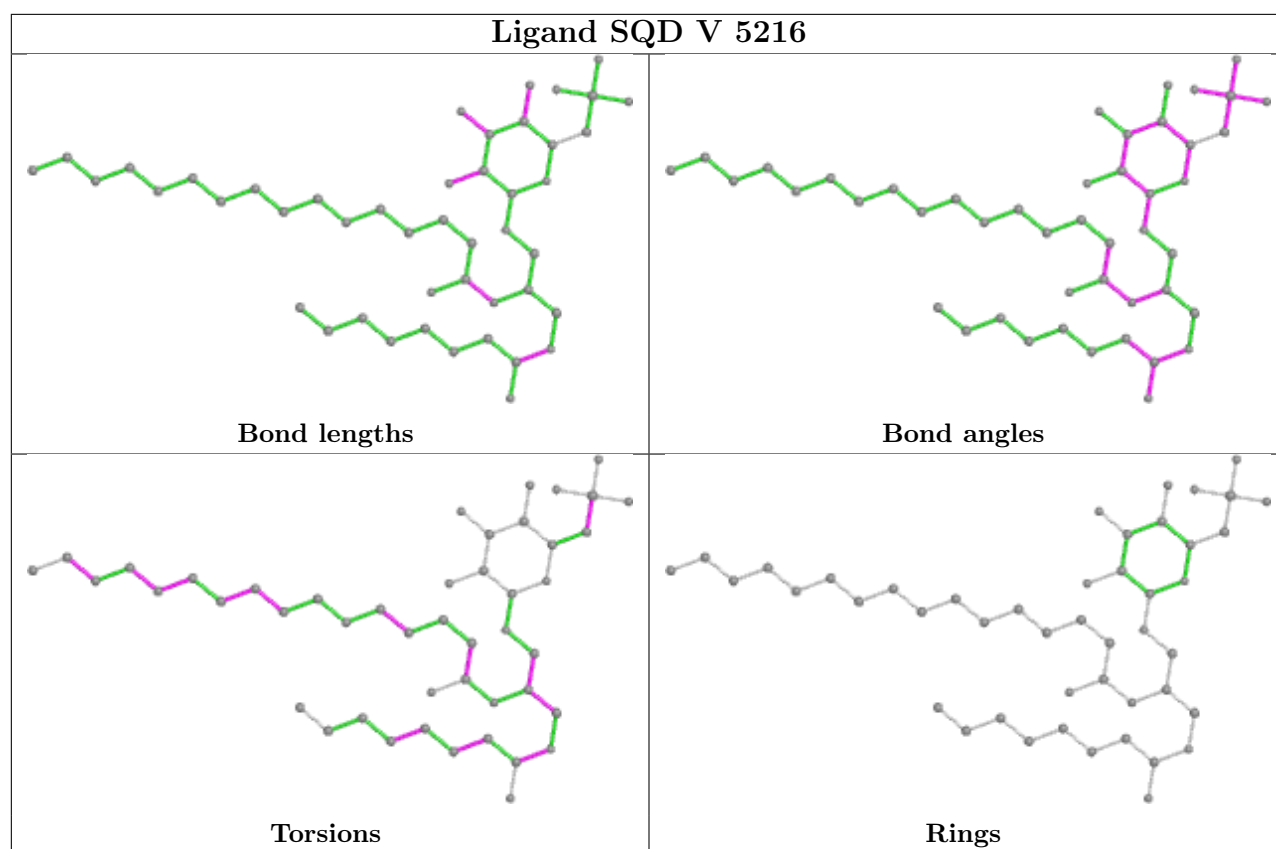
Ligand CLA r 513



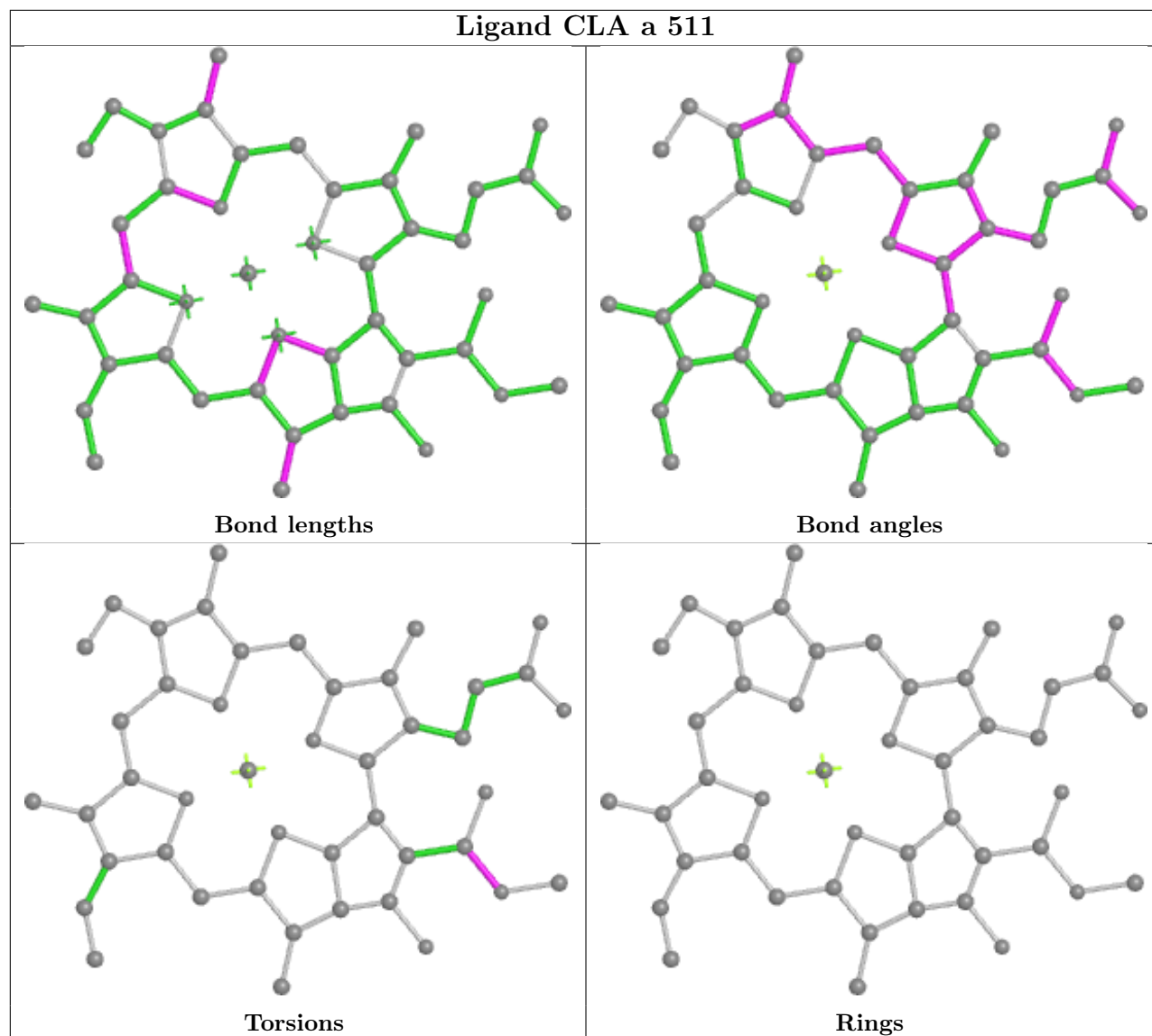


Ligand CLA s 513

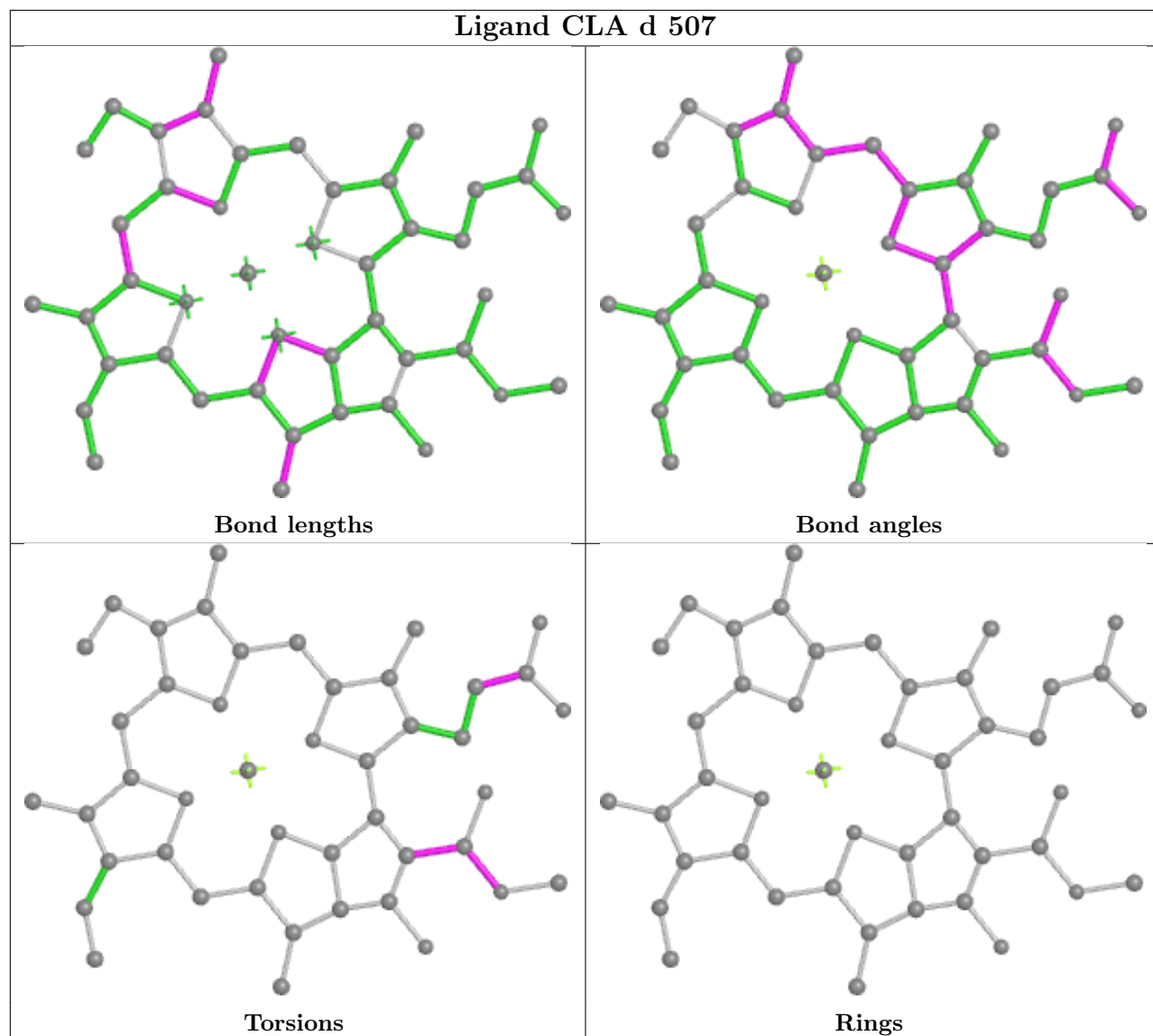




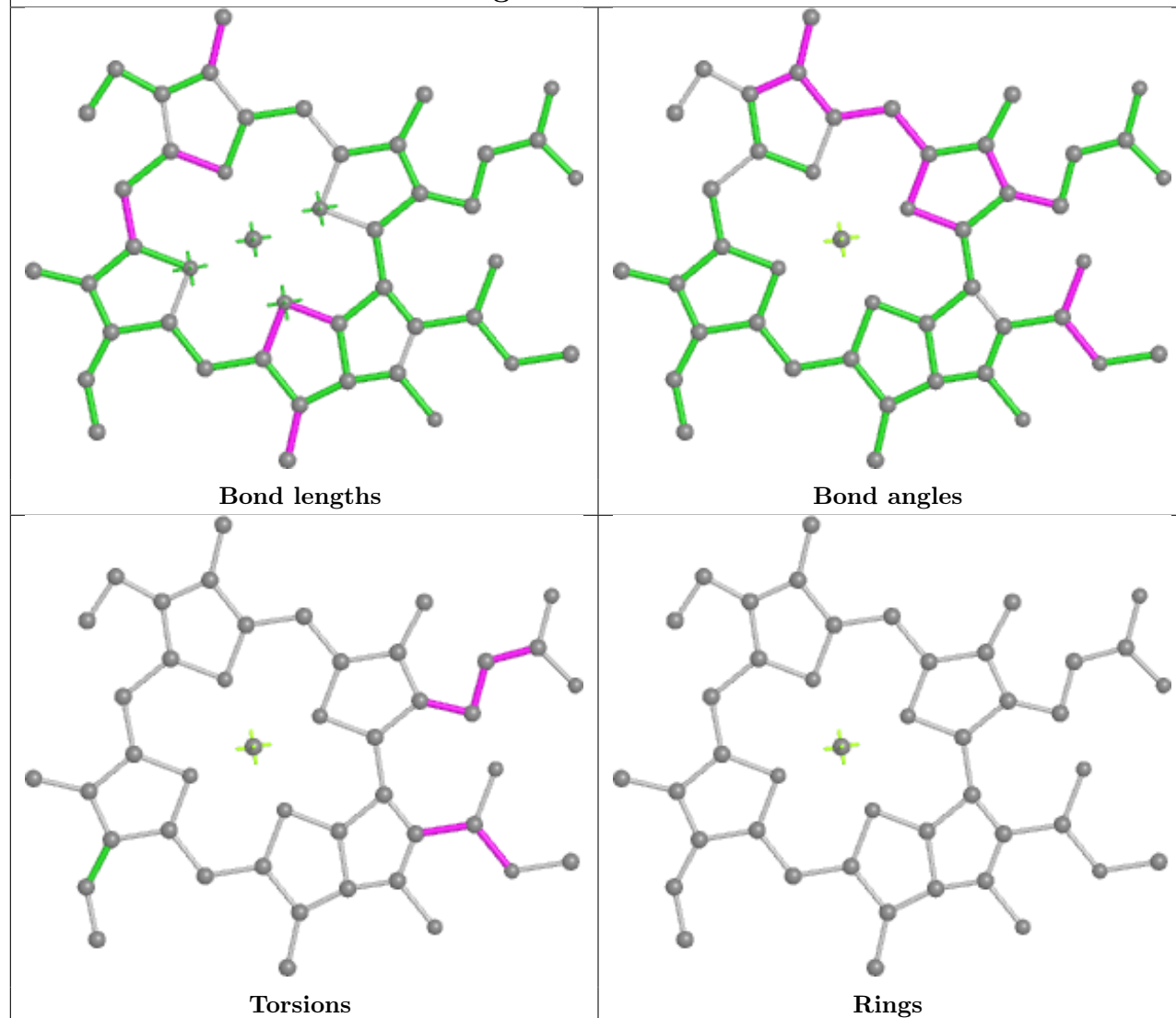
Ligand CLA a 511



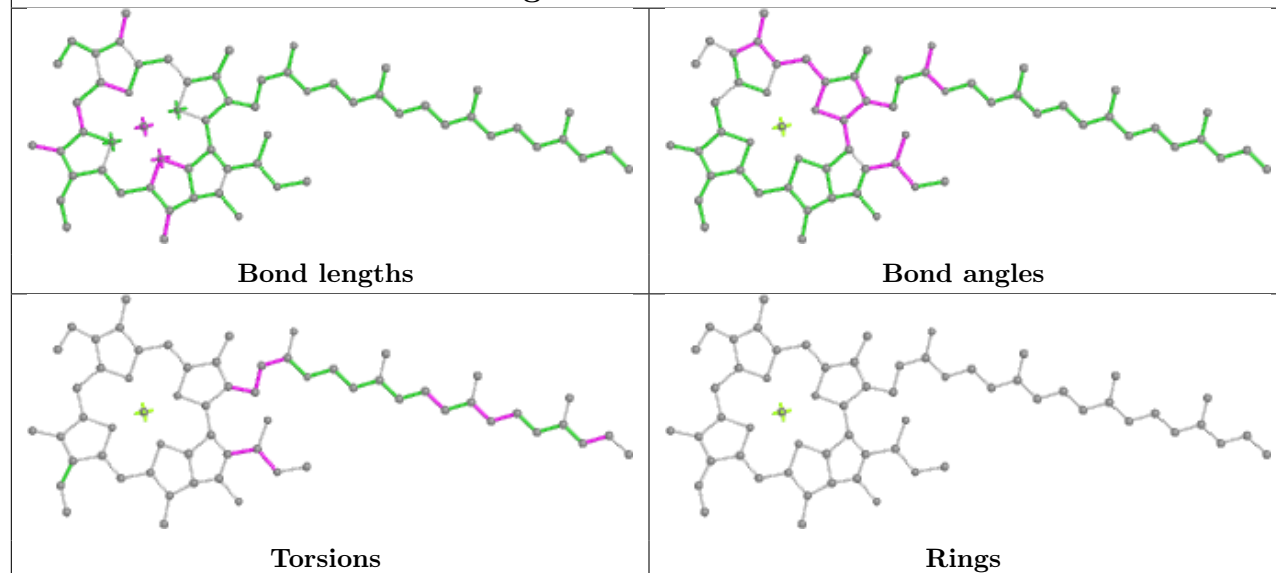
Ligand CLA d 507

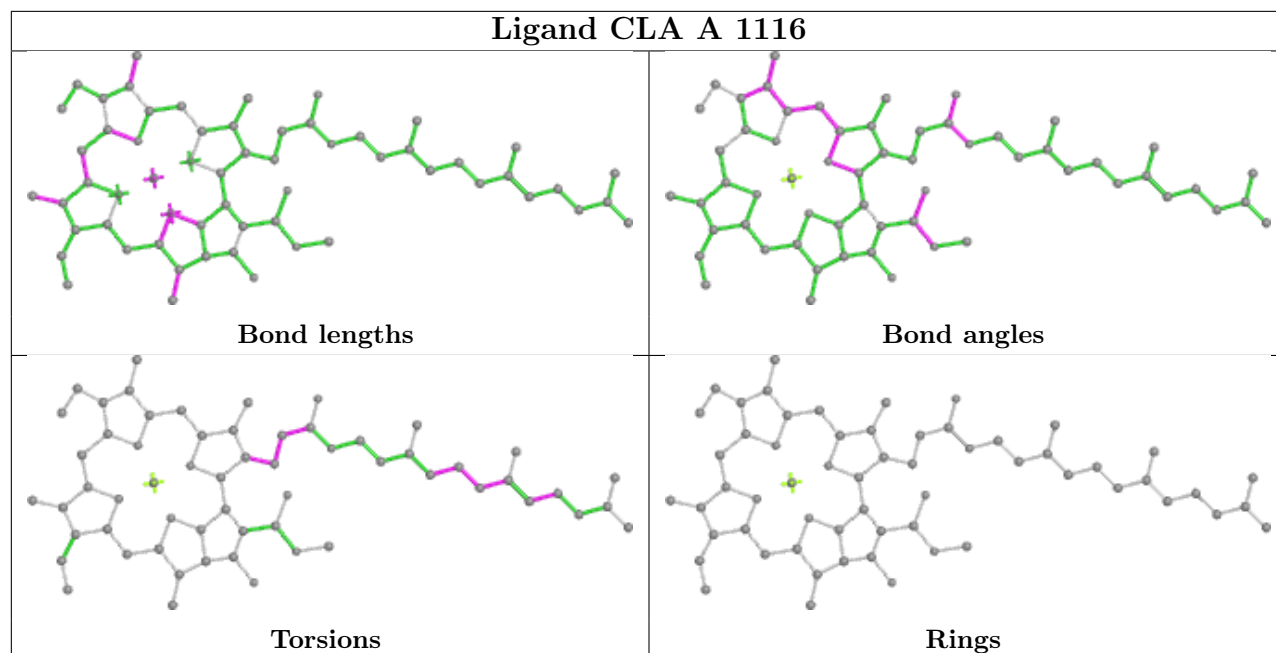
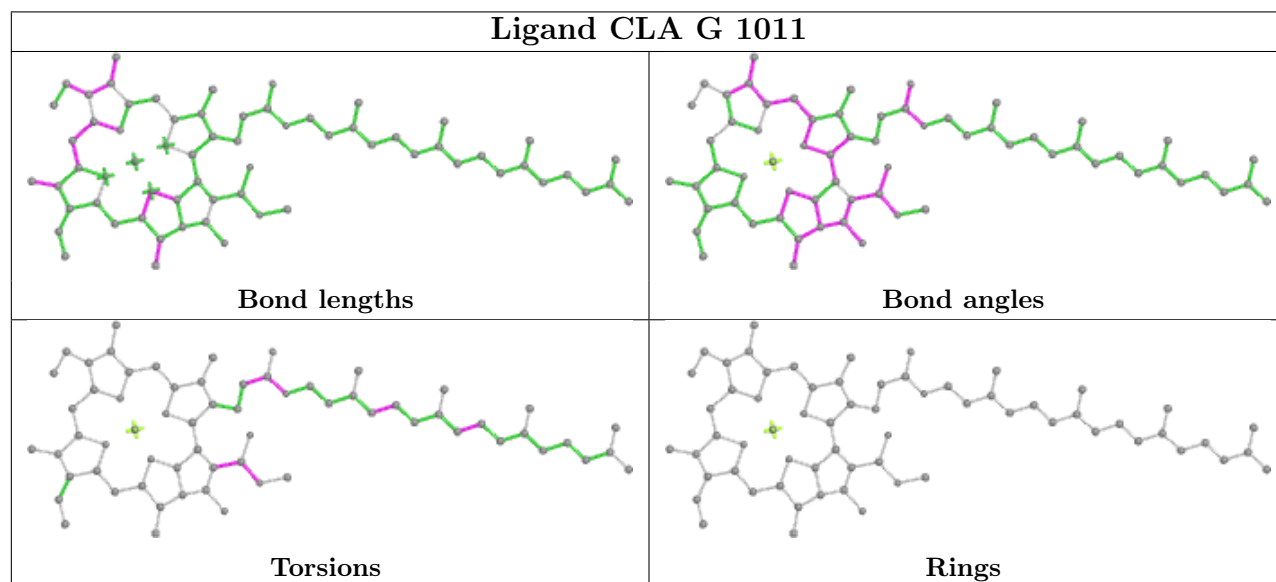


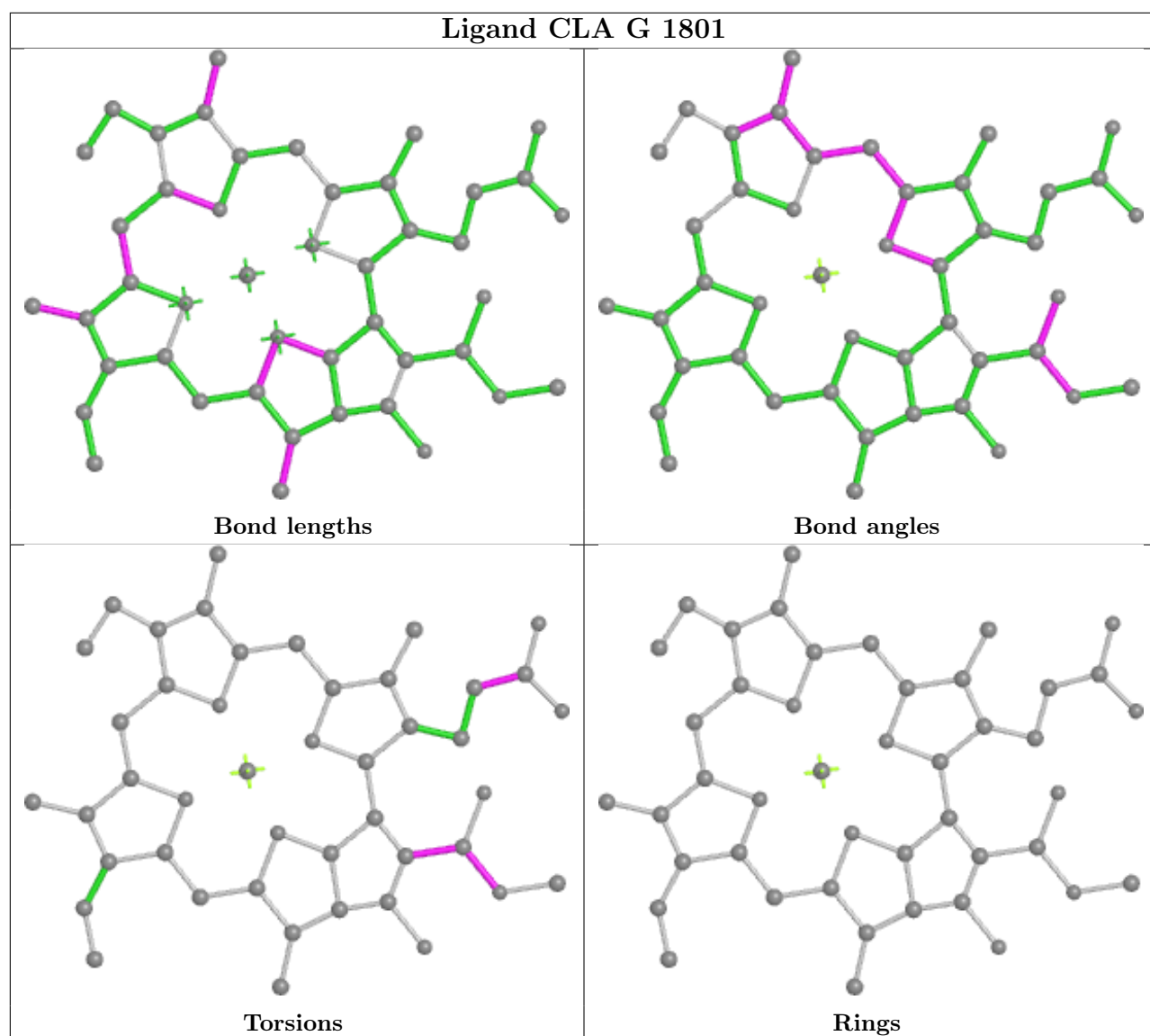
Ligand CLA d 516



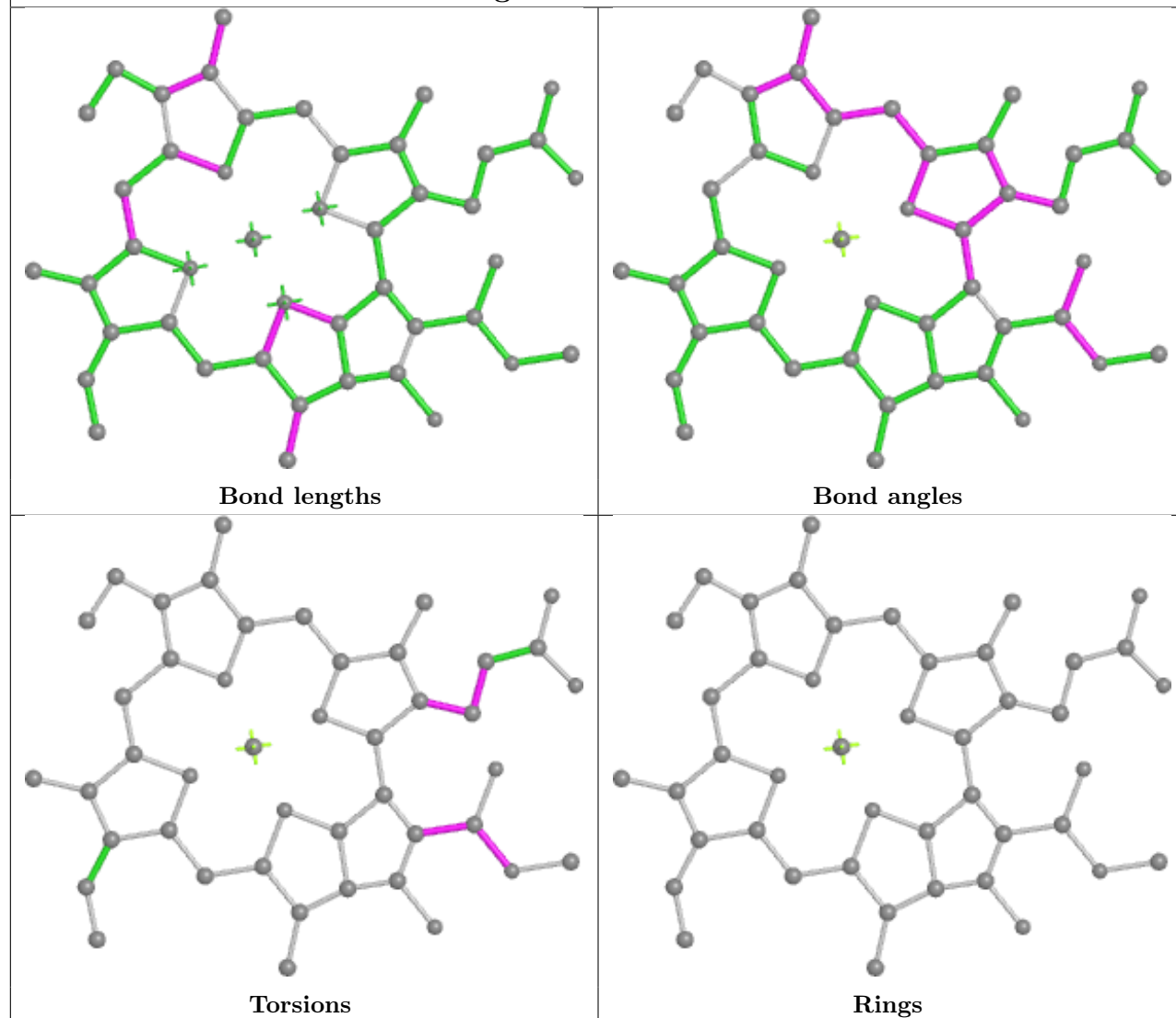
Ligand CLA B 1221



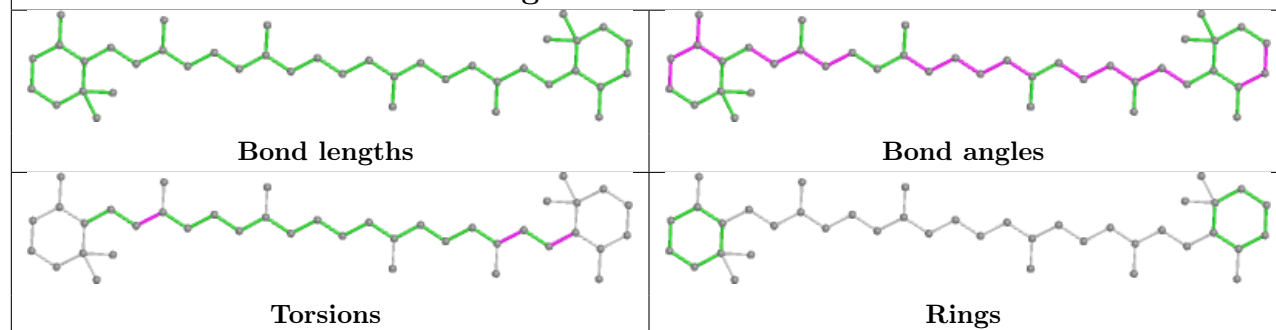
Ligand CLA A 1116**Ligand CLA G 1011**

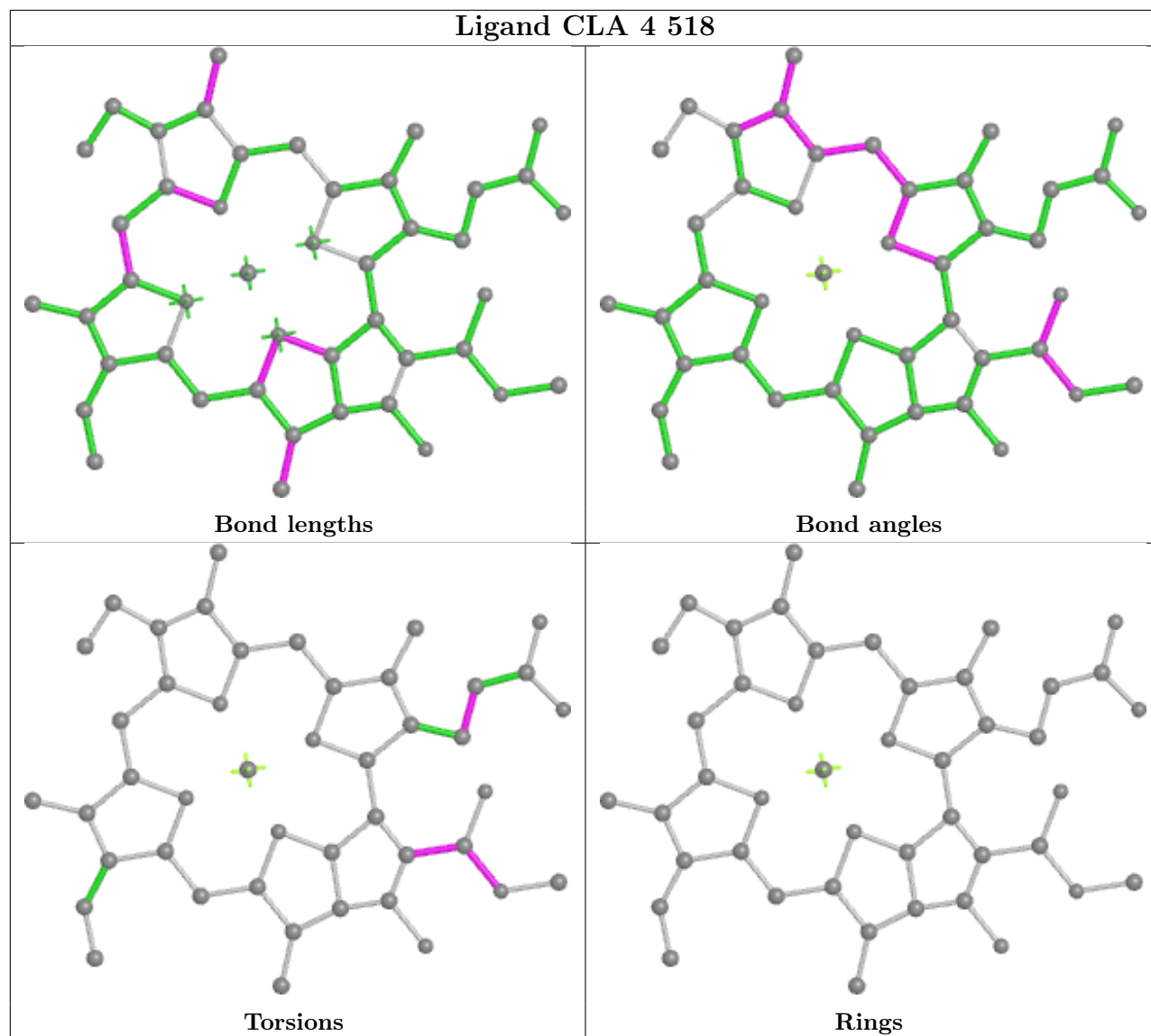
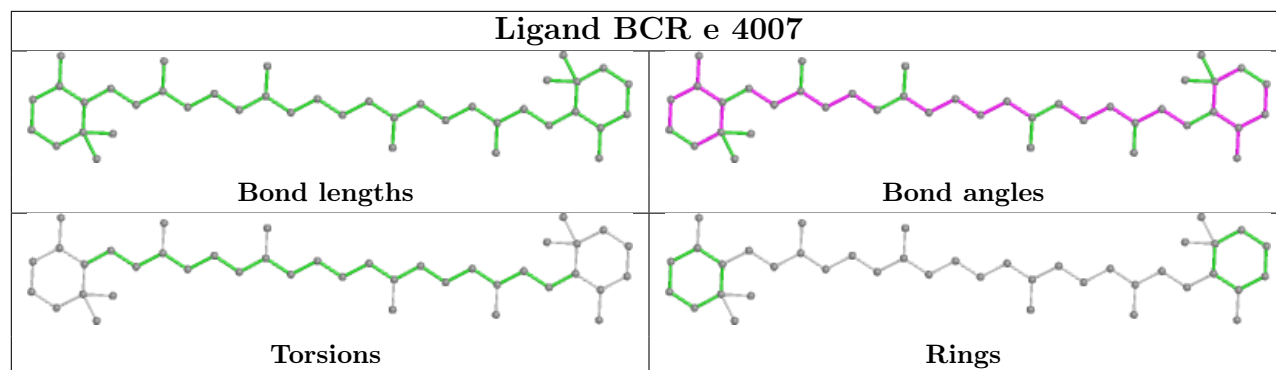


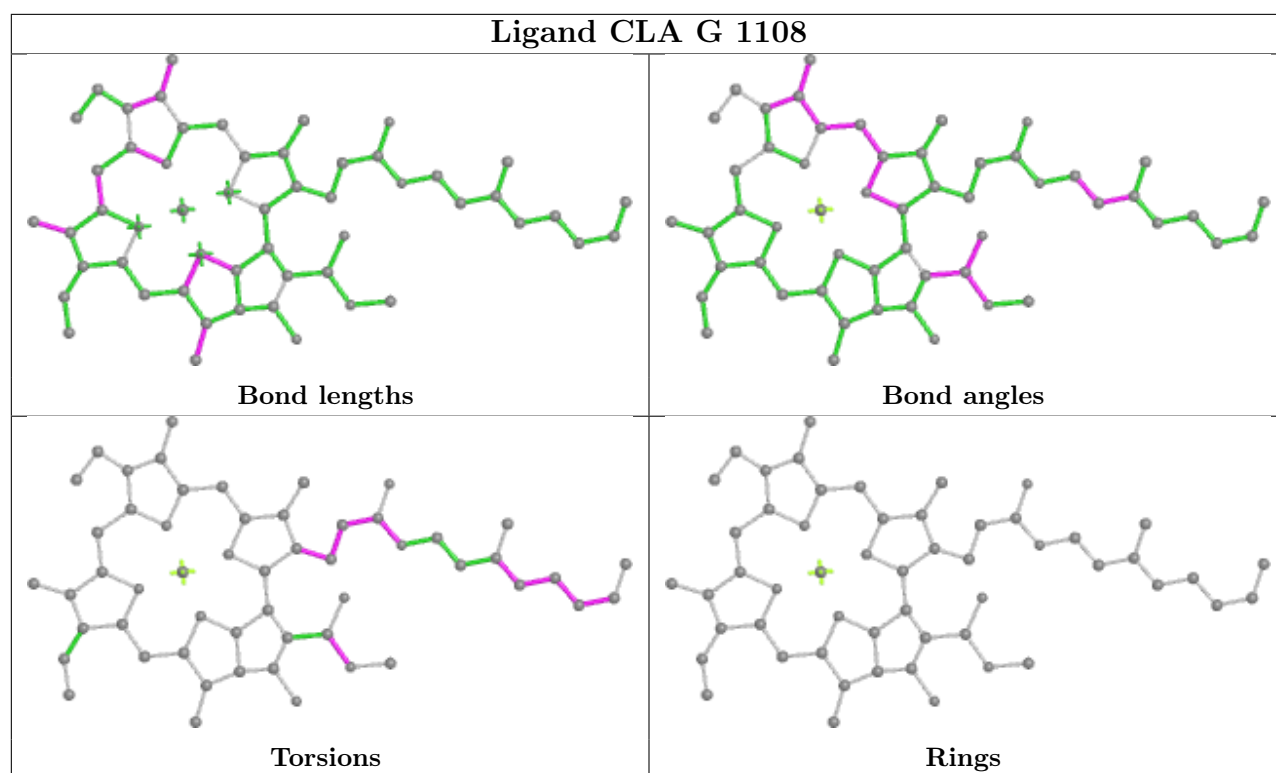
Ligand CLA 2 504

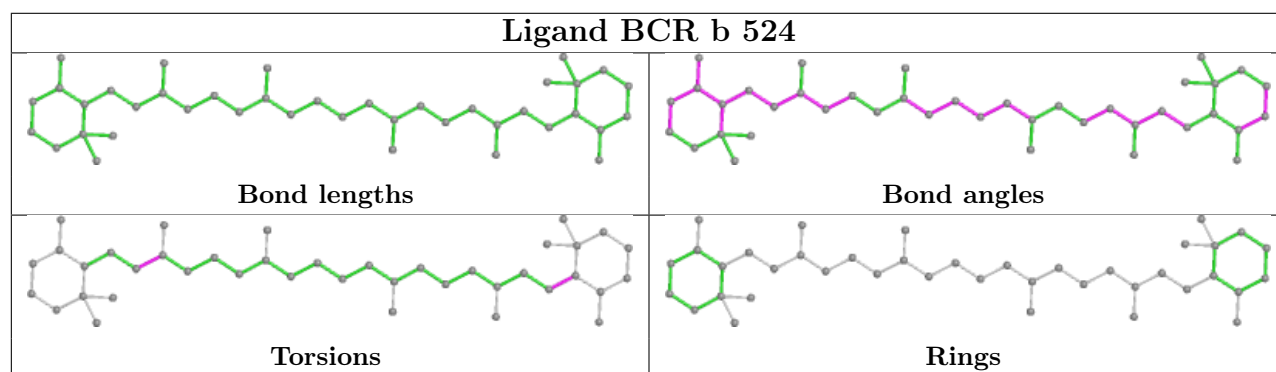
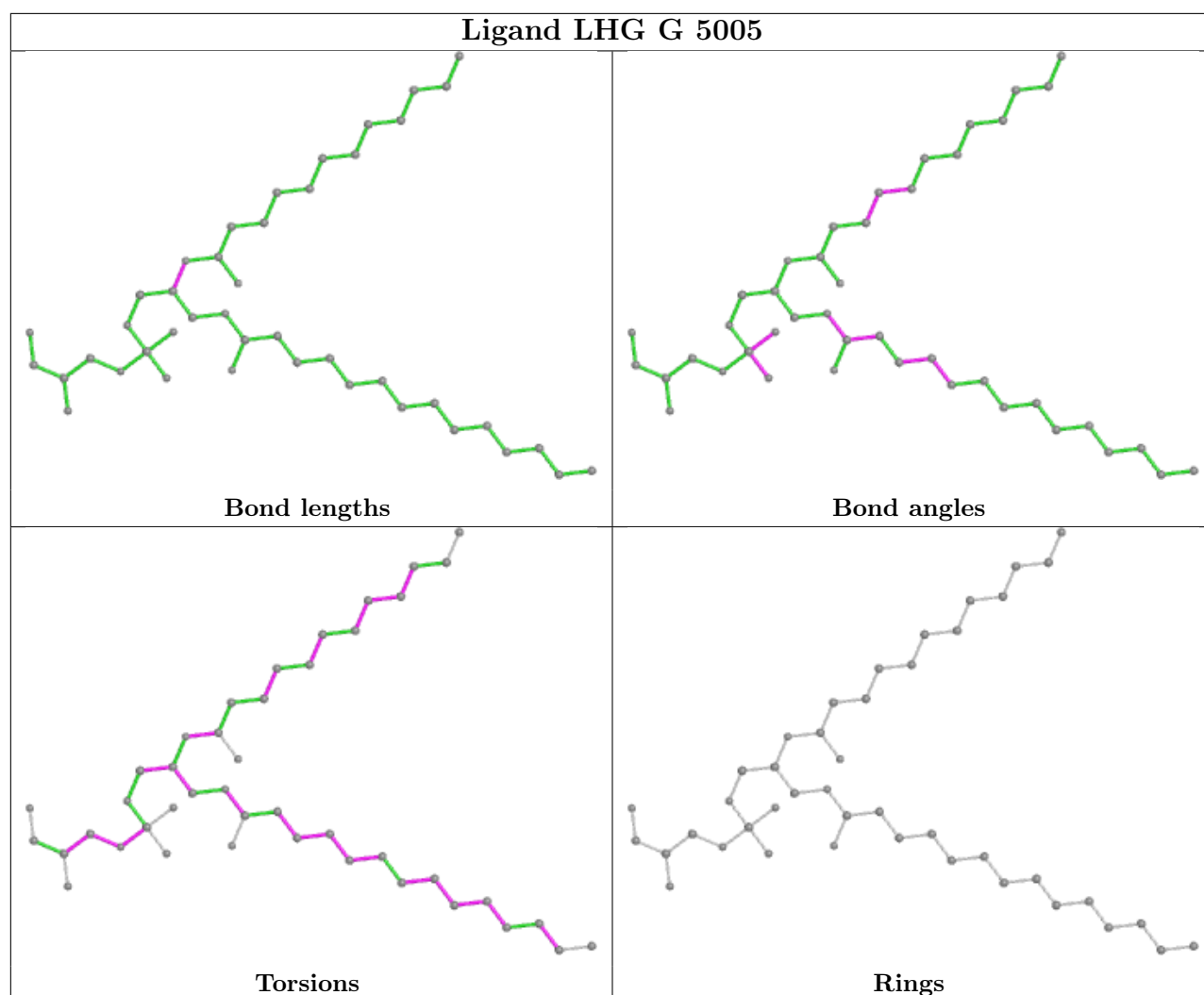


Ligand BCR B 4005

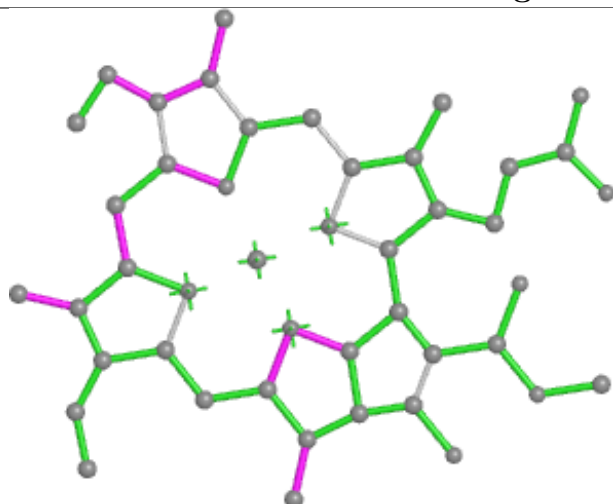




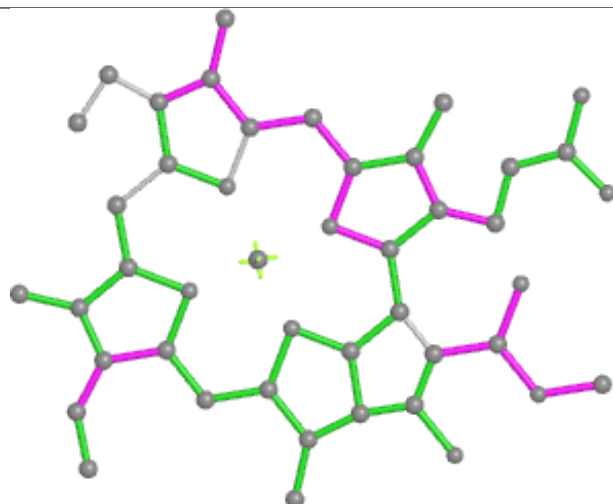




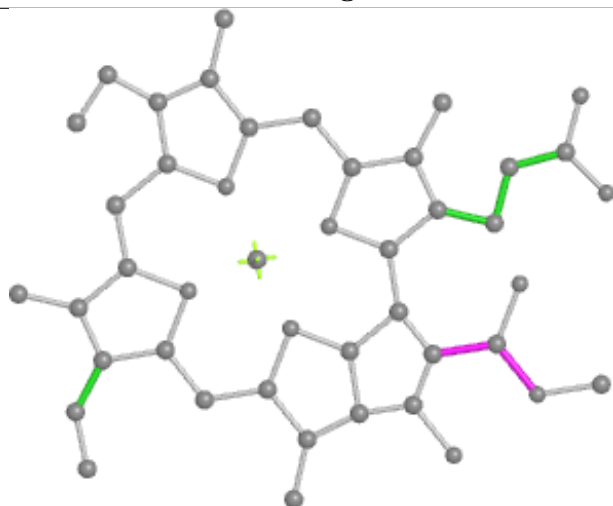
Ligand CLA Y 504



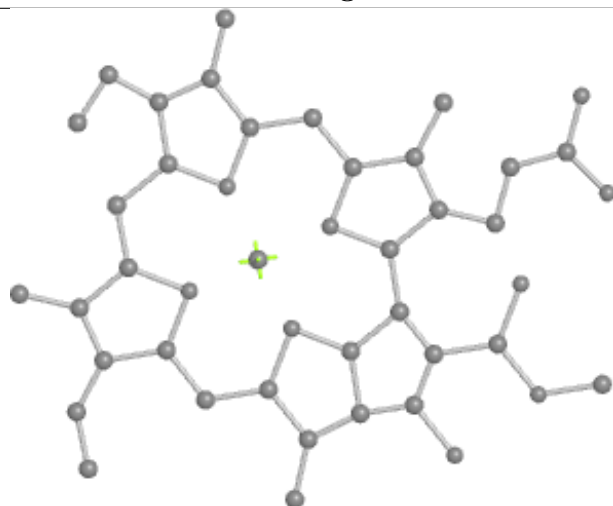
Bond lengths



Bond angles

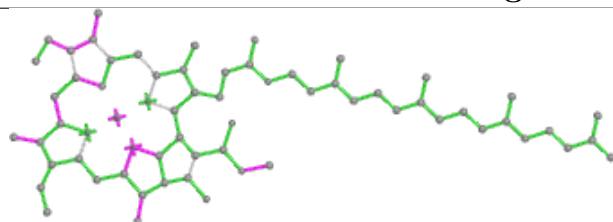


Torsions

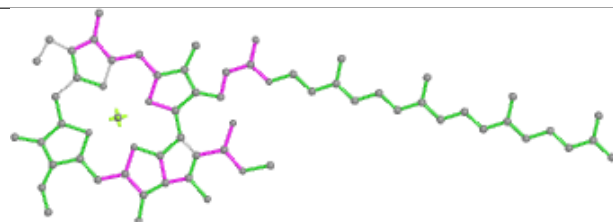


Rings

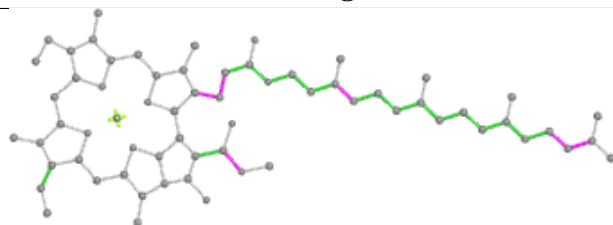
Ligand CLA A 1022



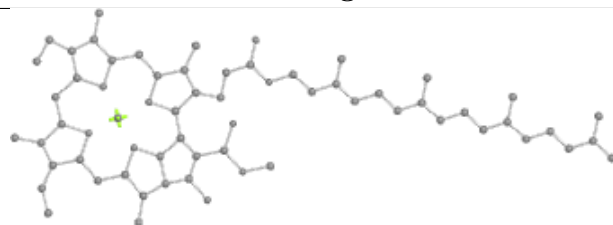
Bond lengths



Bond angles

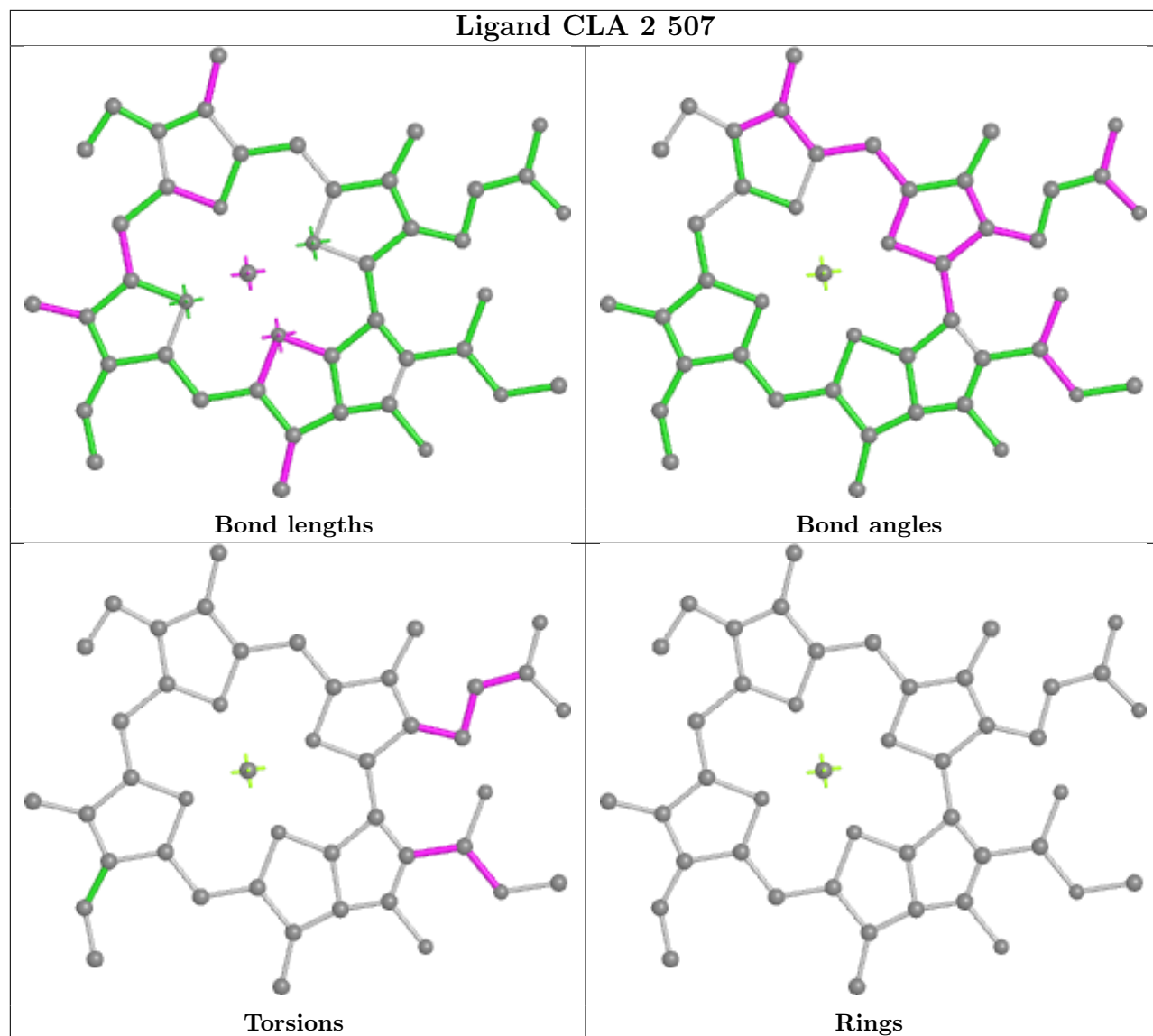


Torsions

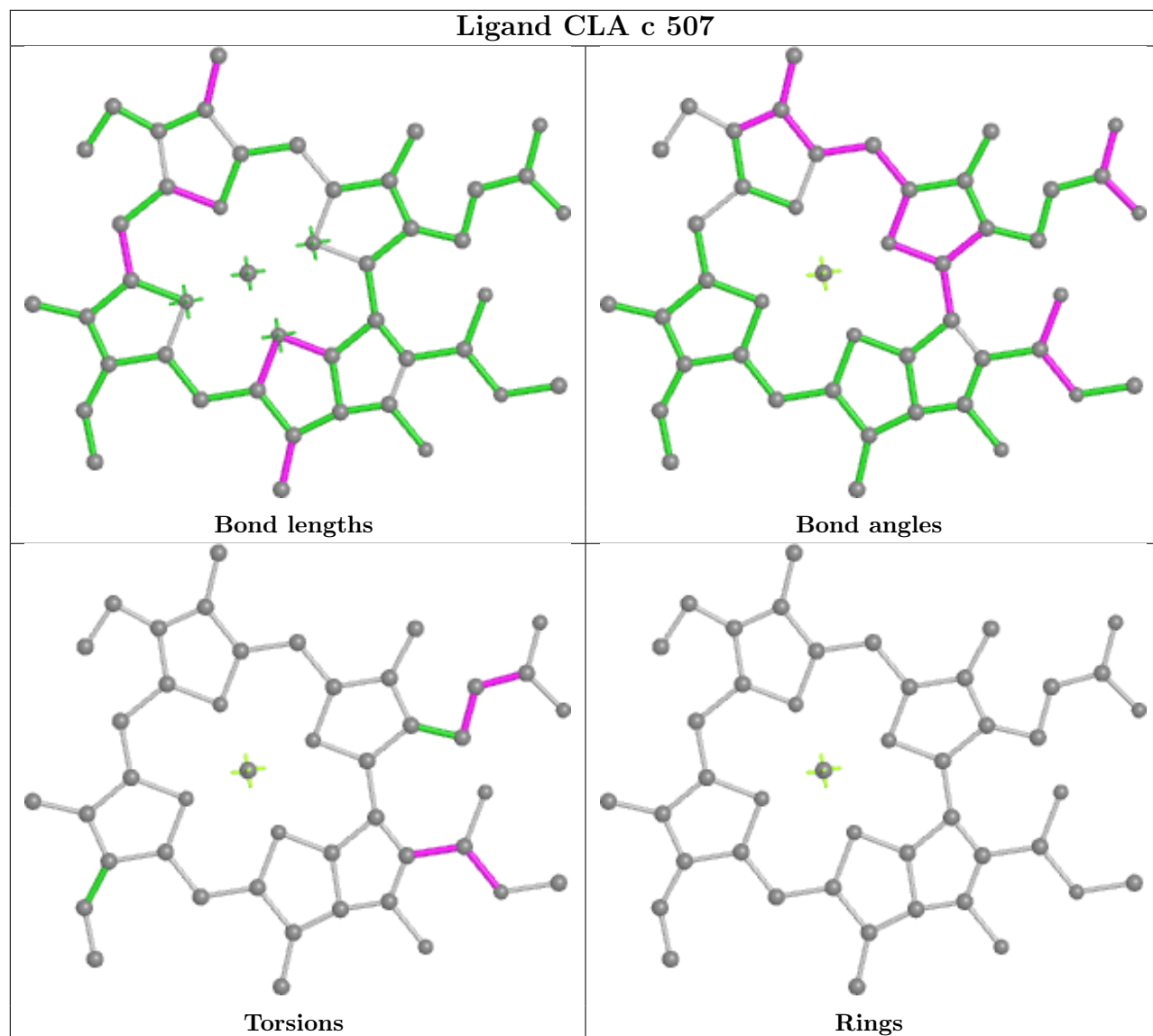


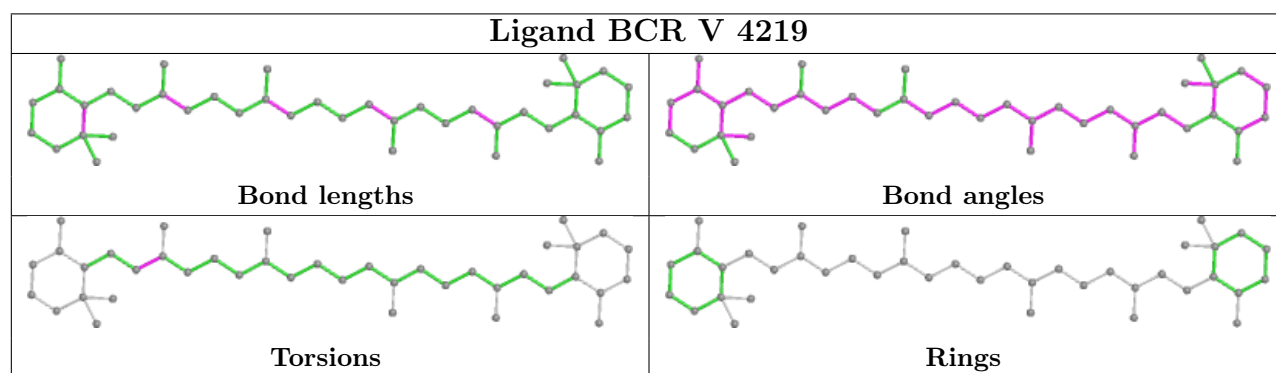
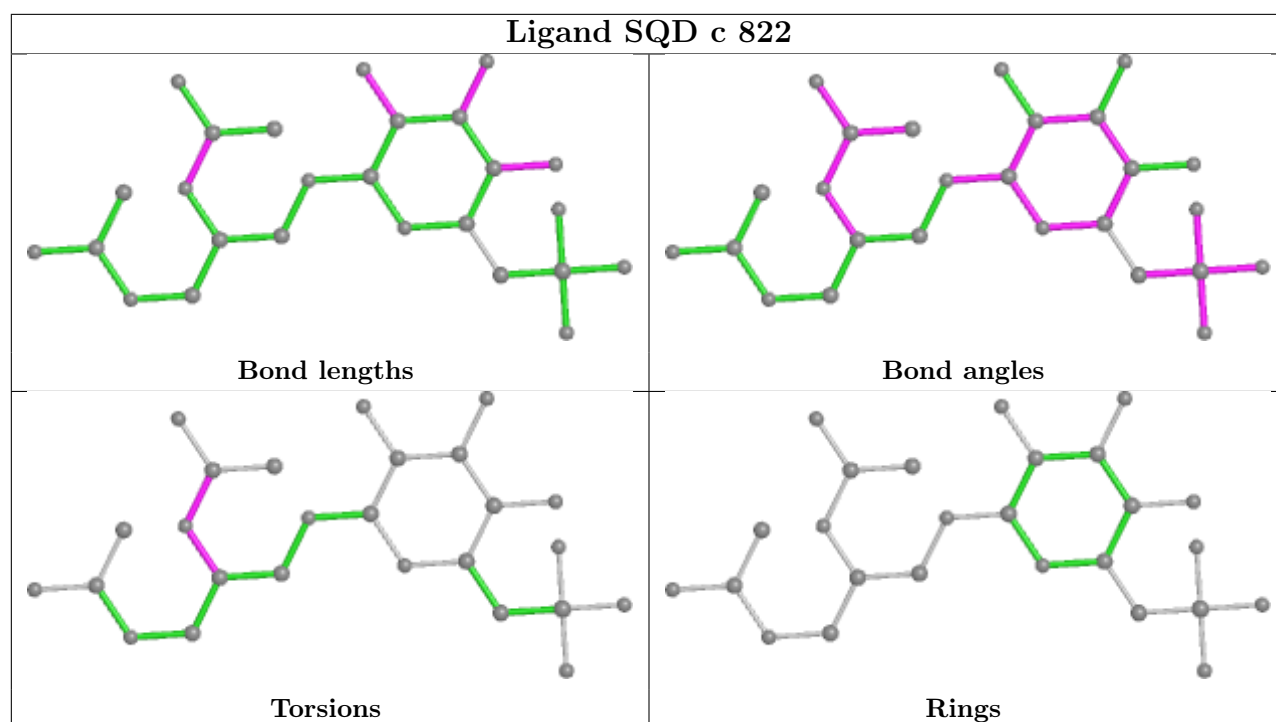
Rings

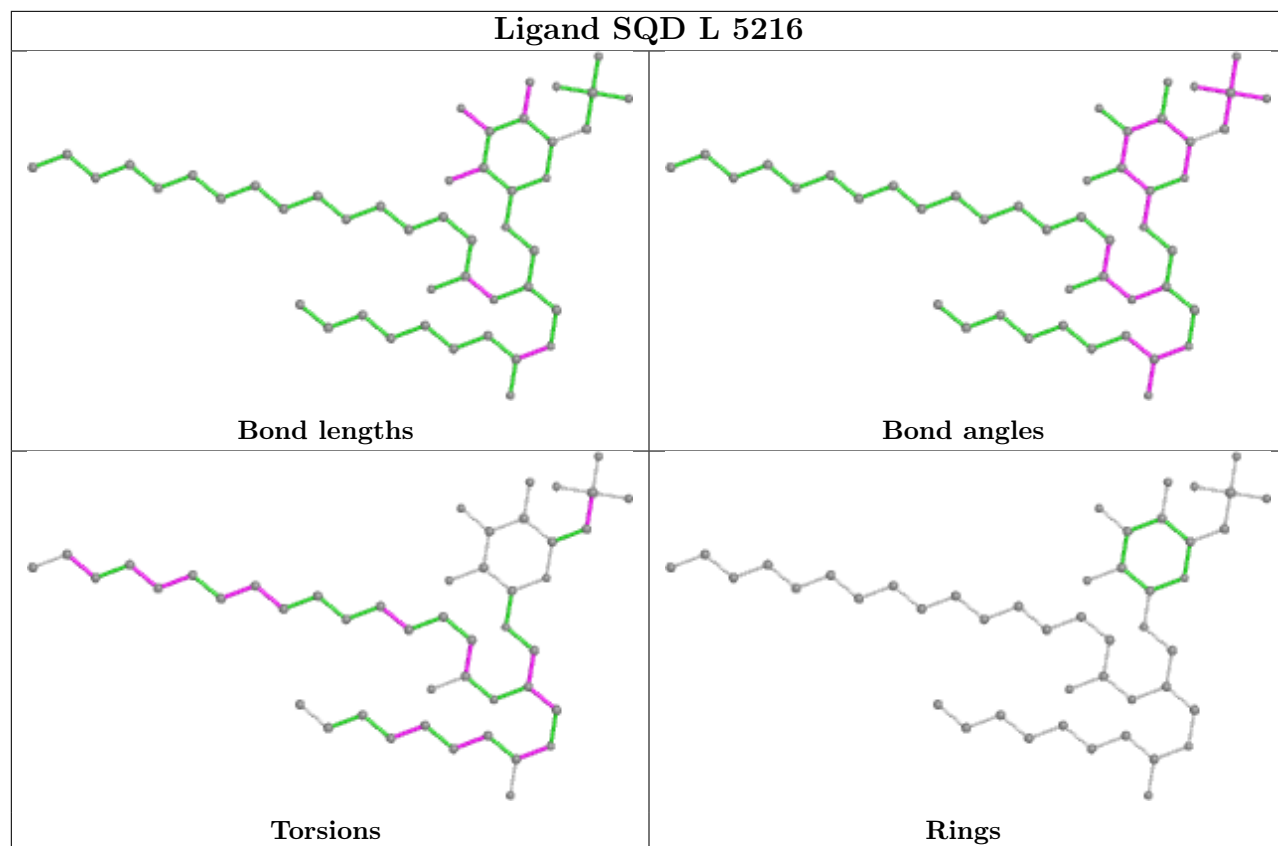
Ligand CLA 2 507



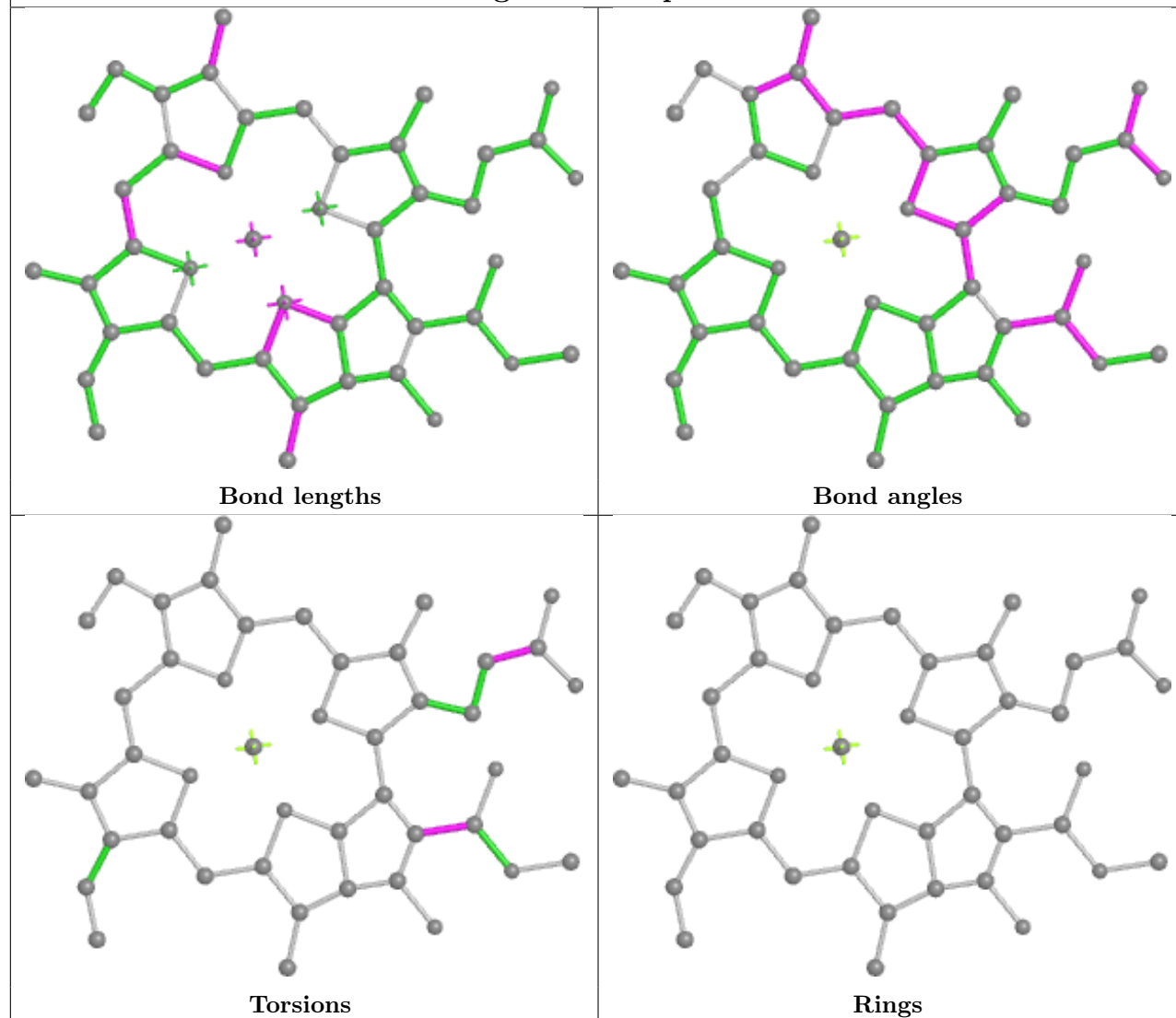
Ligand CLA c 507



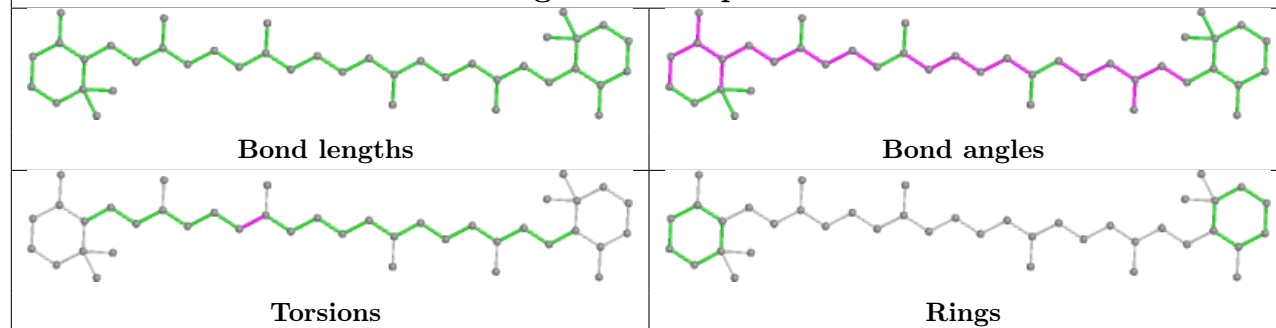


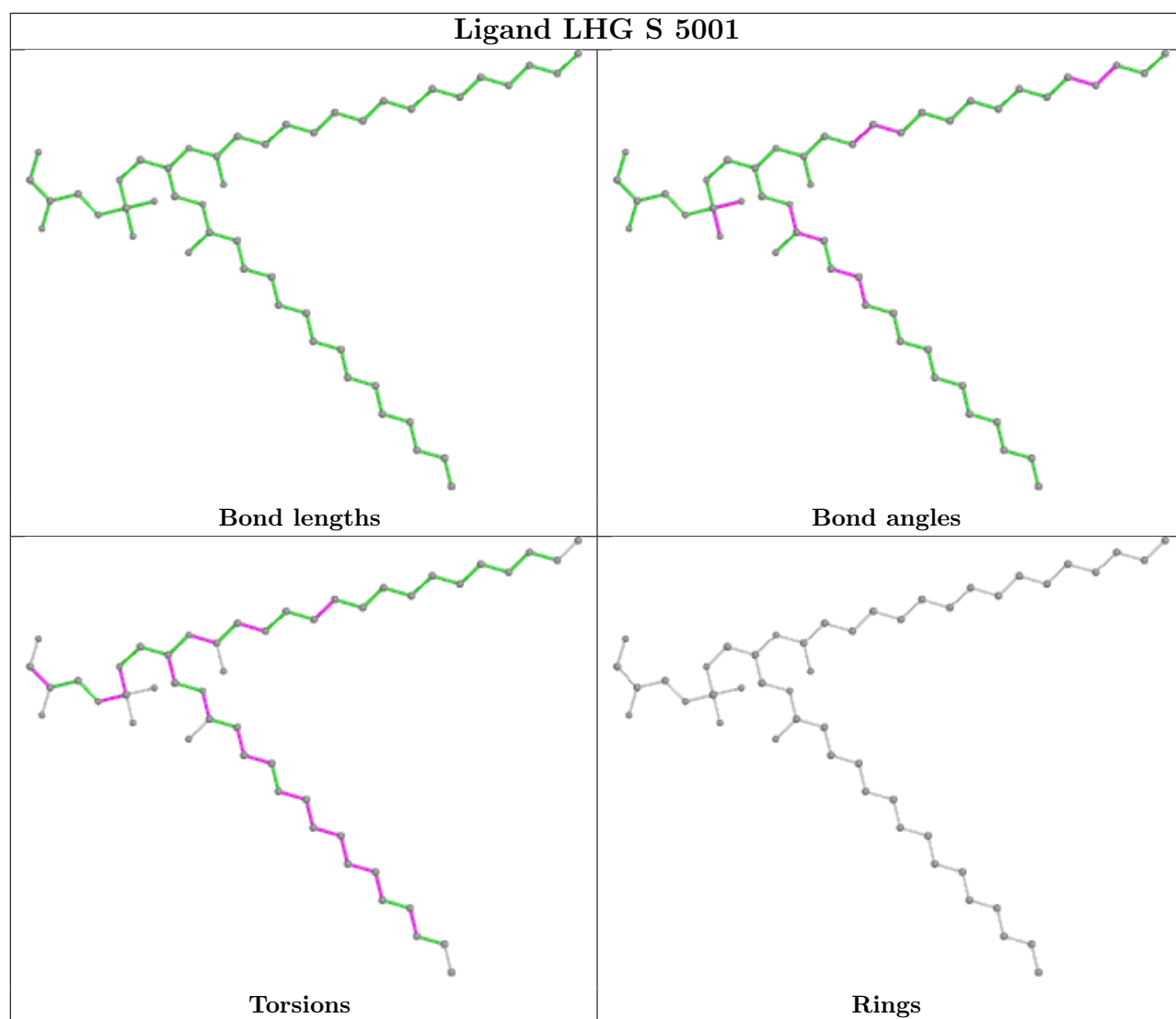


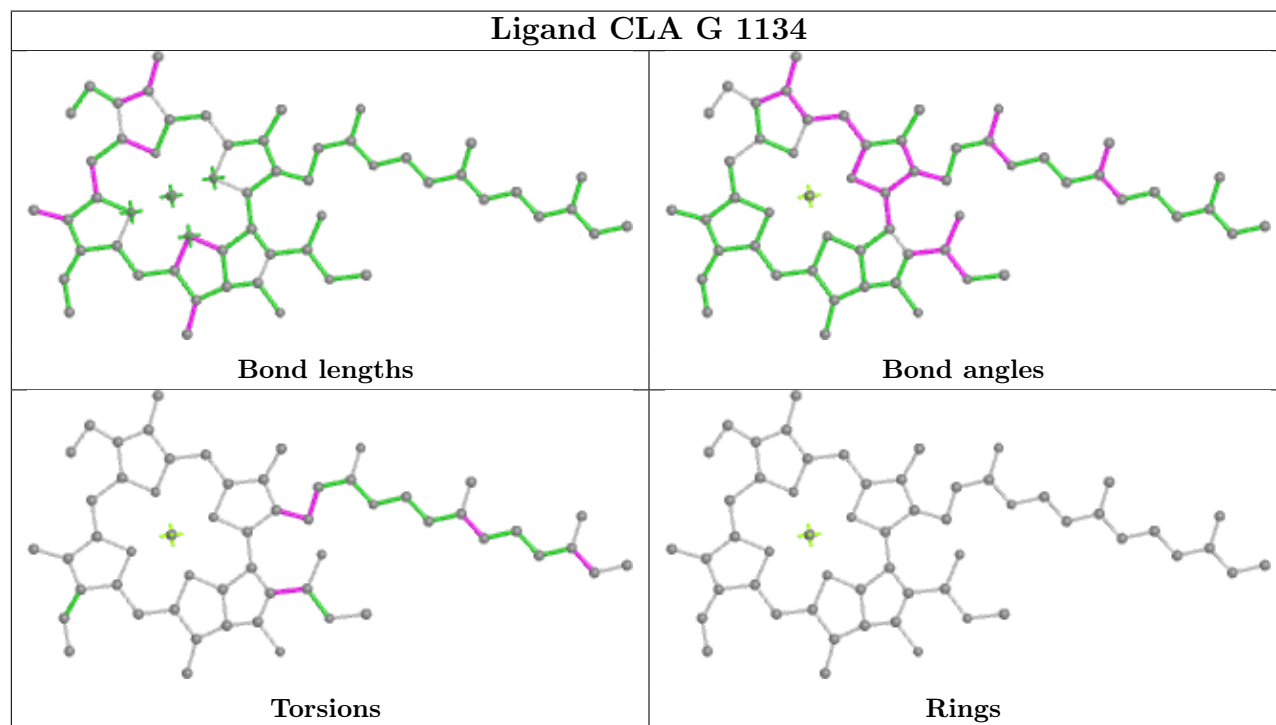
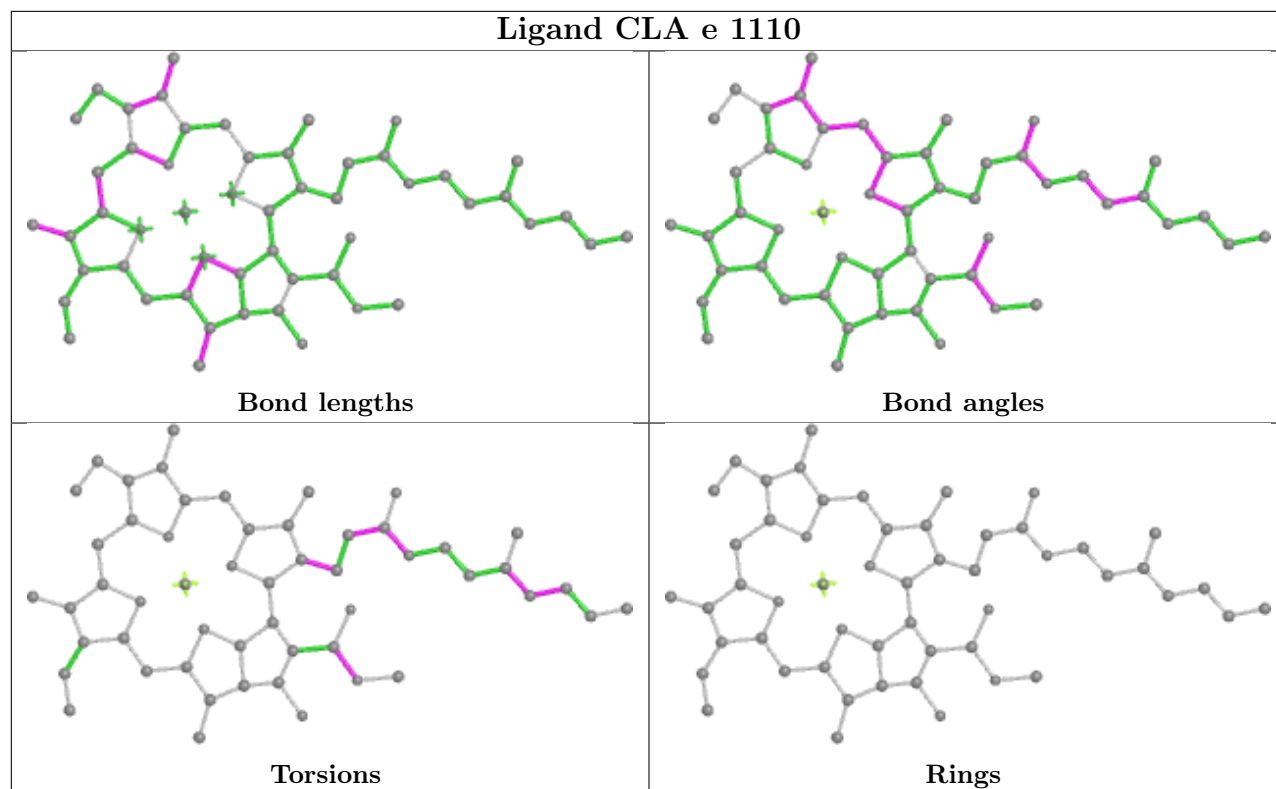
Ligand CLA q 509



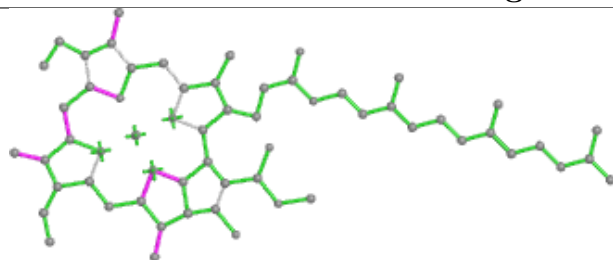
Ligand BCR q 524



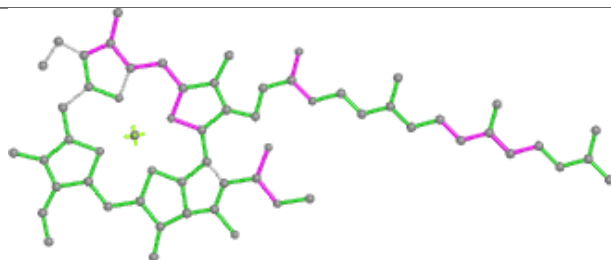




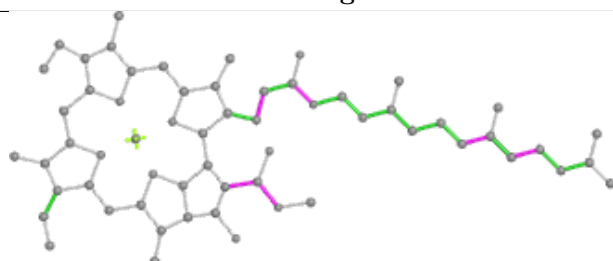
Ligand CLA B 1201



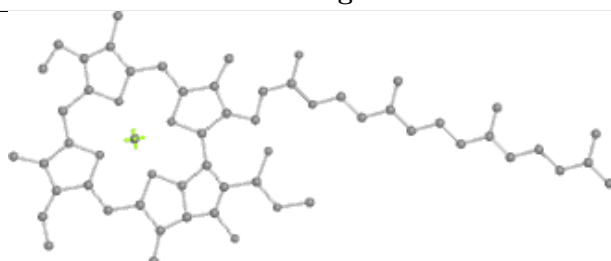
Bond lengths



Bond angles

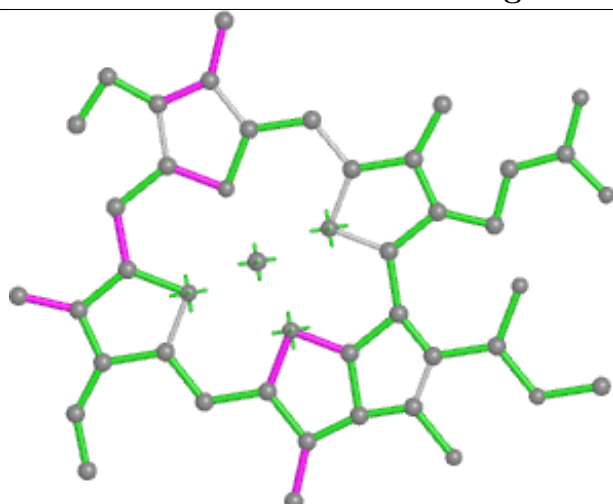


Torsions

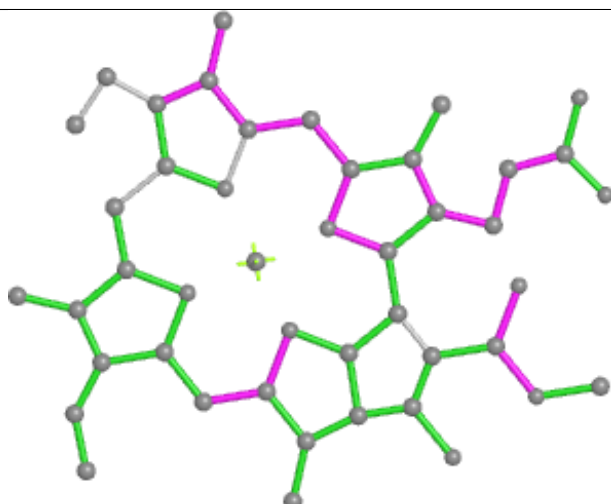


Rings

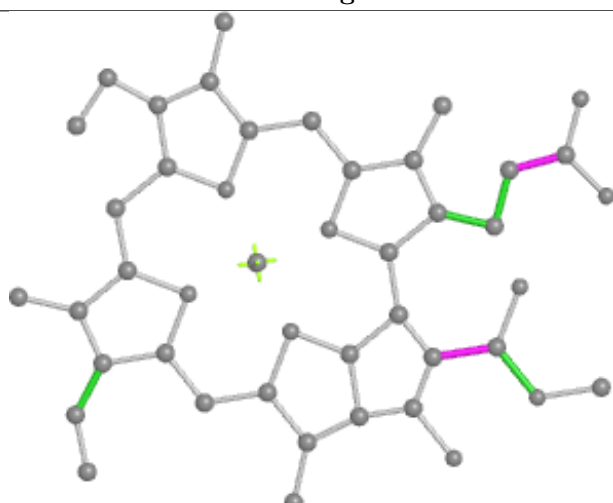
Ligand CLA G 1114



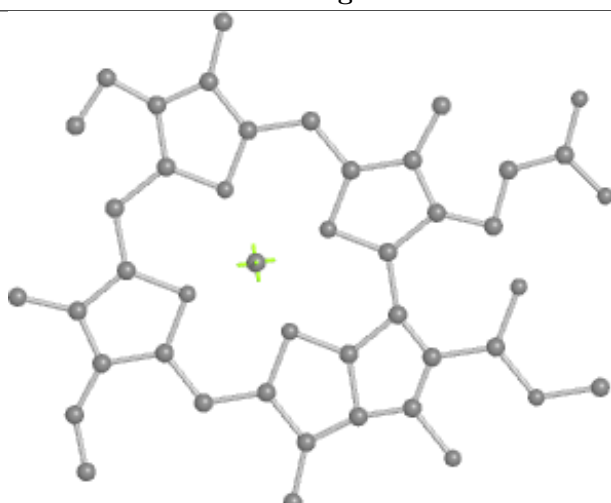
Bond lengths



Bond angles

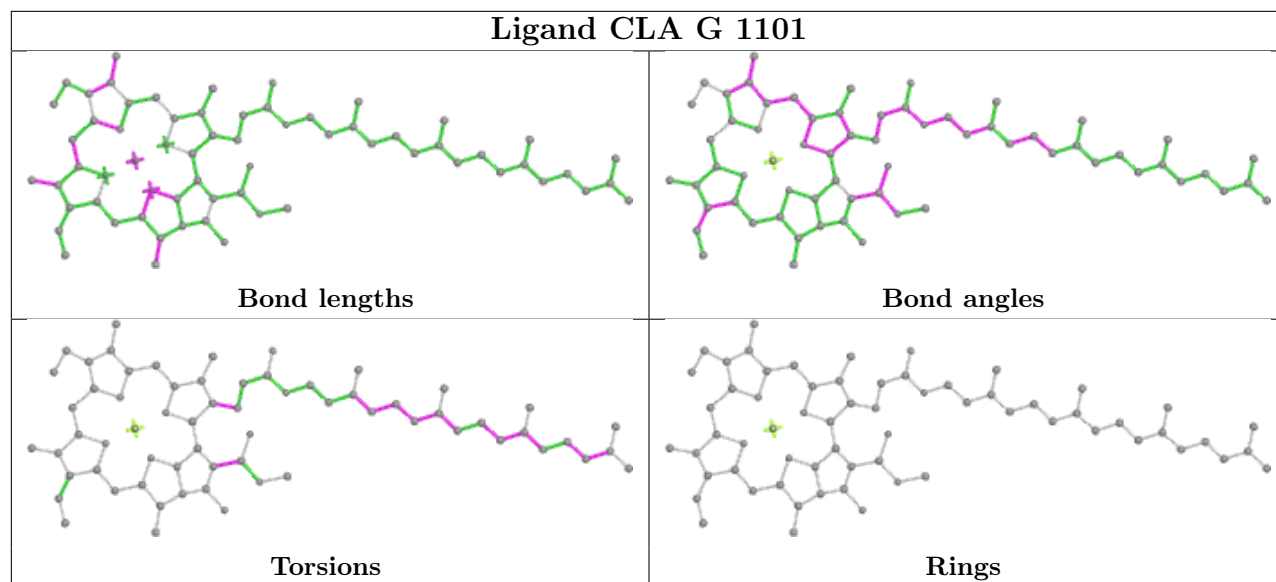


Torsions

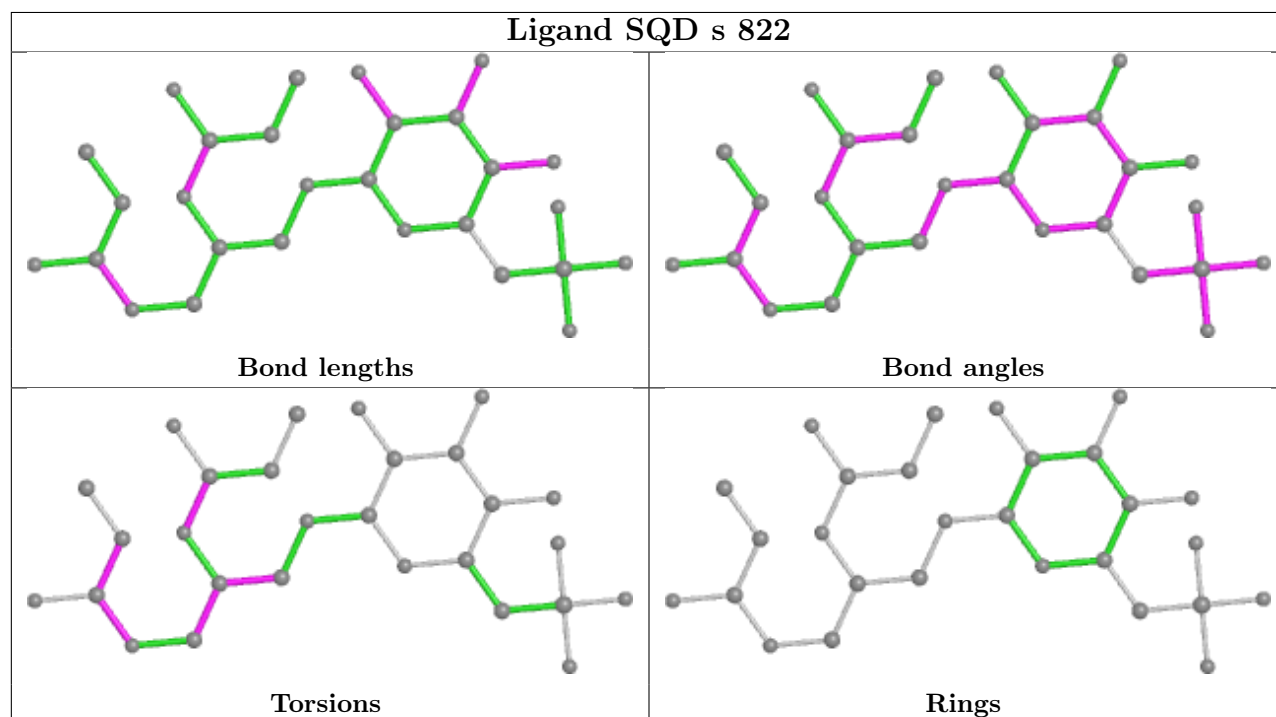


Rings

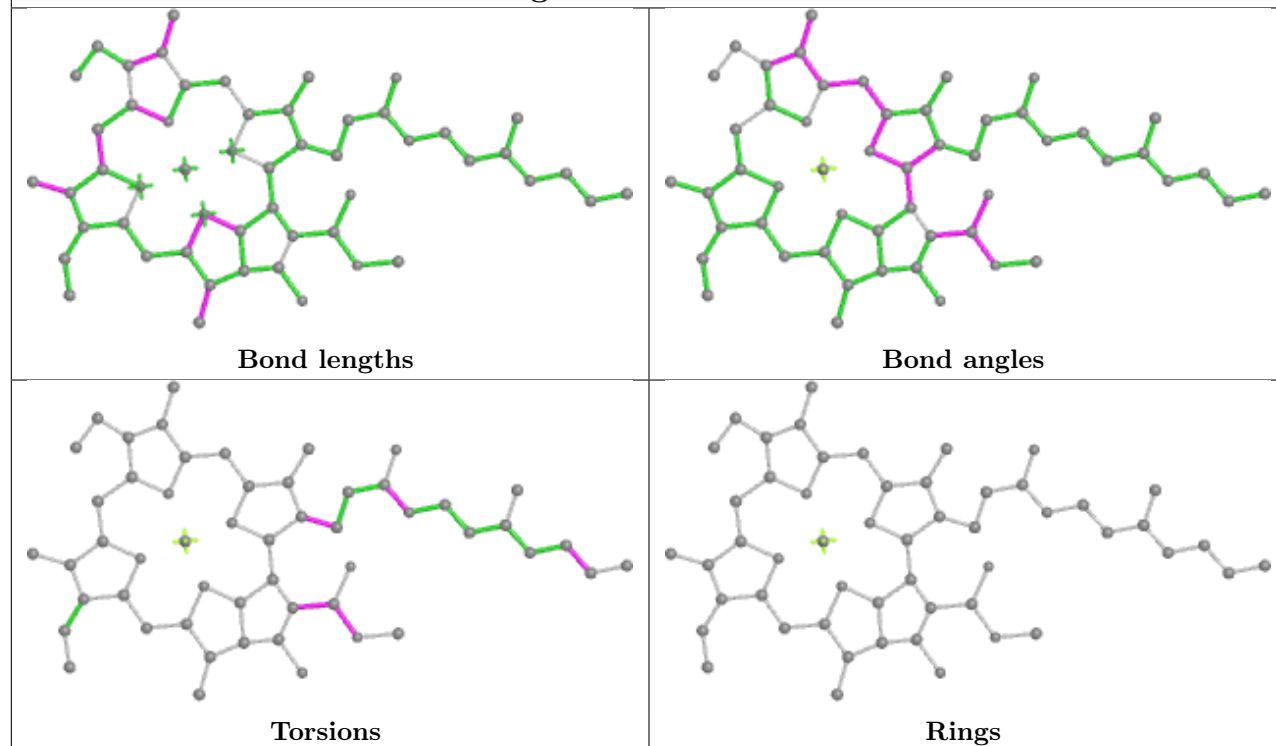
Ligand CLA G 1101



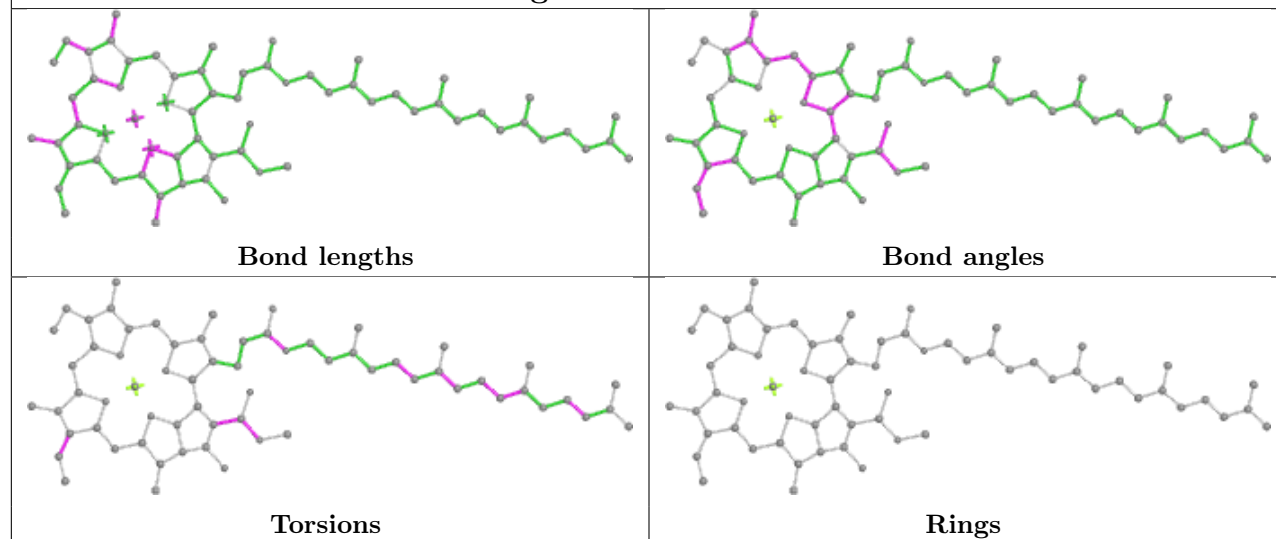
Ligand SQD s 822



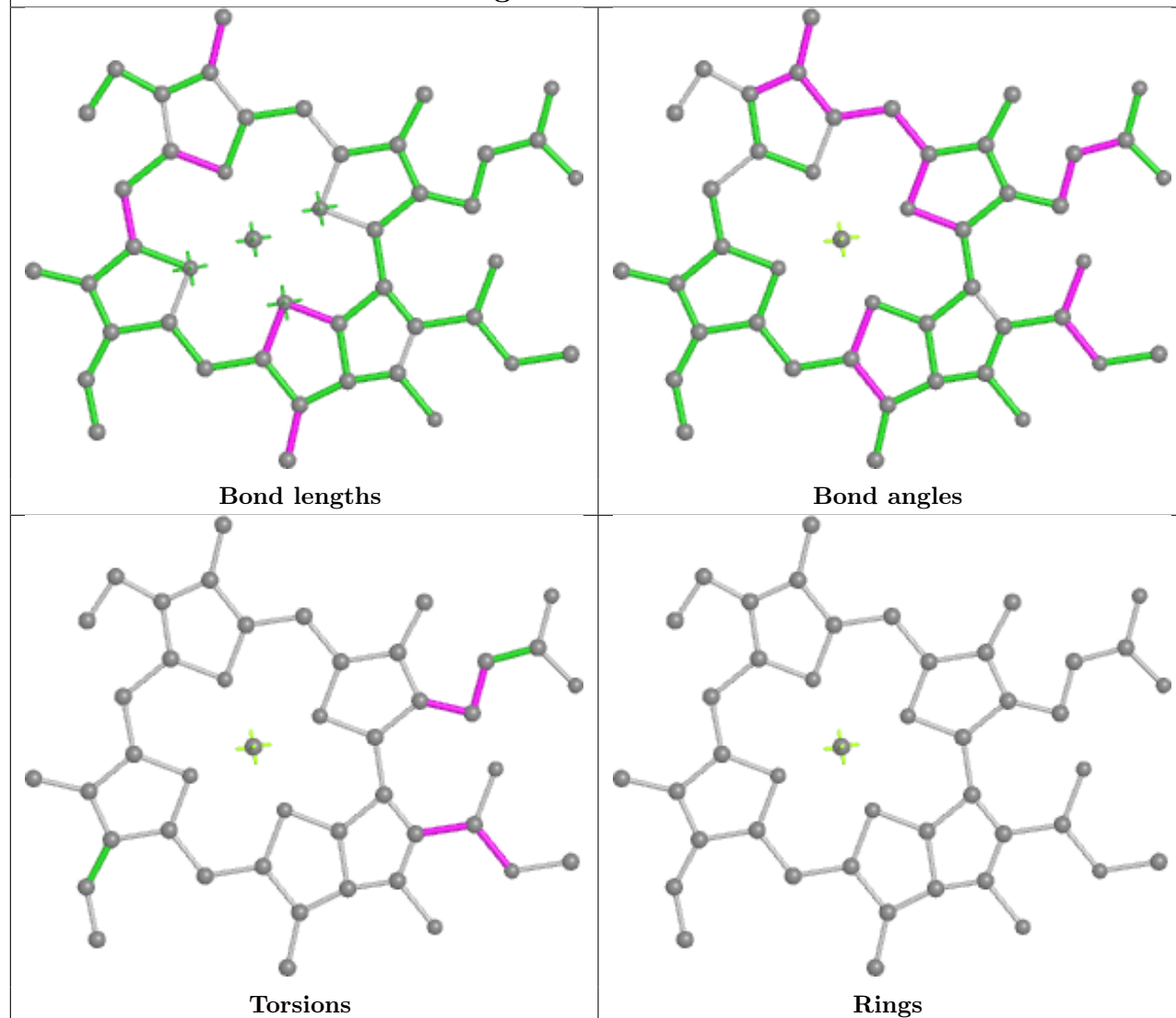
Ligand CLA f 1209



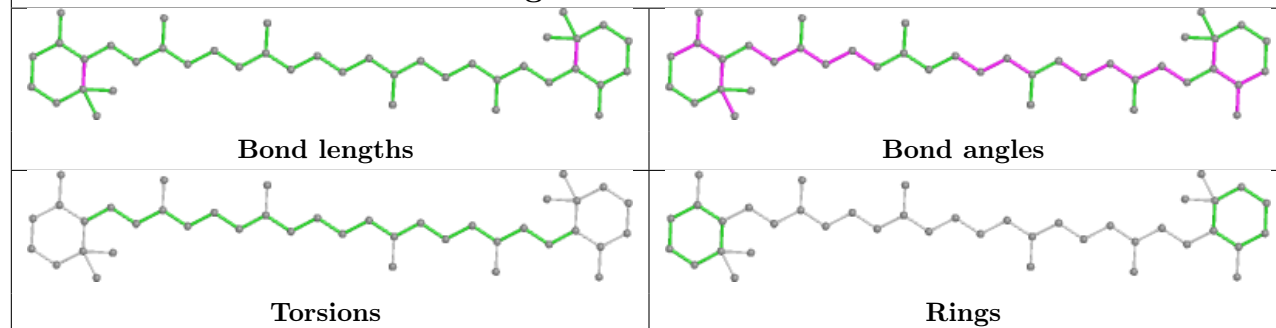
Ligand CLA f 1234

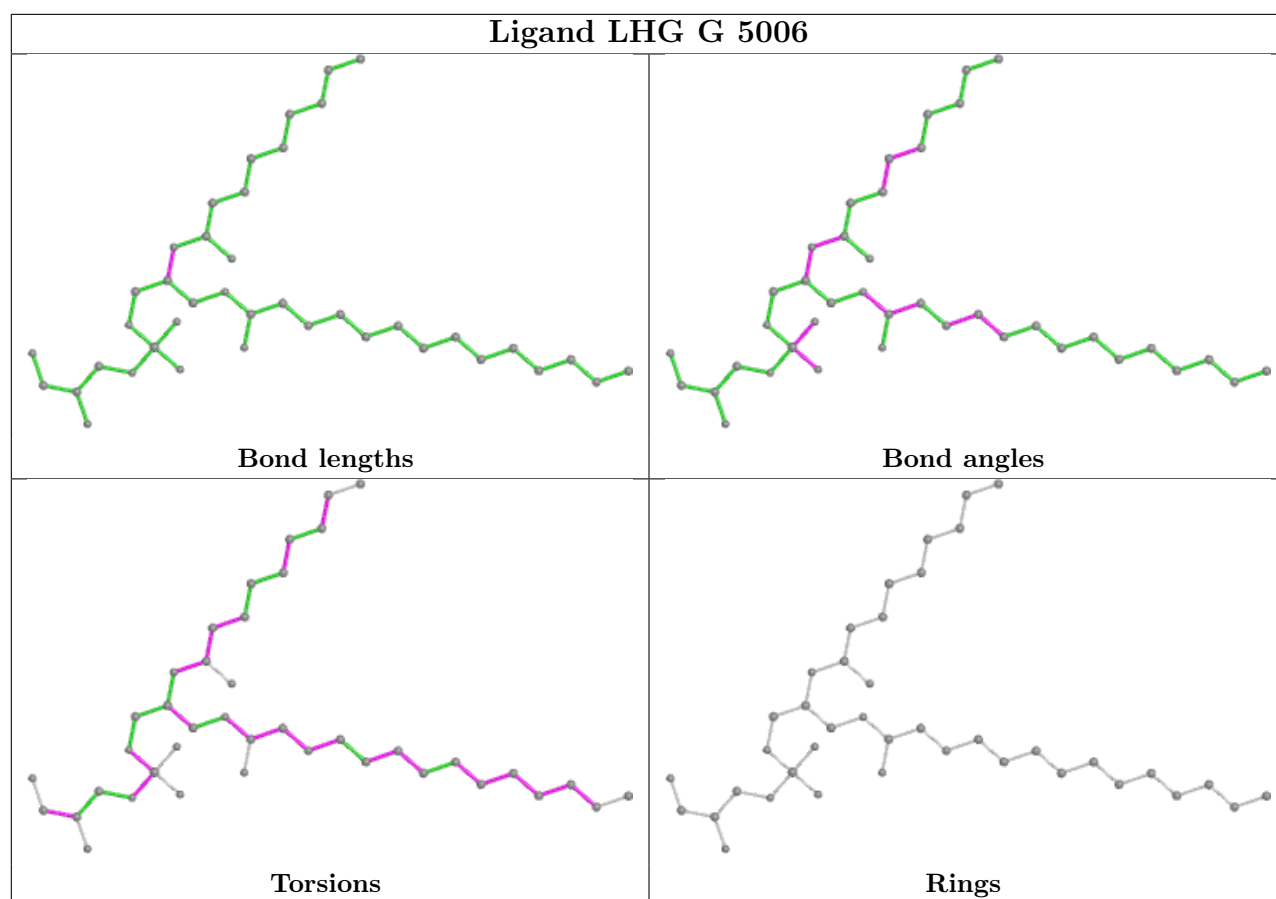


Ligand CLA 3 503

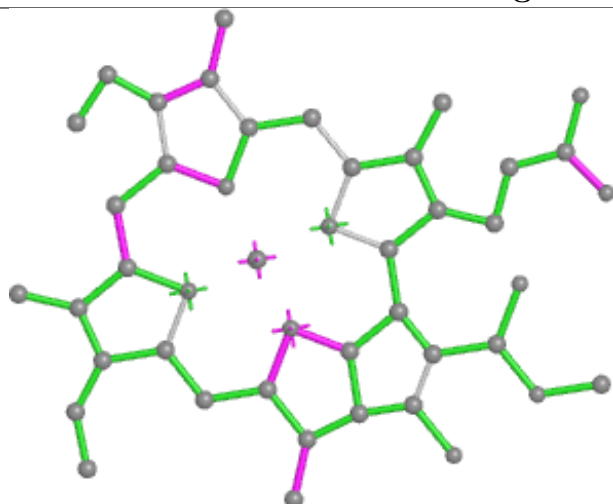


Ligand BCR k 4018

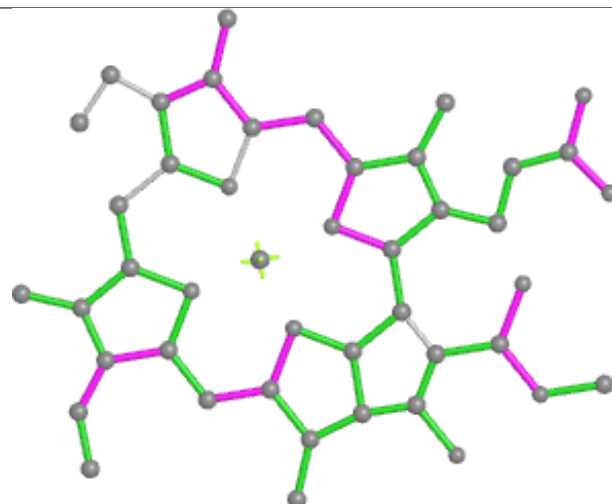




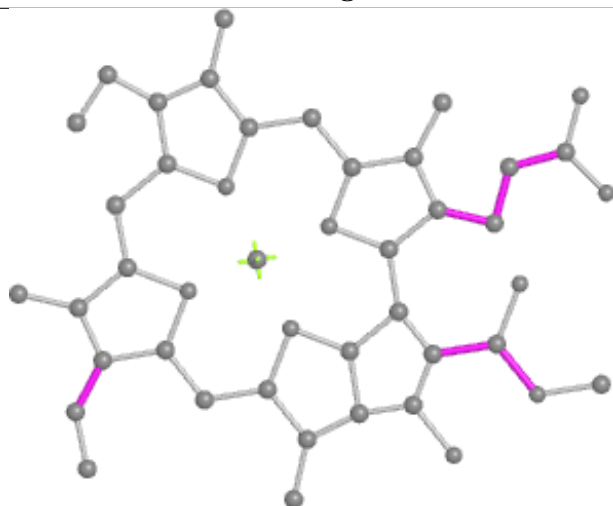
Ligand CLA Y 516



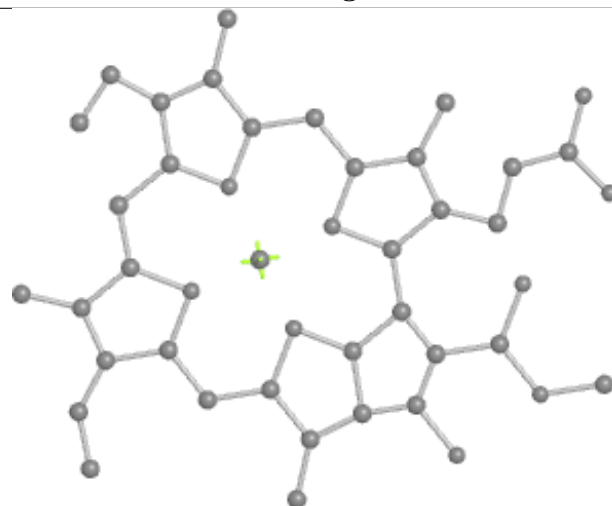
Bond lengths



Bond angles

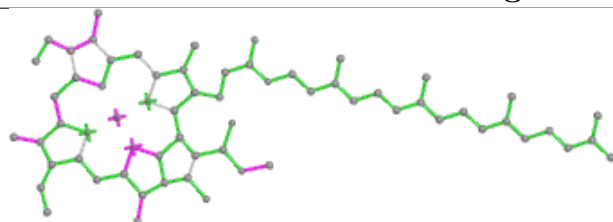


Torsions

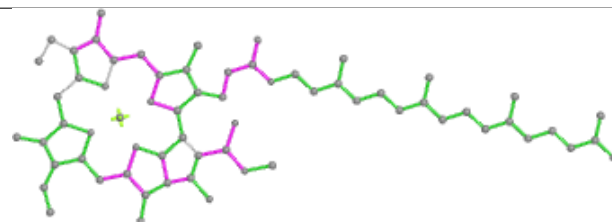


Rings

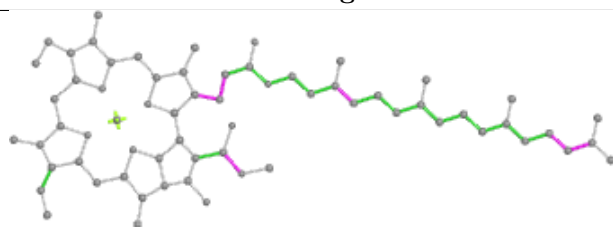
Ligand CLA G 1022



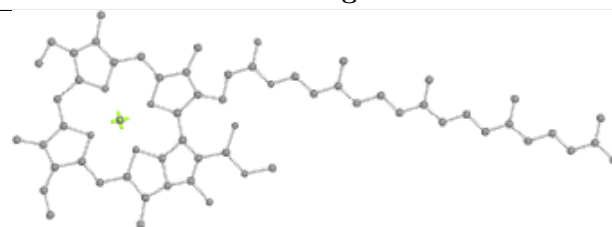
Bond lengths



Bond angles

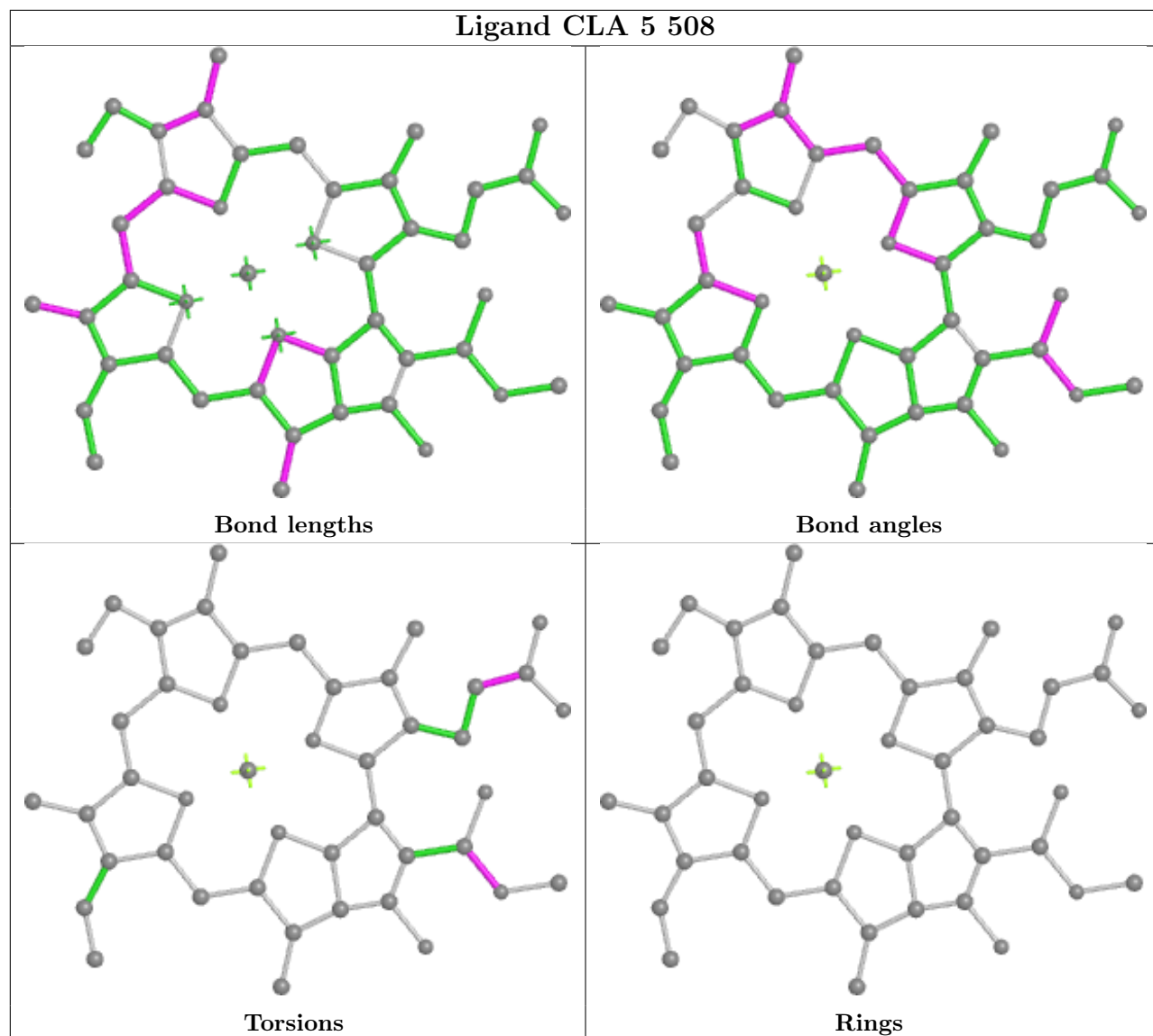


Torsions

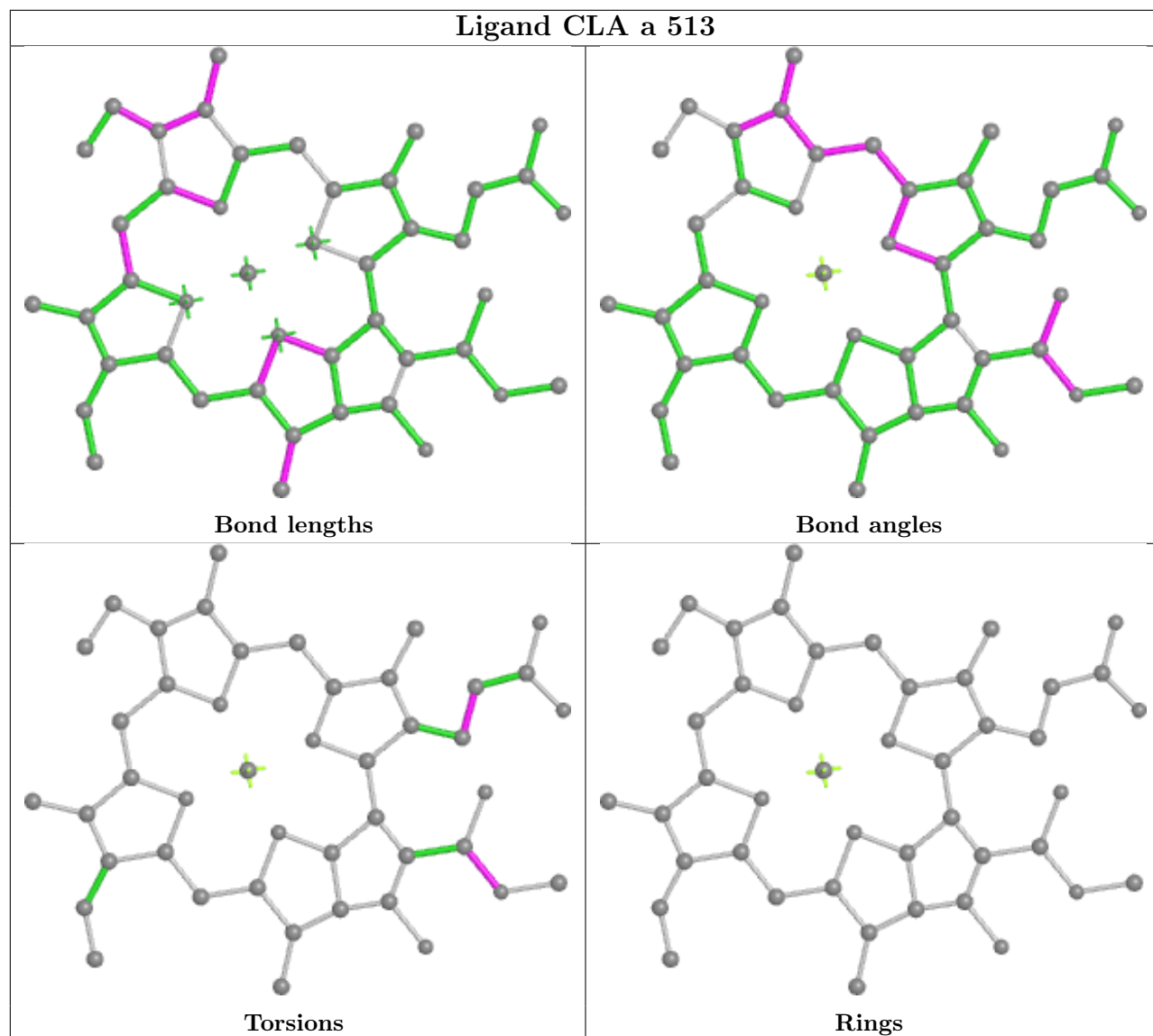


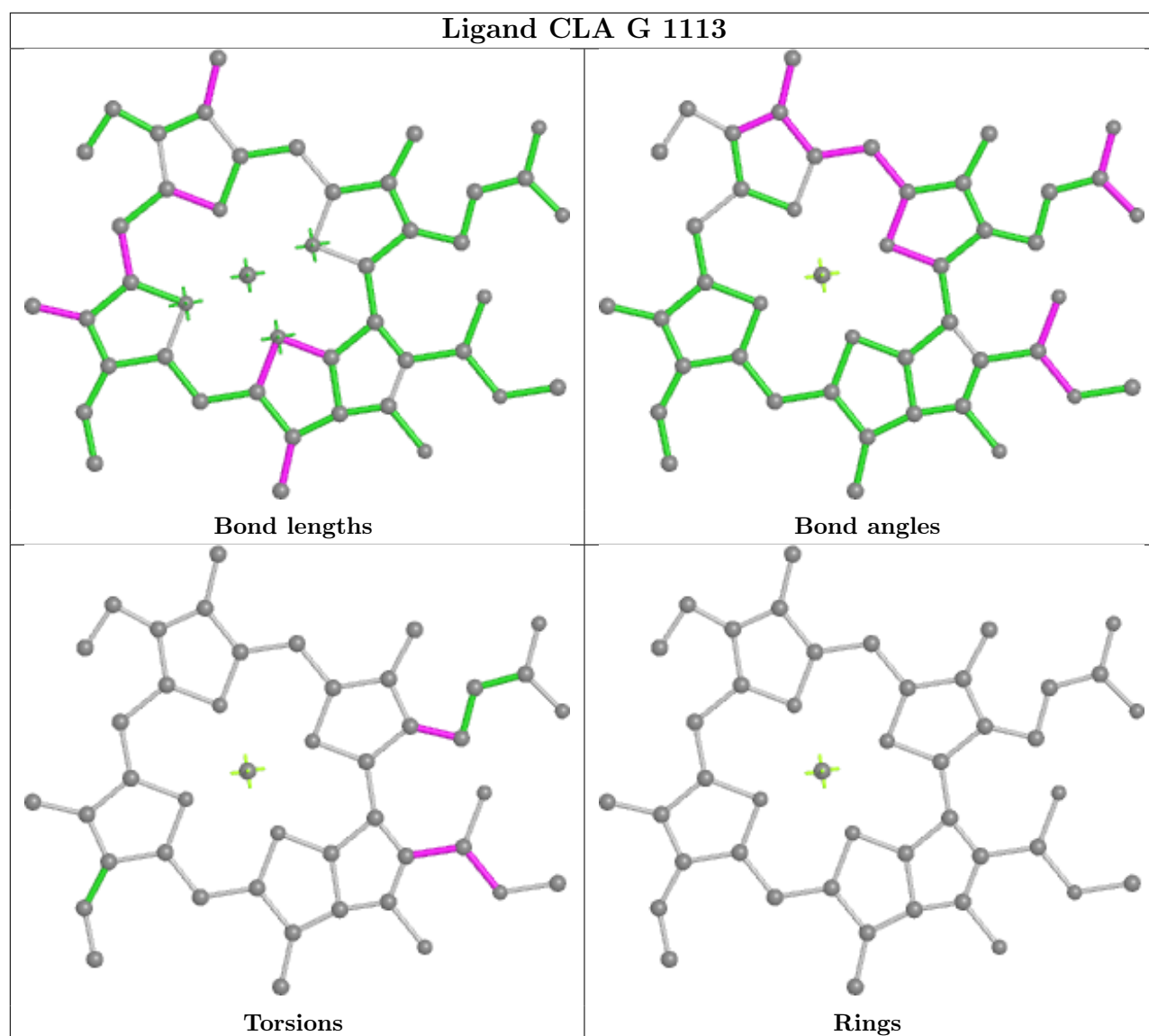
Rings

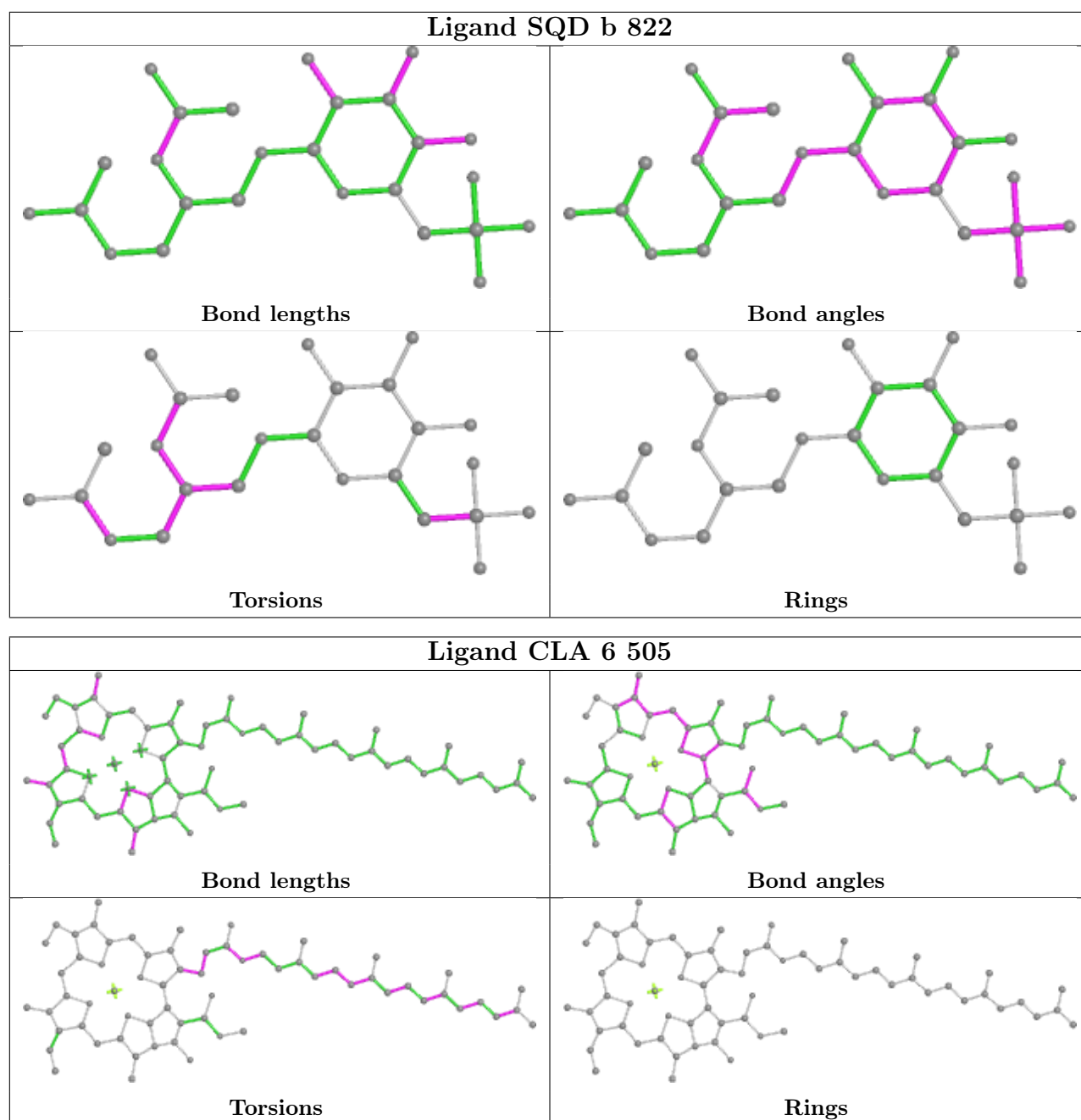
Ligand CLA 5 508



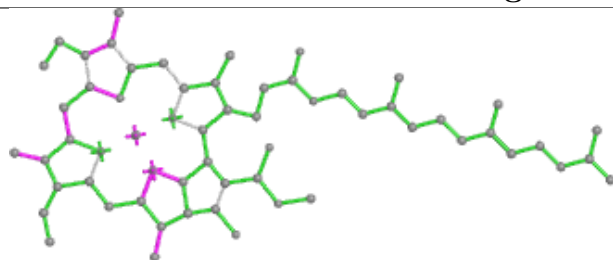
Ligand CLA a 513



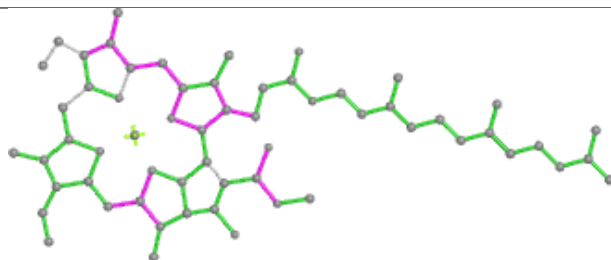




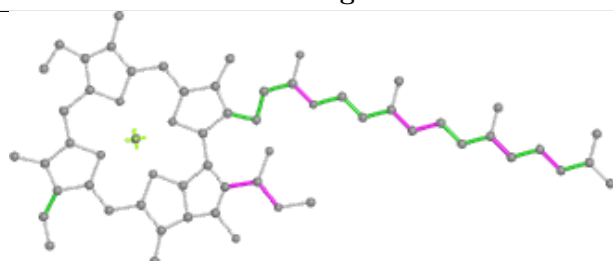
Ligand CLA A 1124



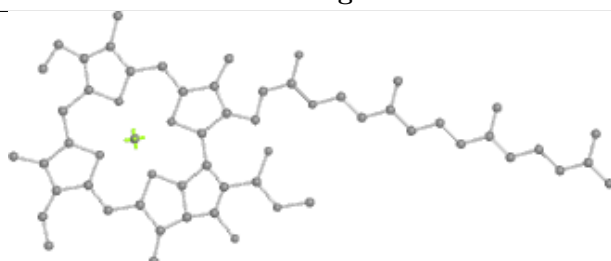
Bond lengths



Bond angles

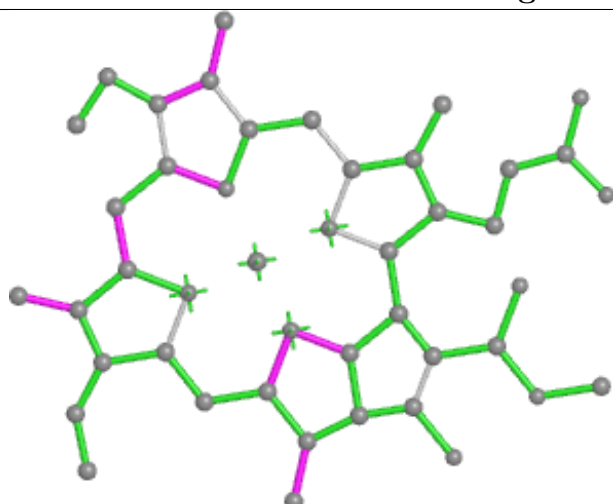


Torsions

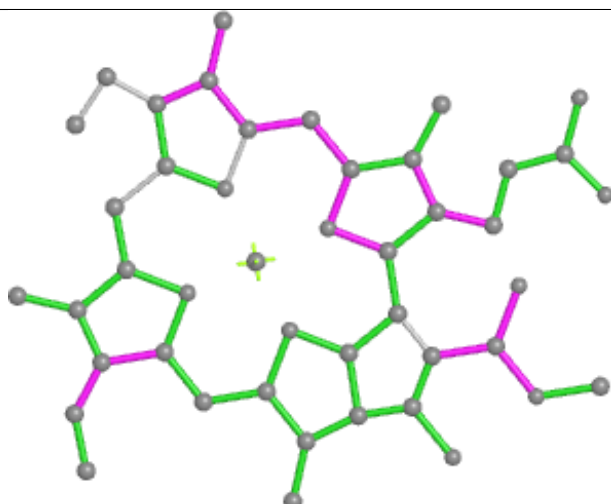


Rings

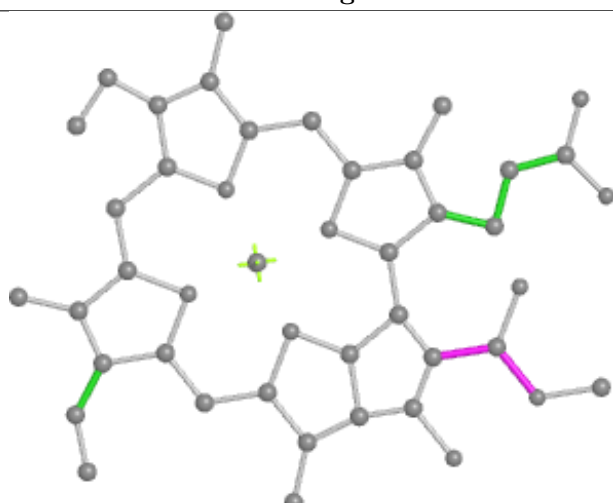
Ligand CLA 1 504



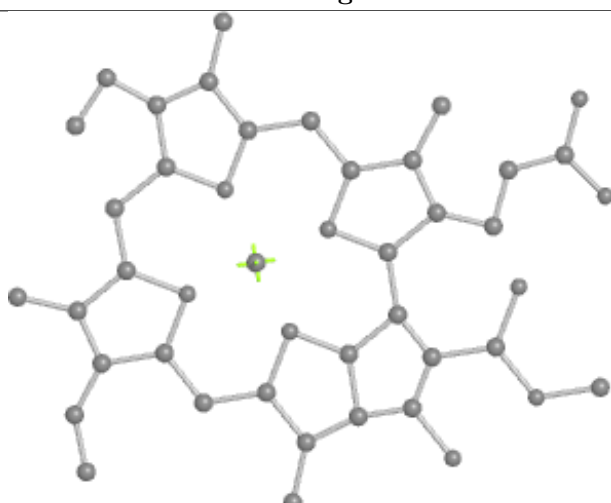
Bond lengths



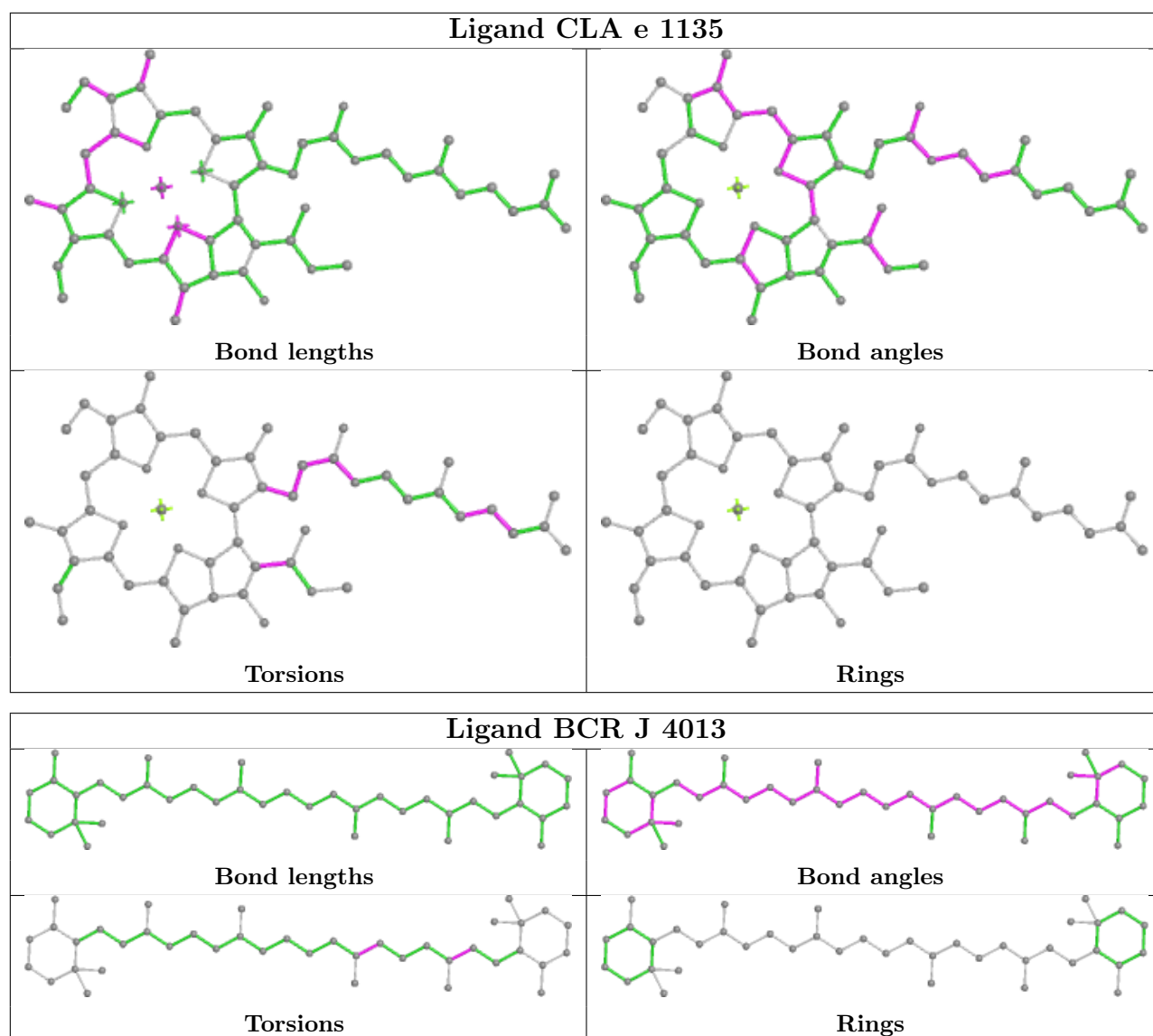
Bond angles



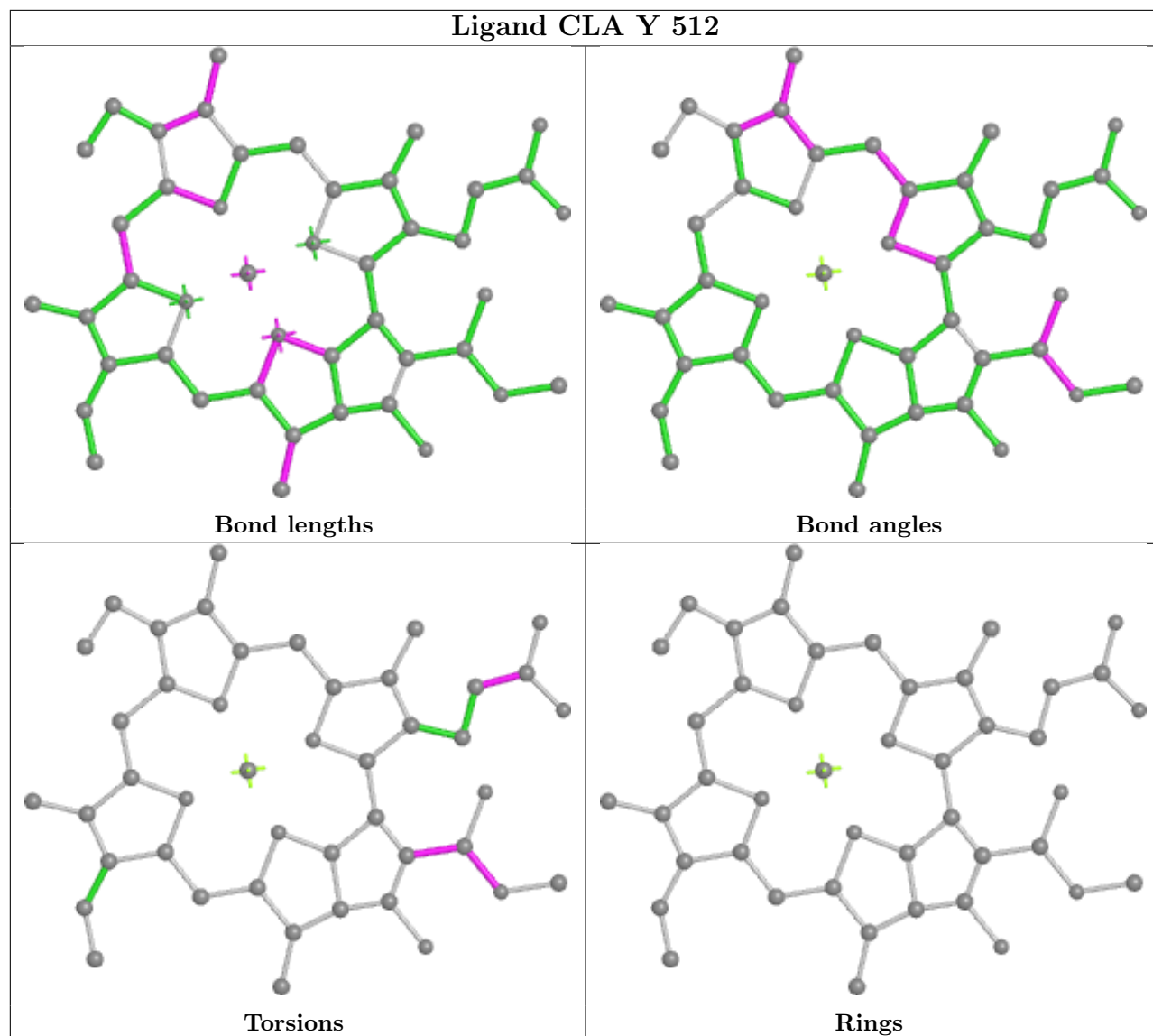
Torsions



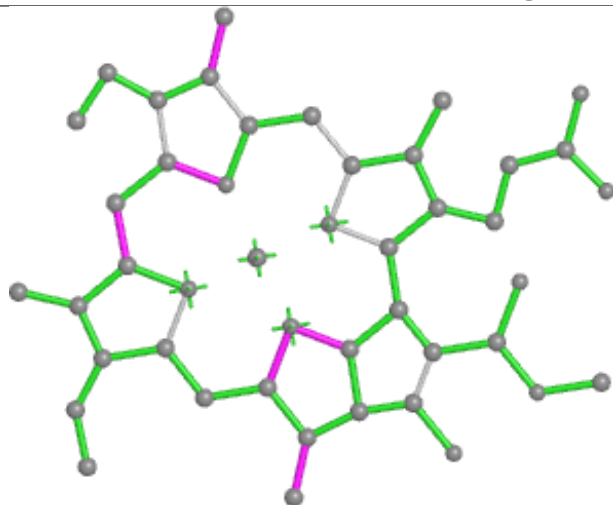
Rings



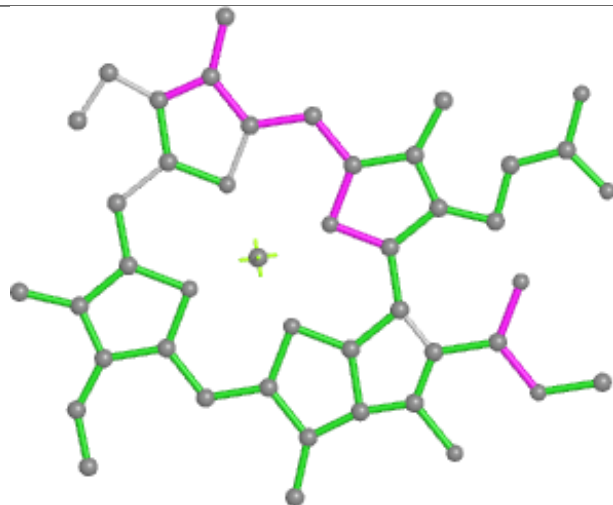
Ligand CLA Y 512



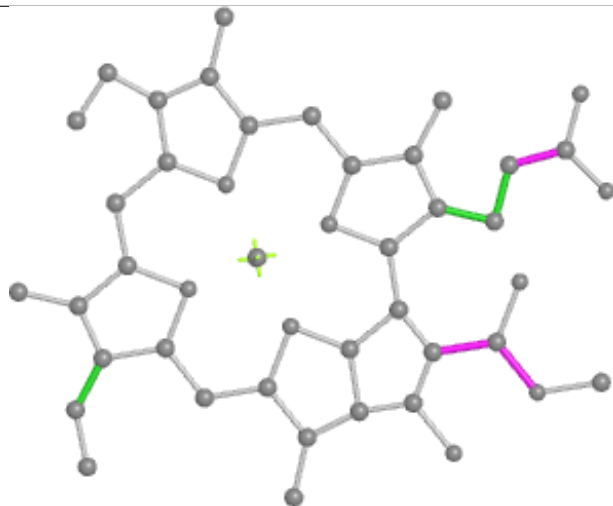
Ligand CLA t 510



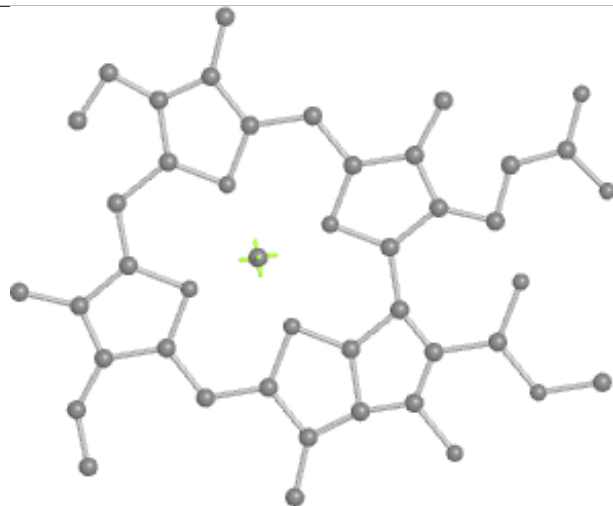
Bond lengths



Bond angles

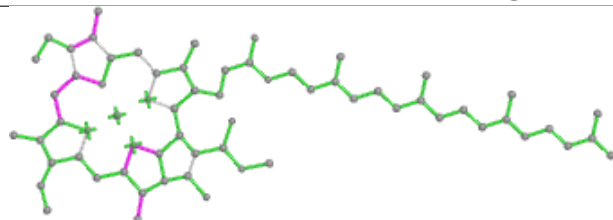


Torsions

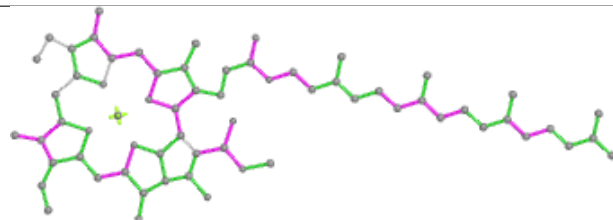


Rings

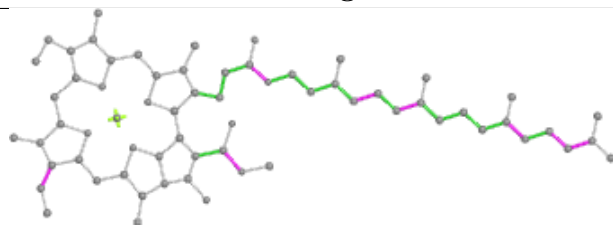
Ligand CLA B 1239



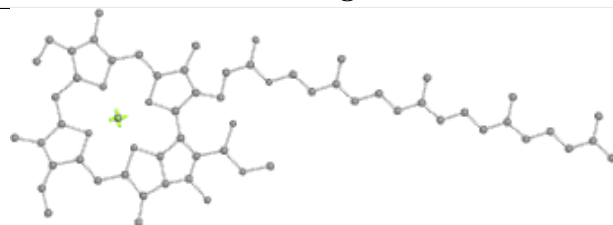
Bond lengths



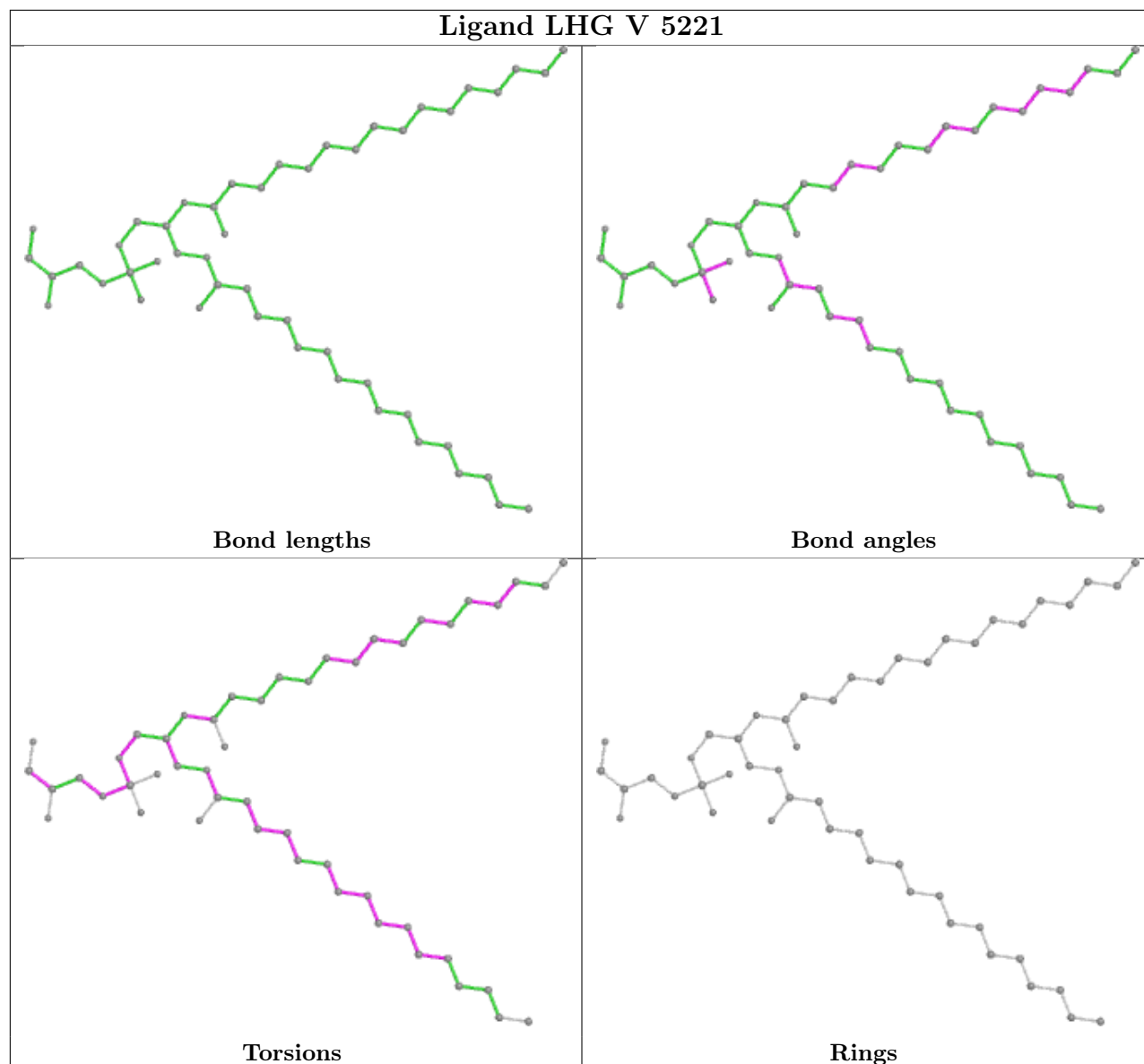
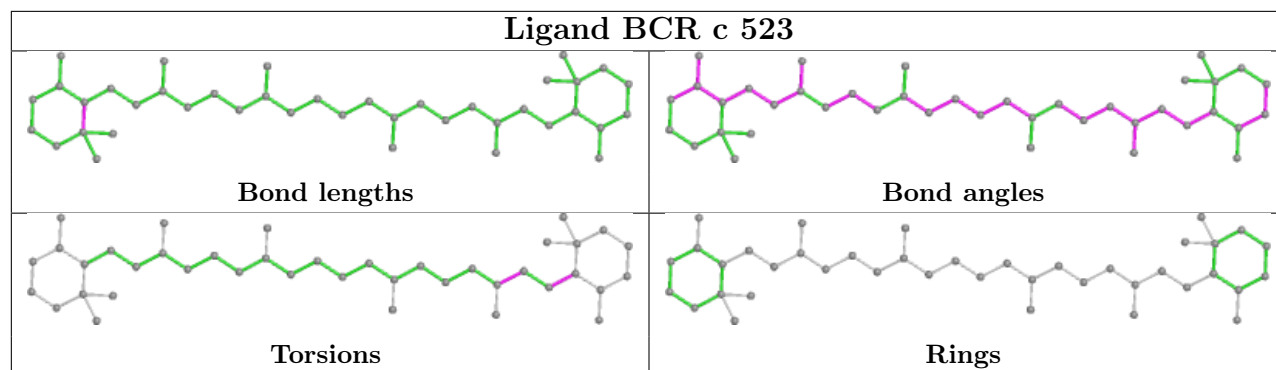
Bond angles

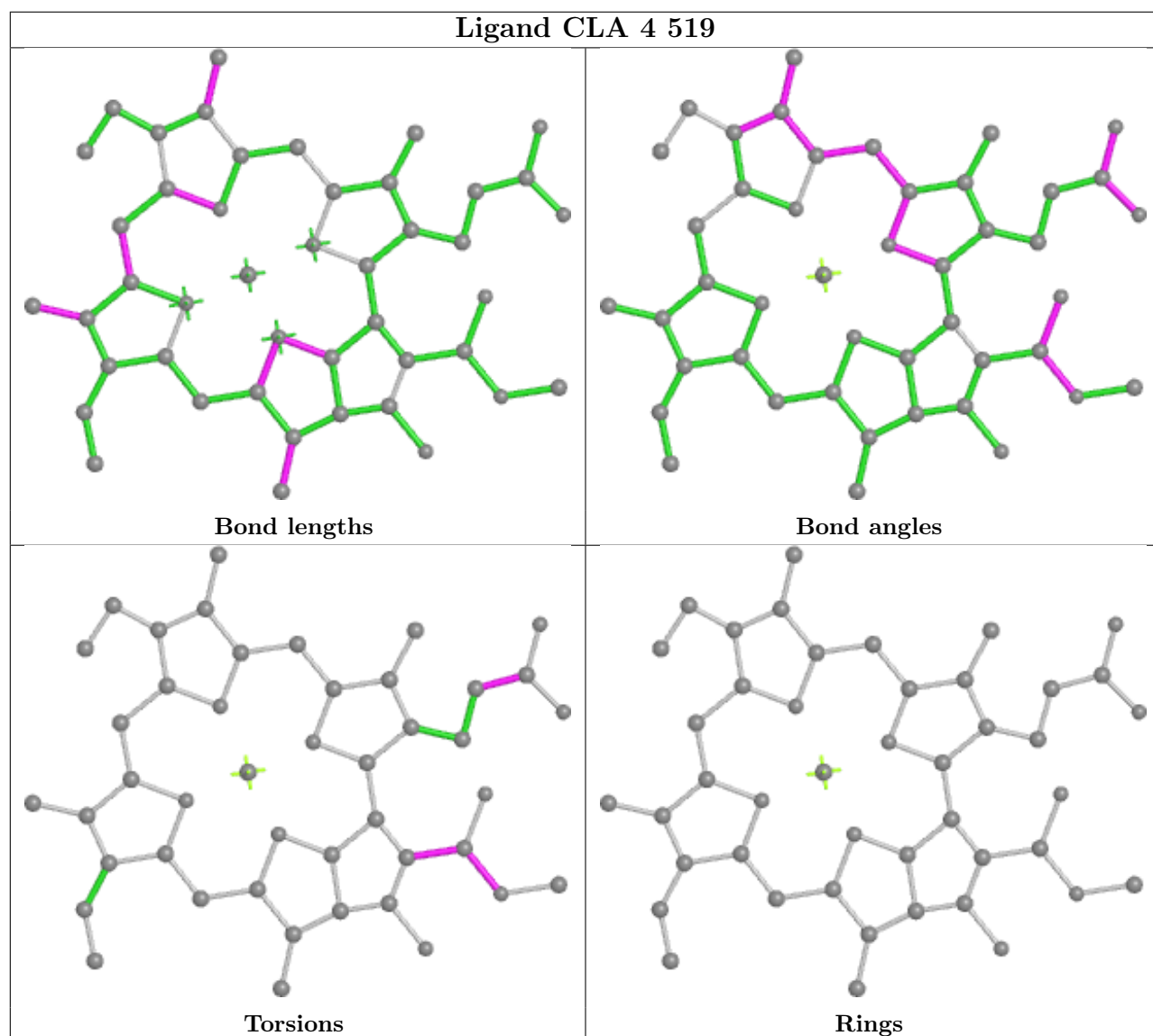
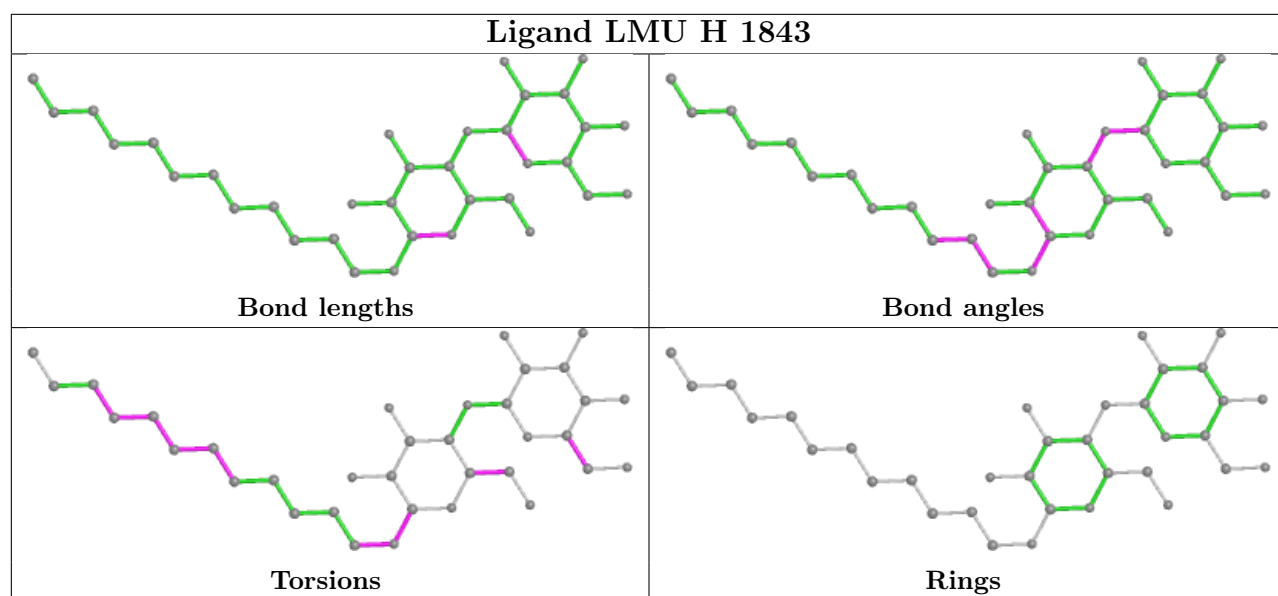


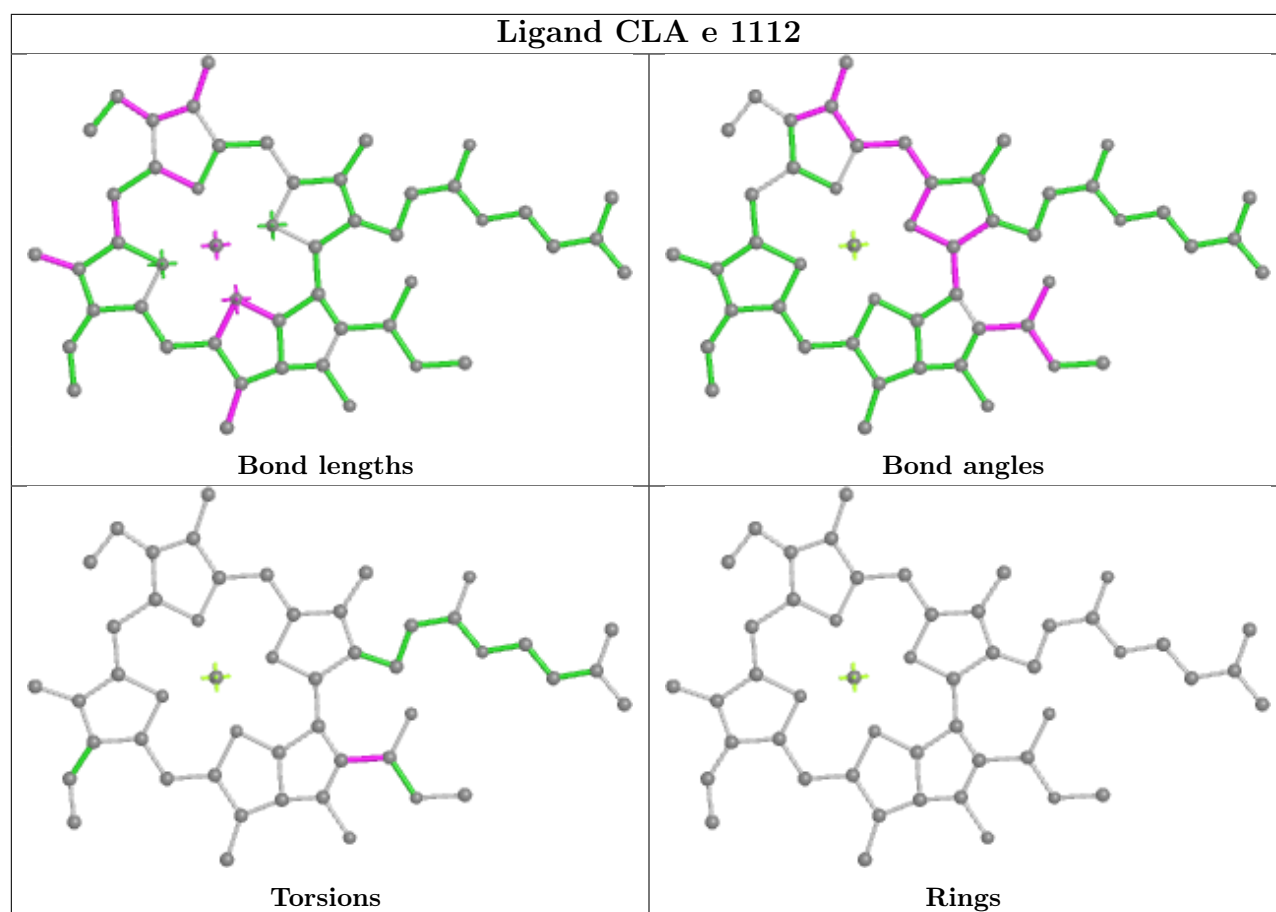
Torsions



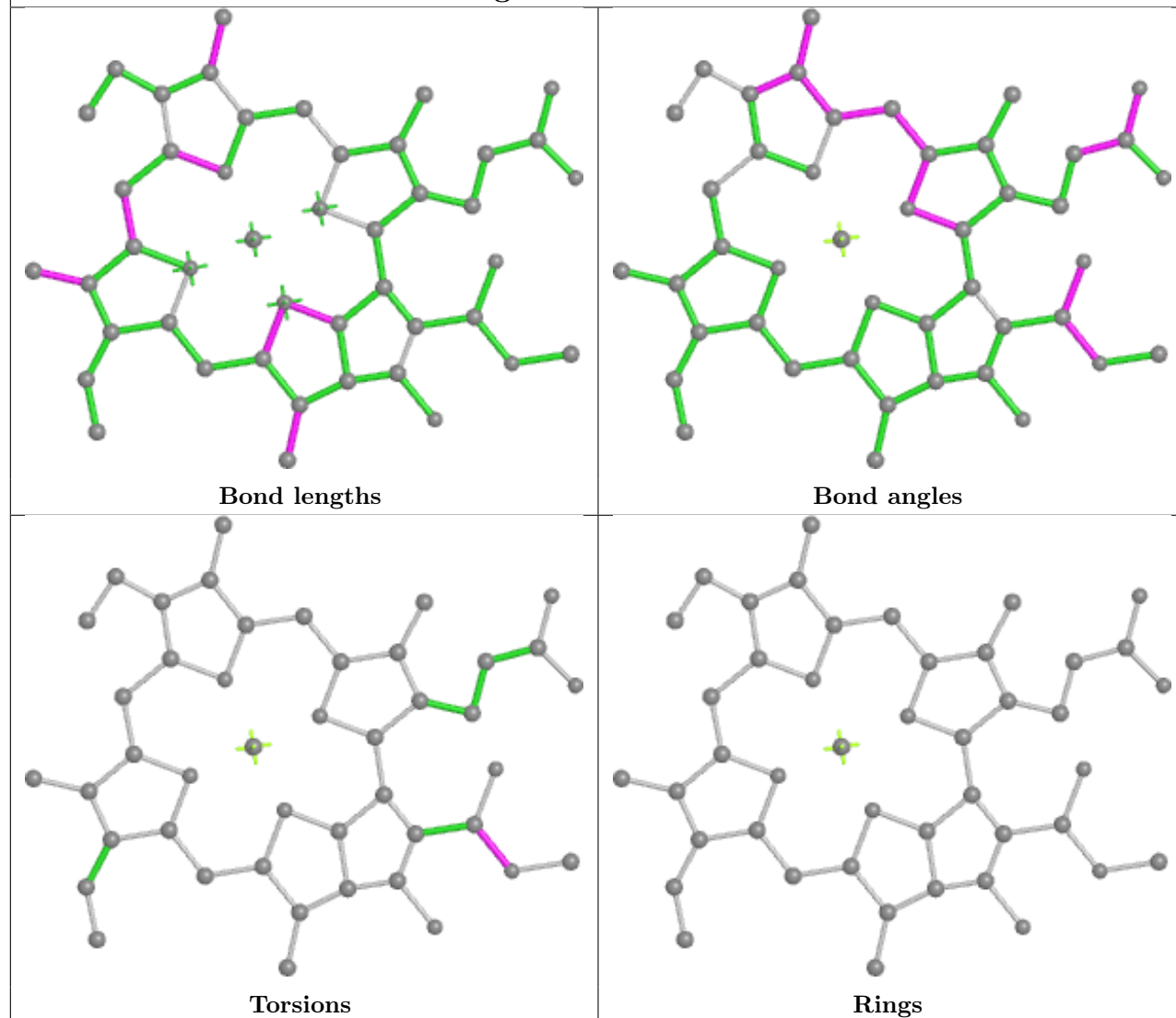
Rings



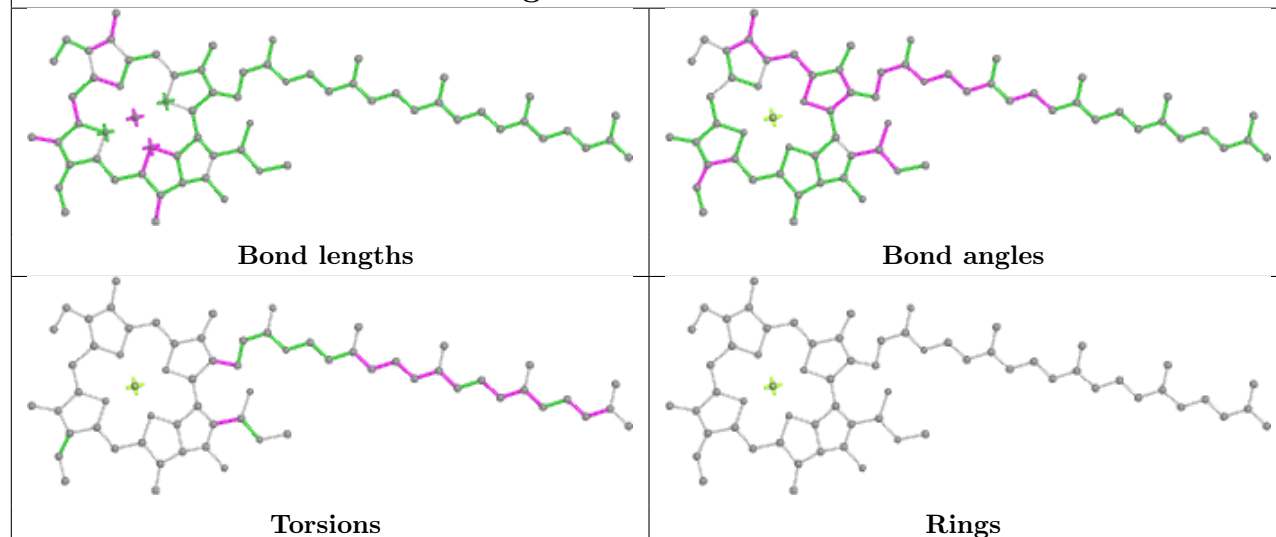




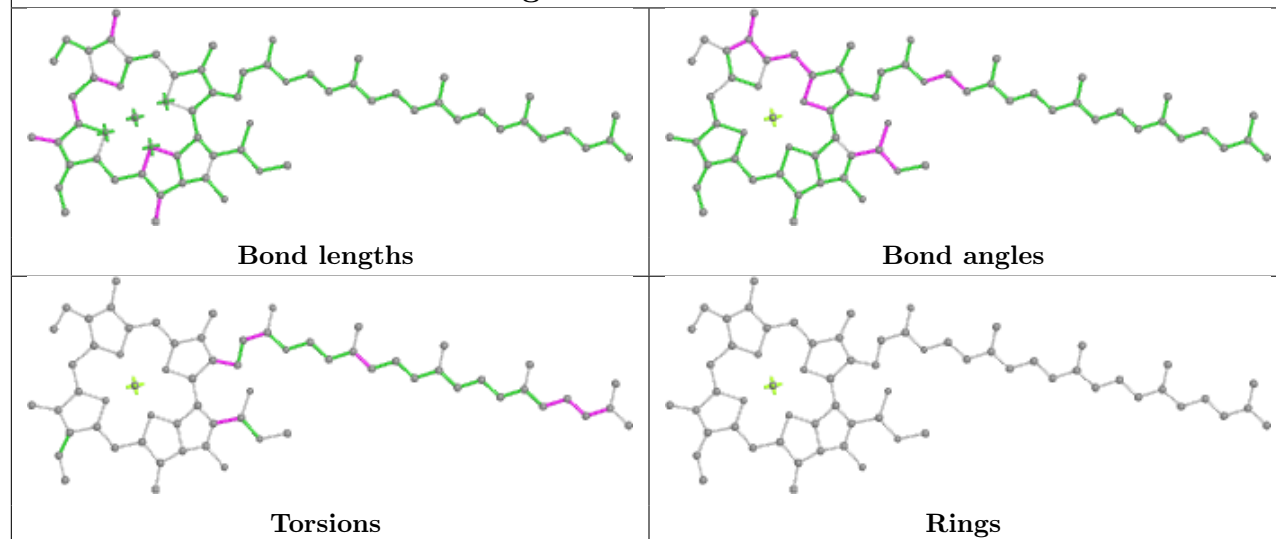
Ligand CLA 3 509



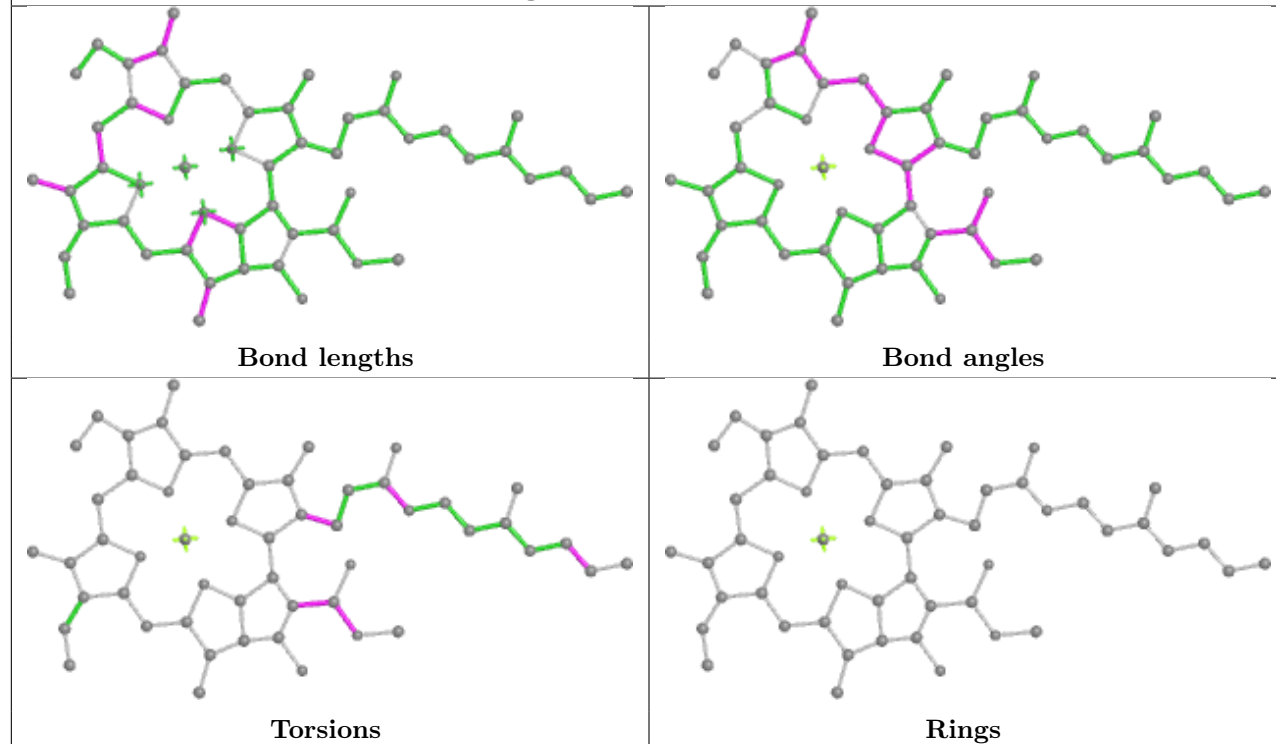
Ligand CLA A 1101



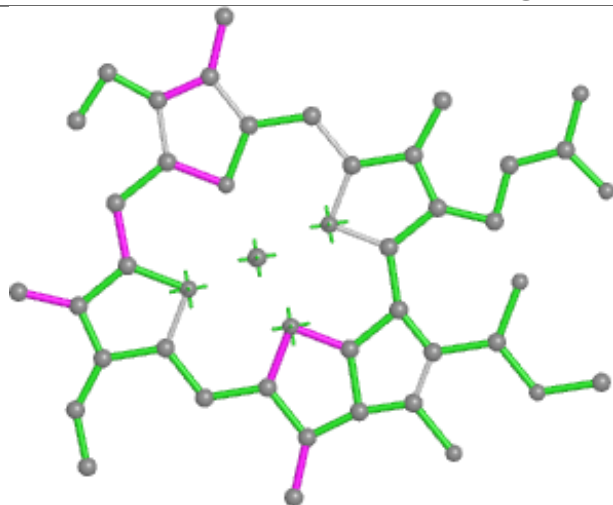
Ligand CLA H 1202



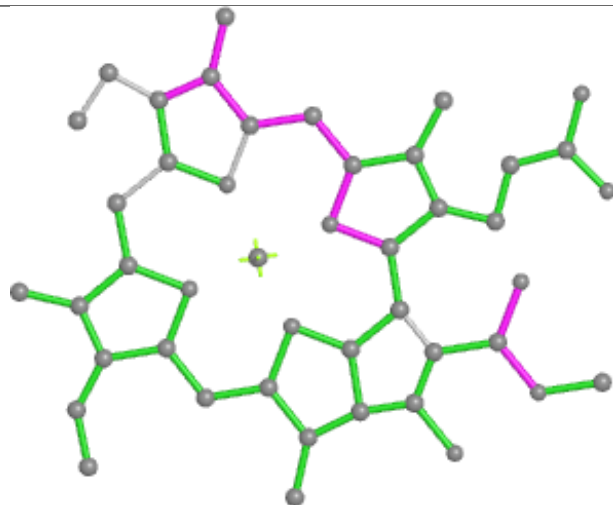
Ligand CLA H 1209



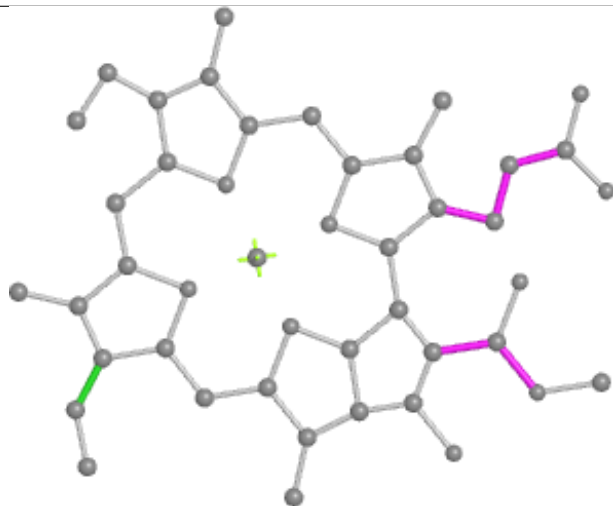
Ligand CLA u 517



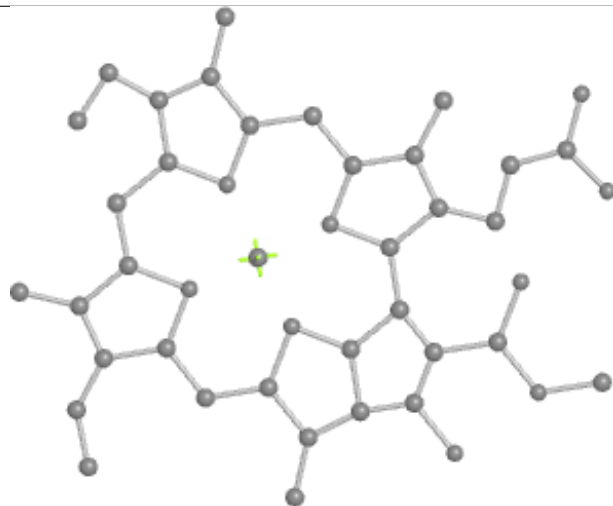
Bond lengths



Bond angles

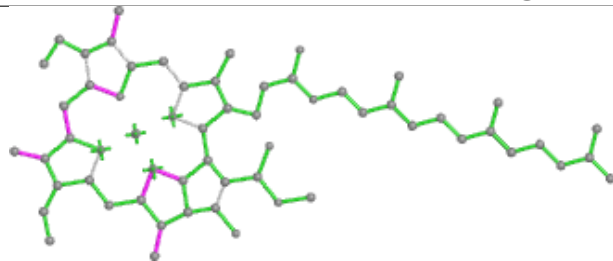


Torsions

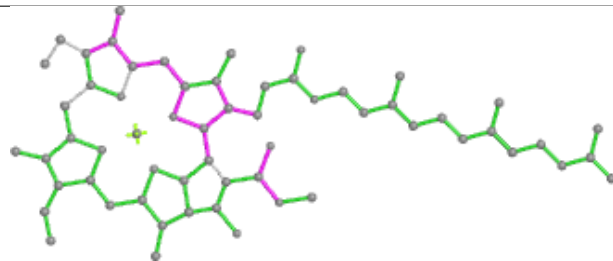


Rings

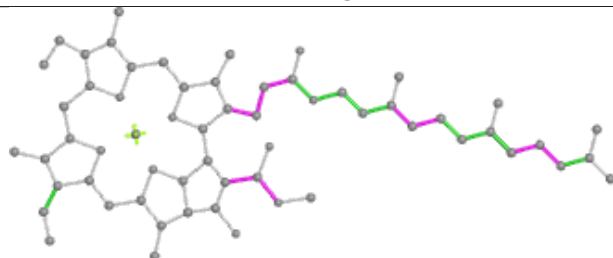
Ligand CLA 2 501



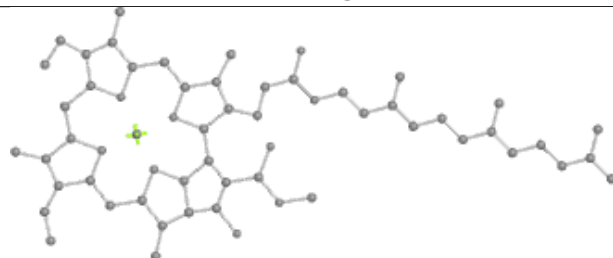
Bond lengths



Bond angles

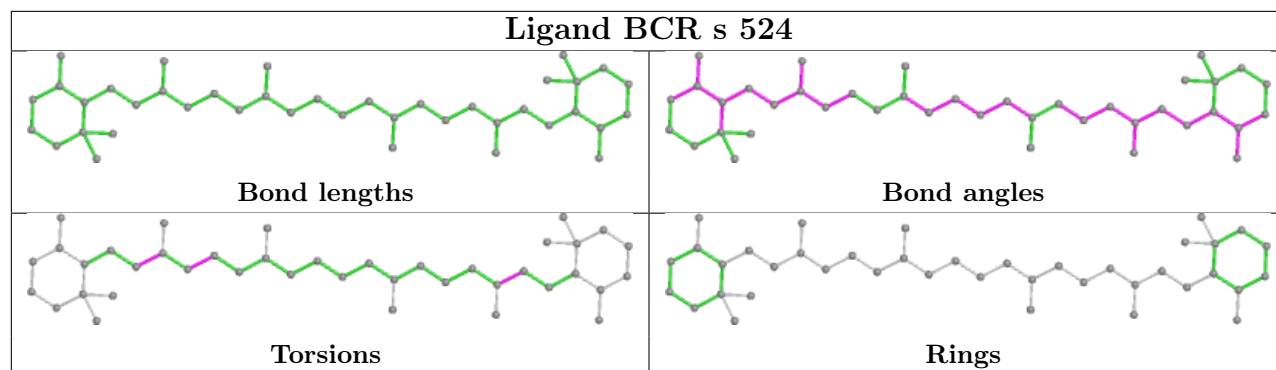


Torsions

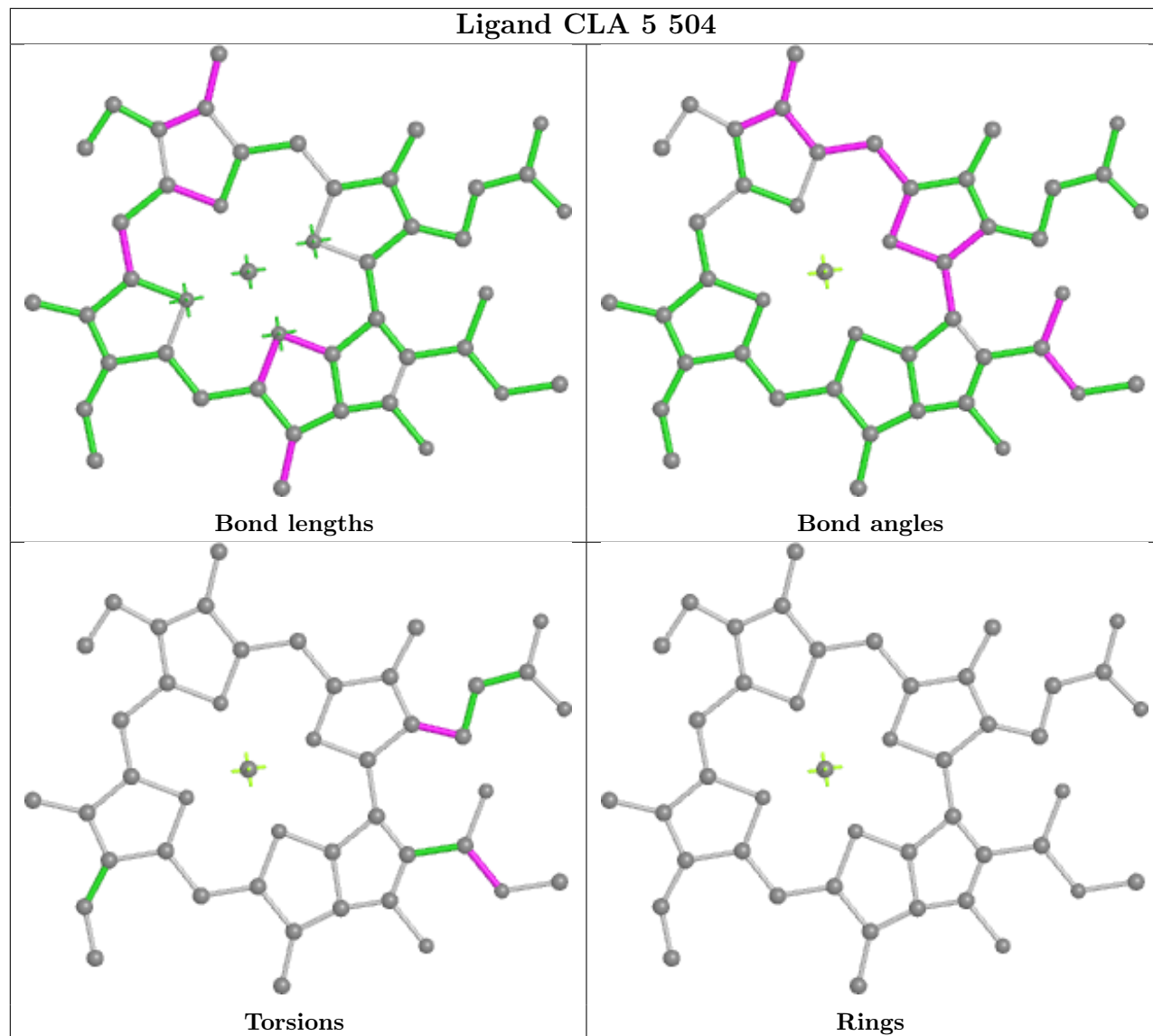


Rings

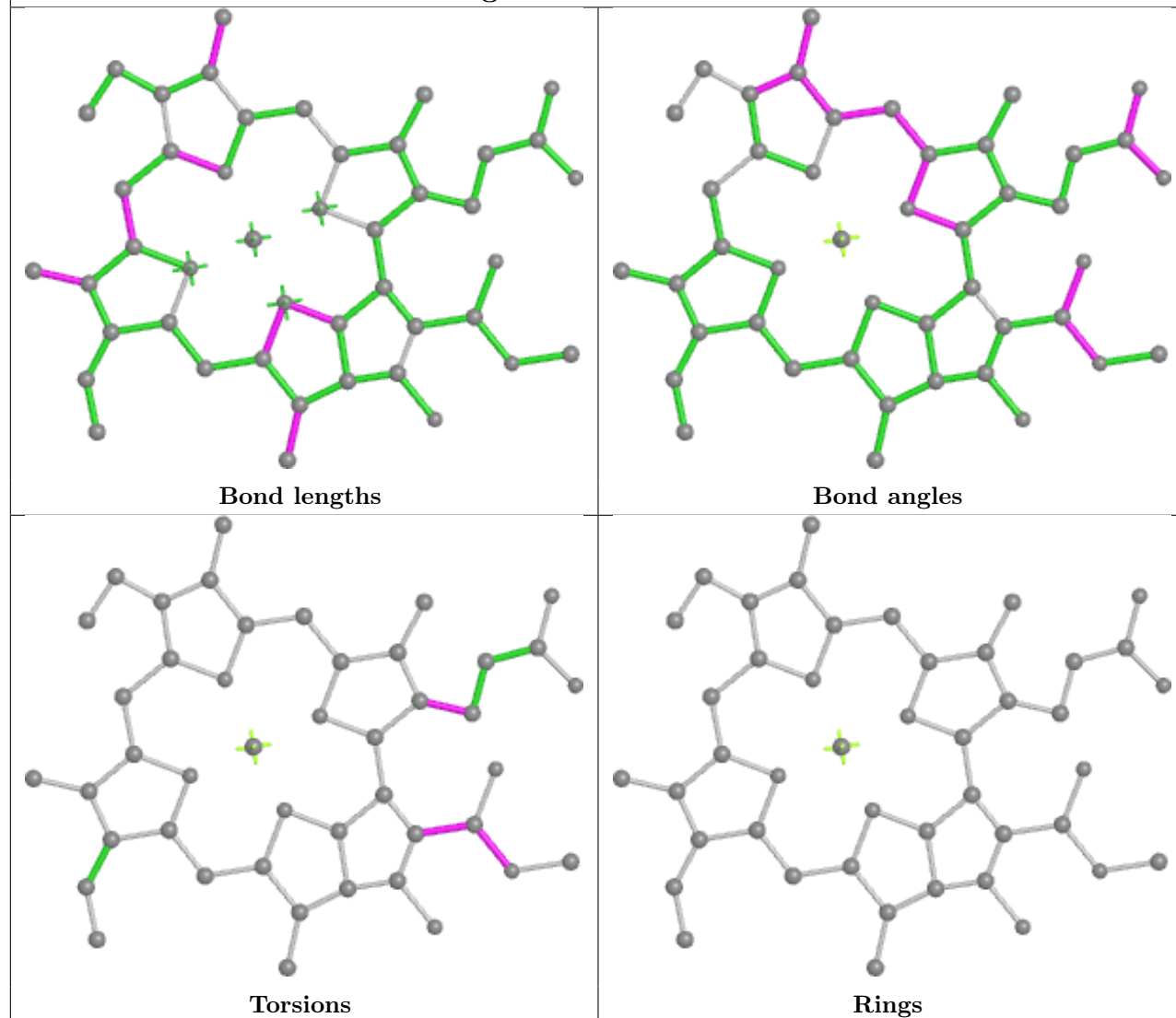
Ligand BCR s 524



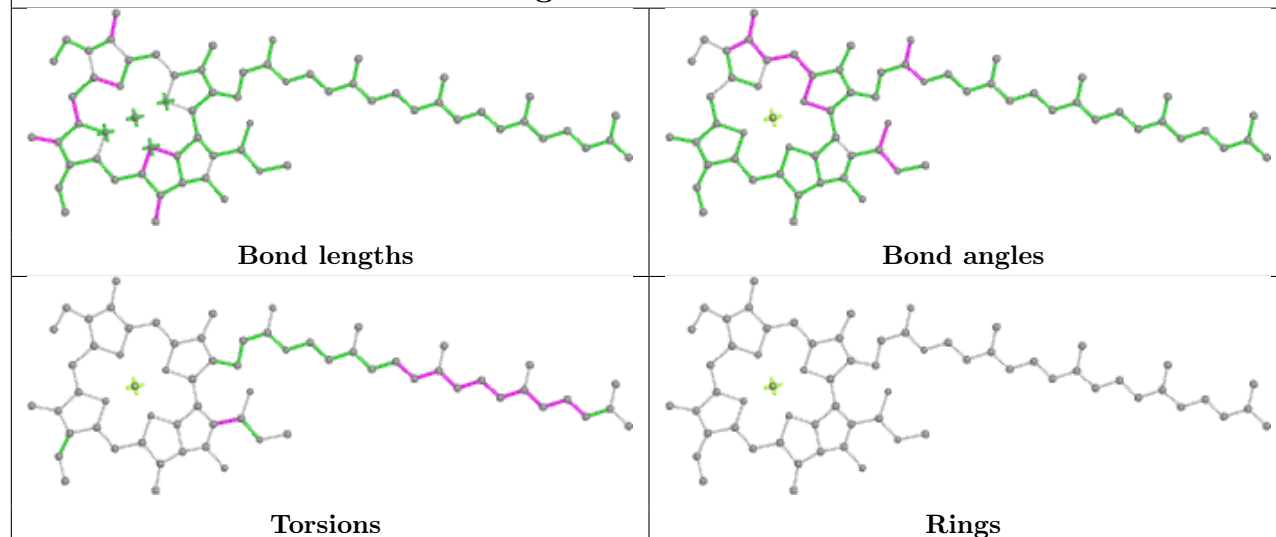
Ligand CLA 5 504

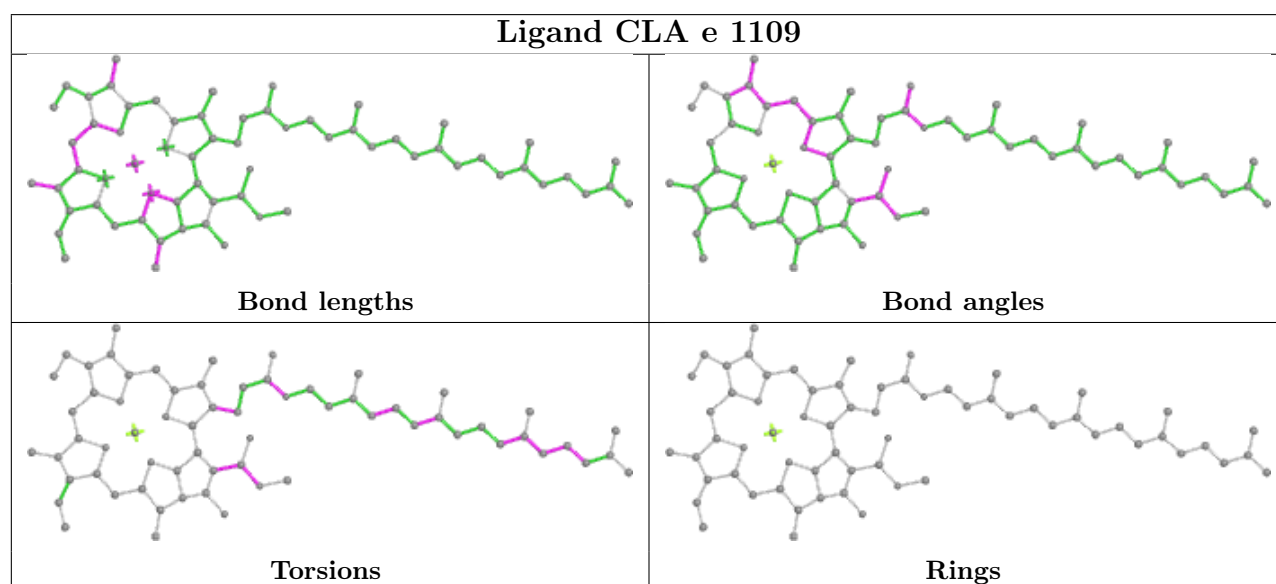
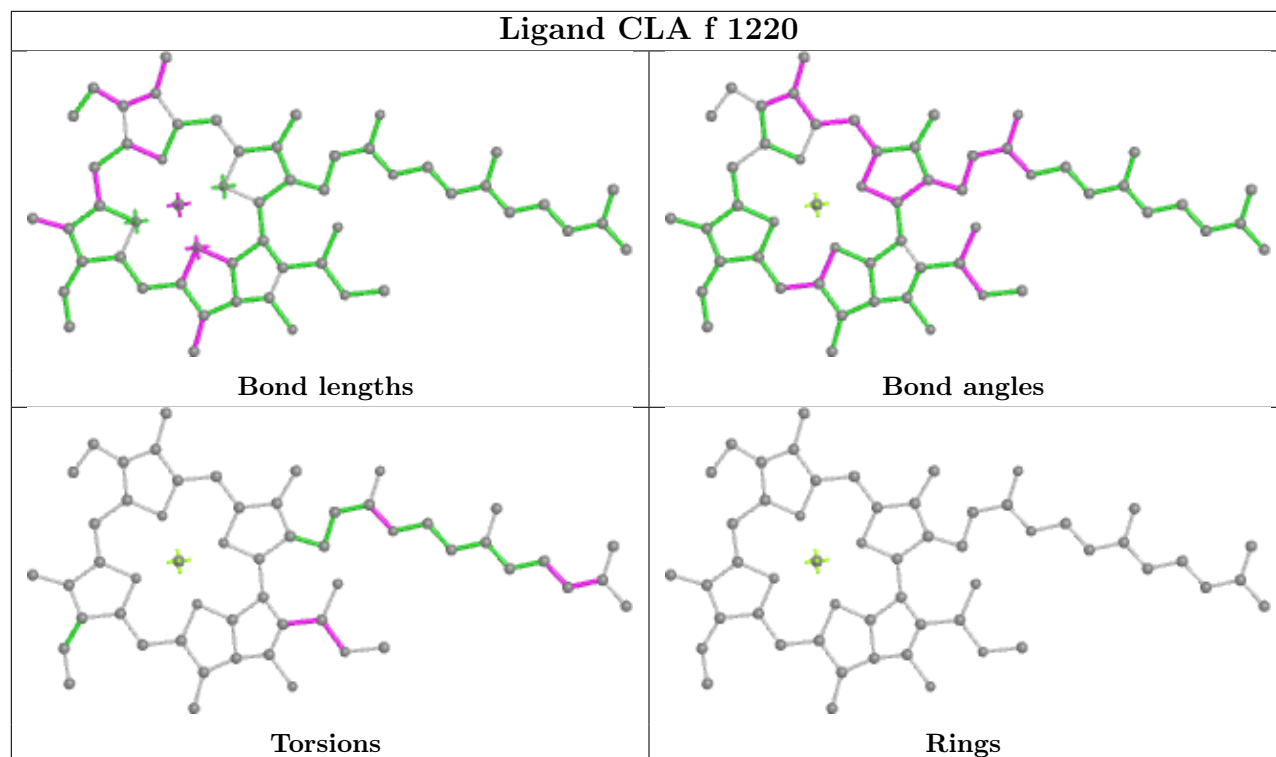
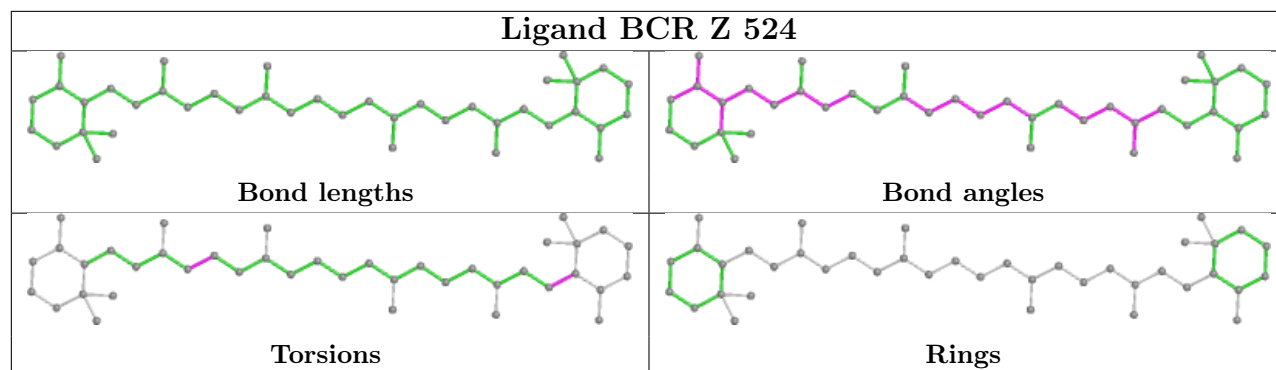


Ligand CLA A 1113

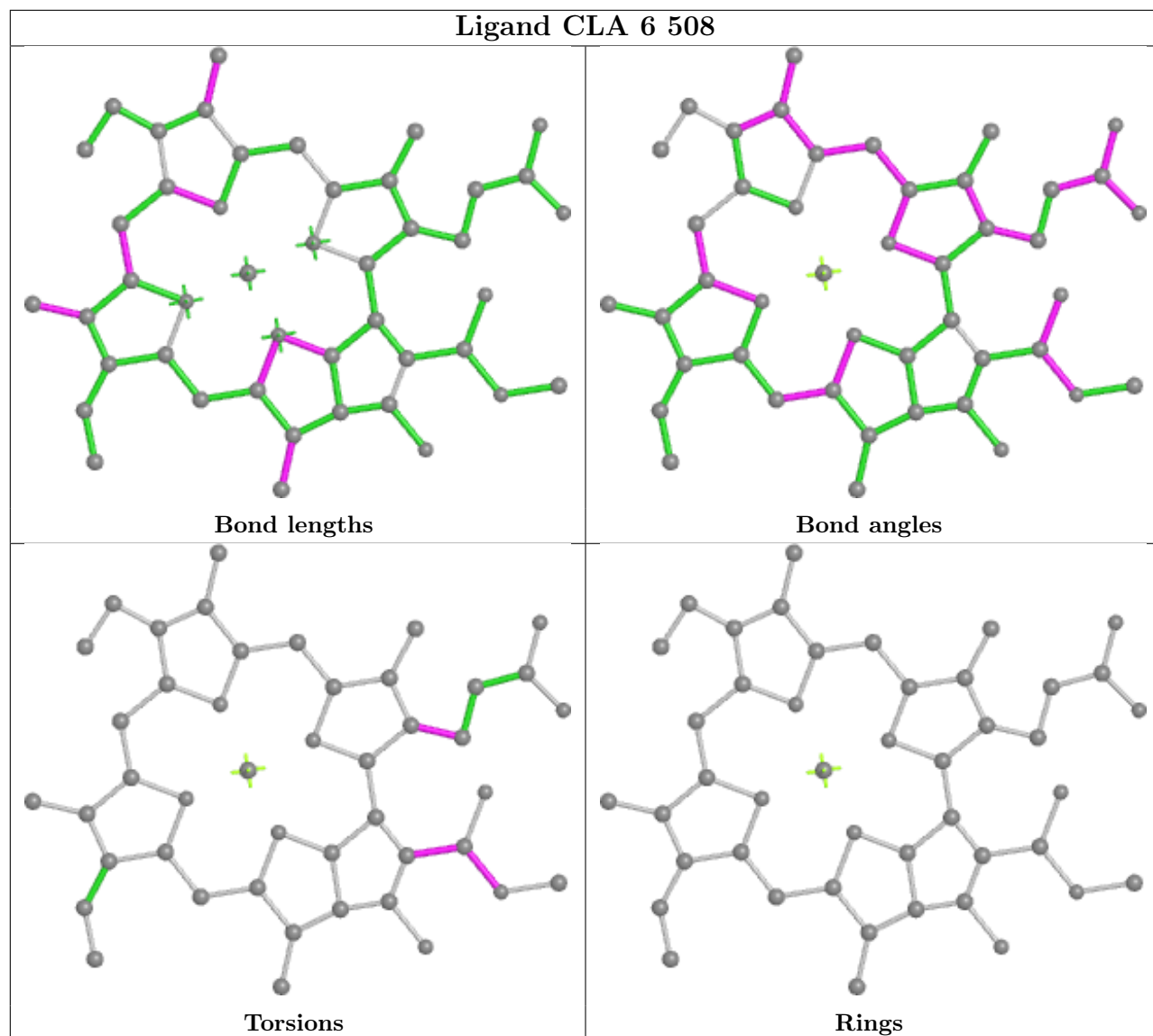


Ligand CLA u 509

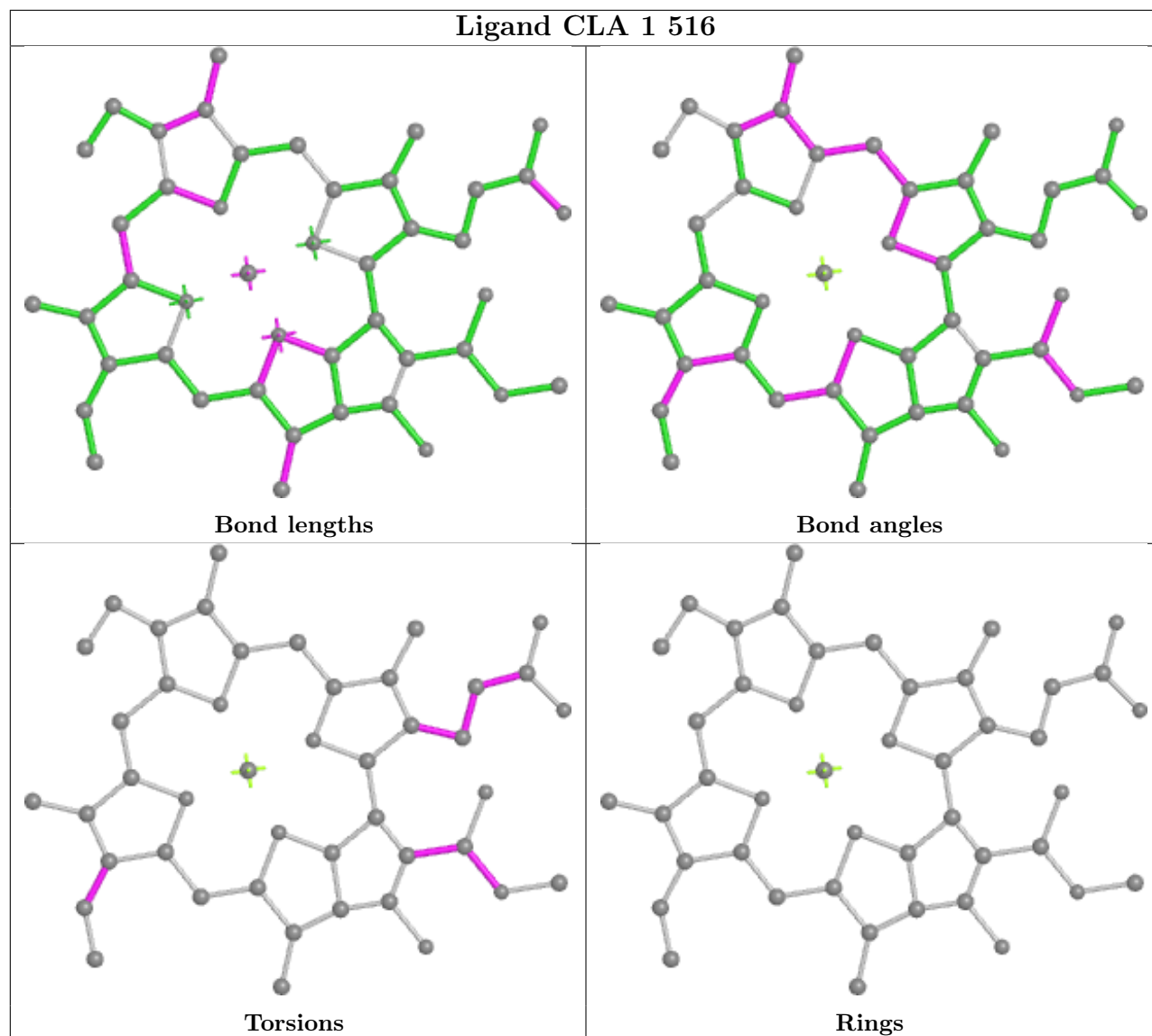




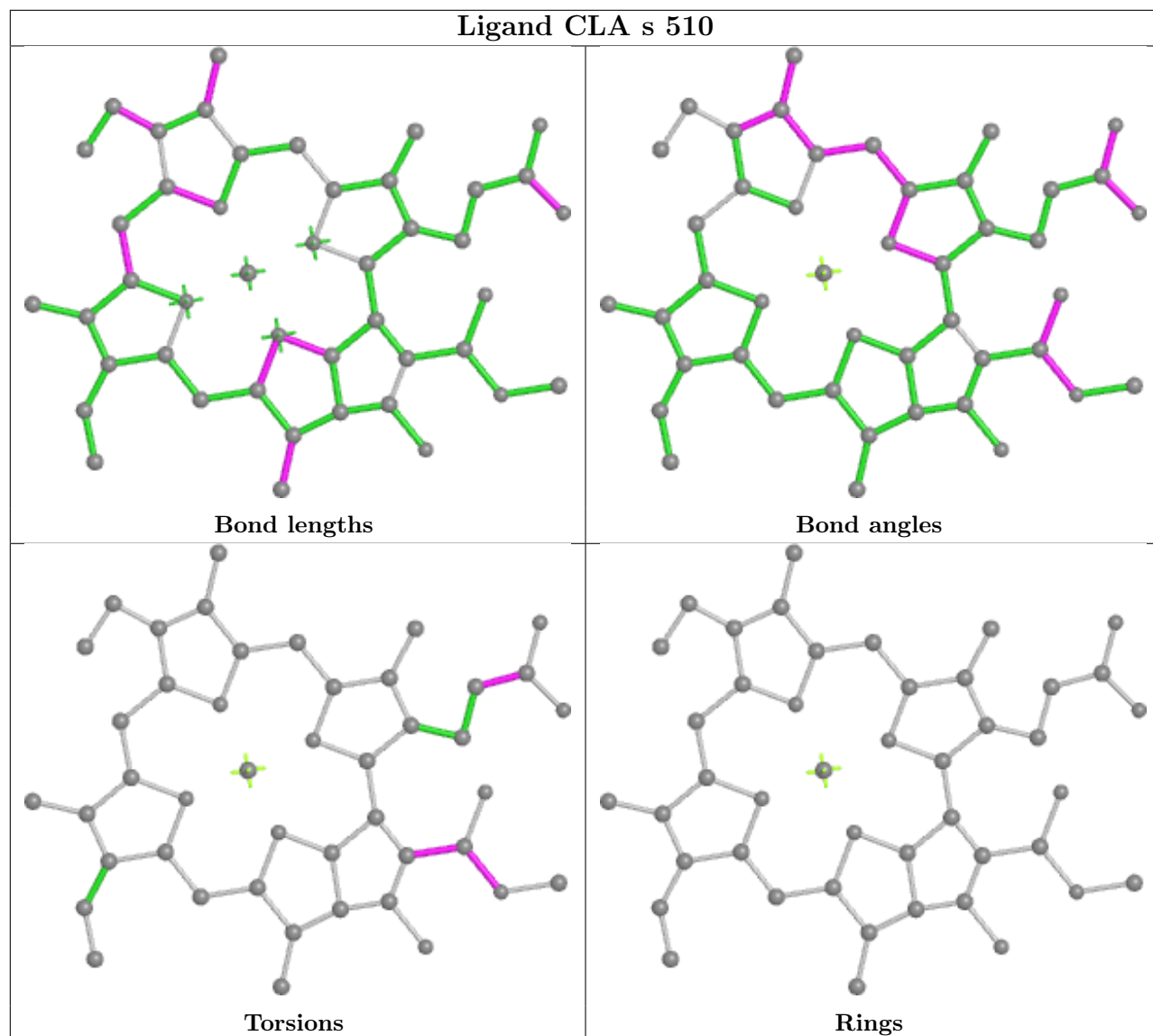
Ligand CLA 6 508



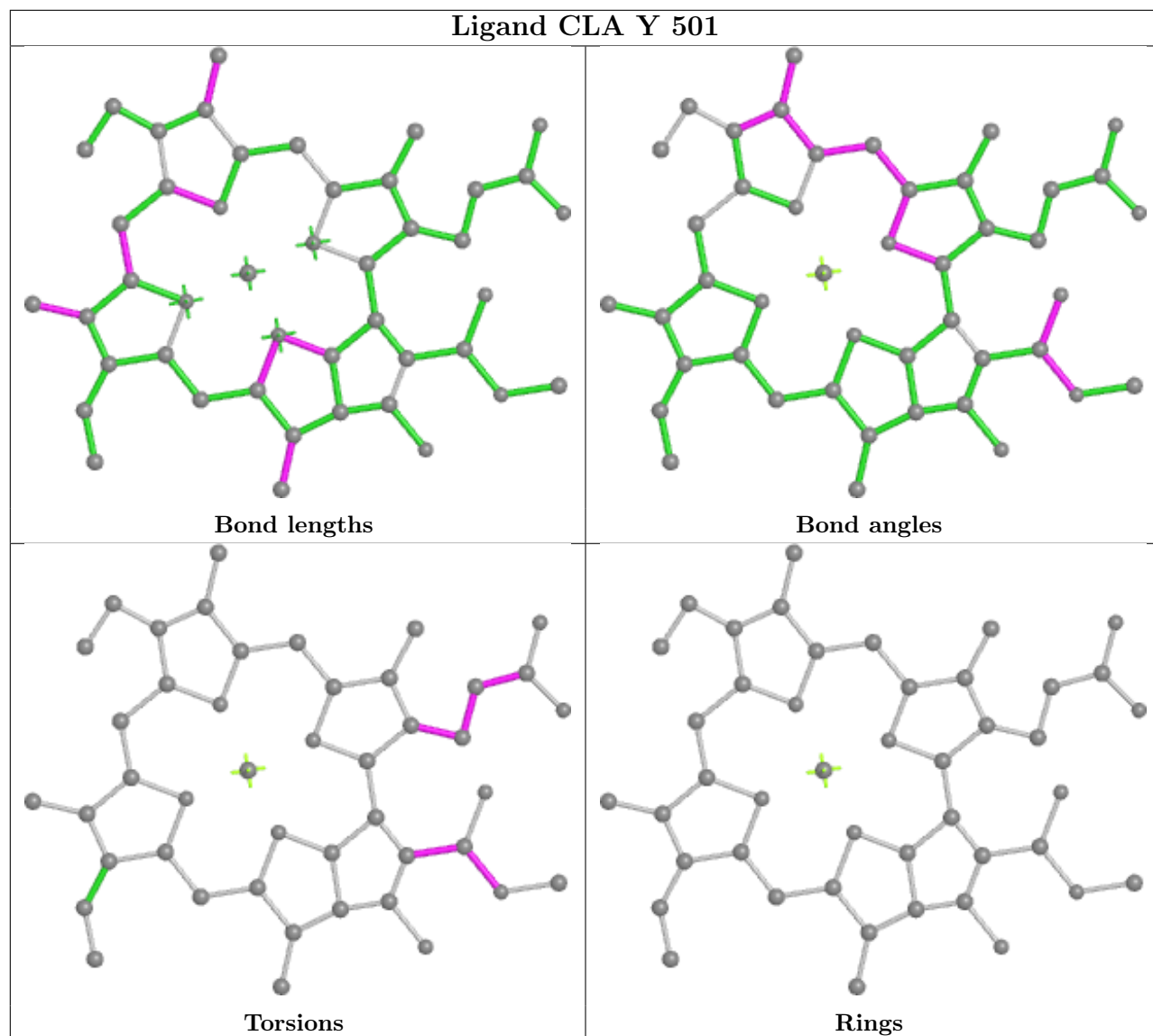
Ligand CLA 1 516



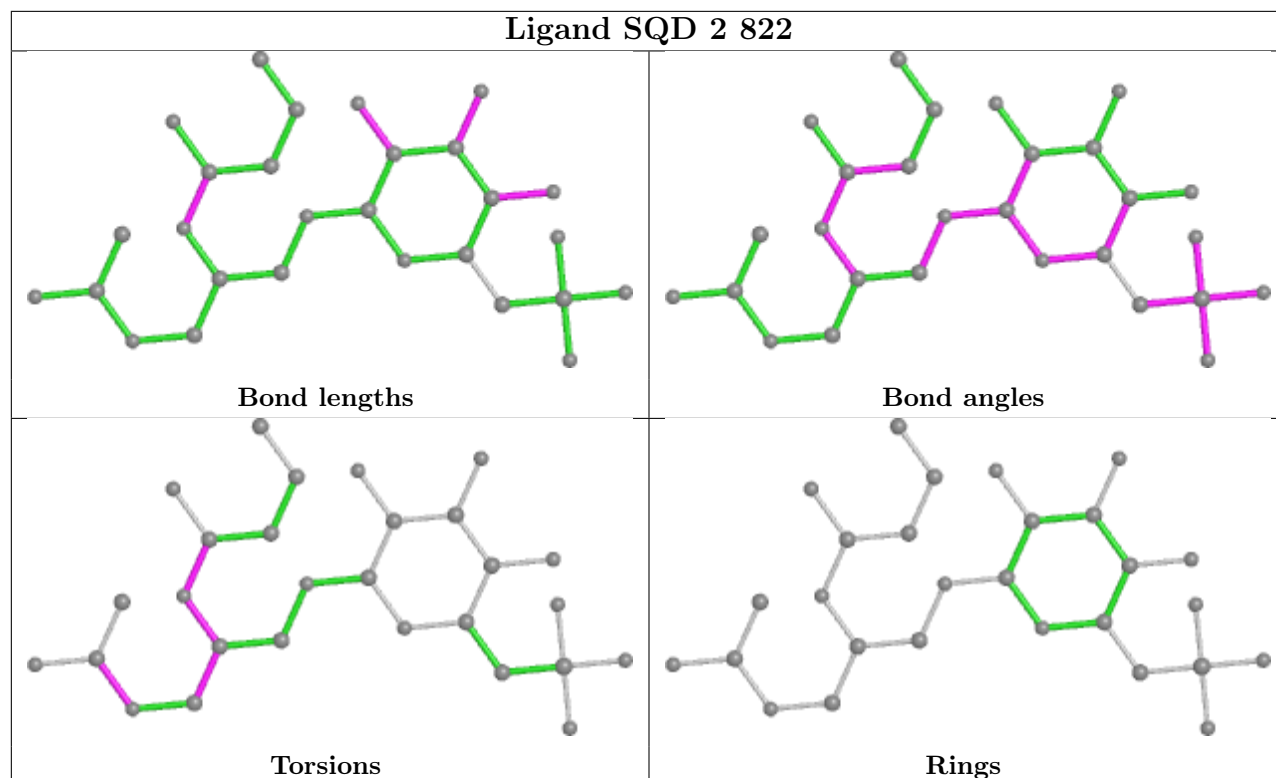
Ligand CLA s 510



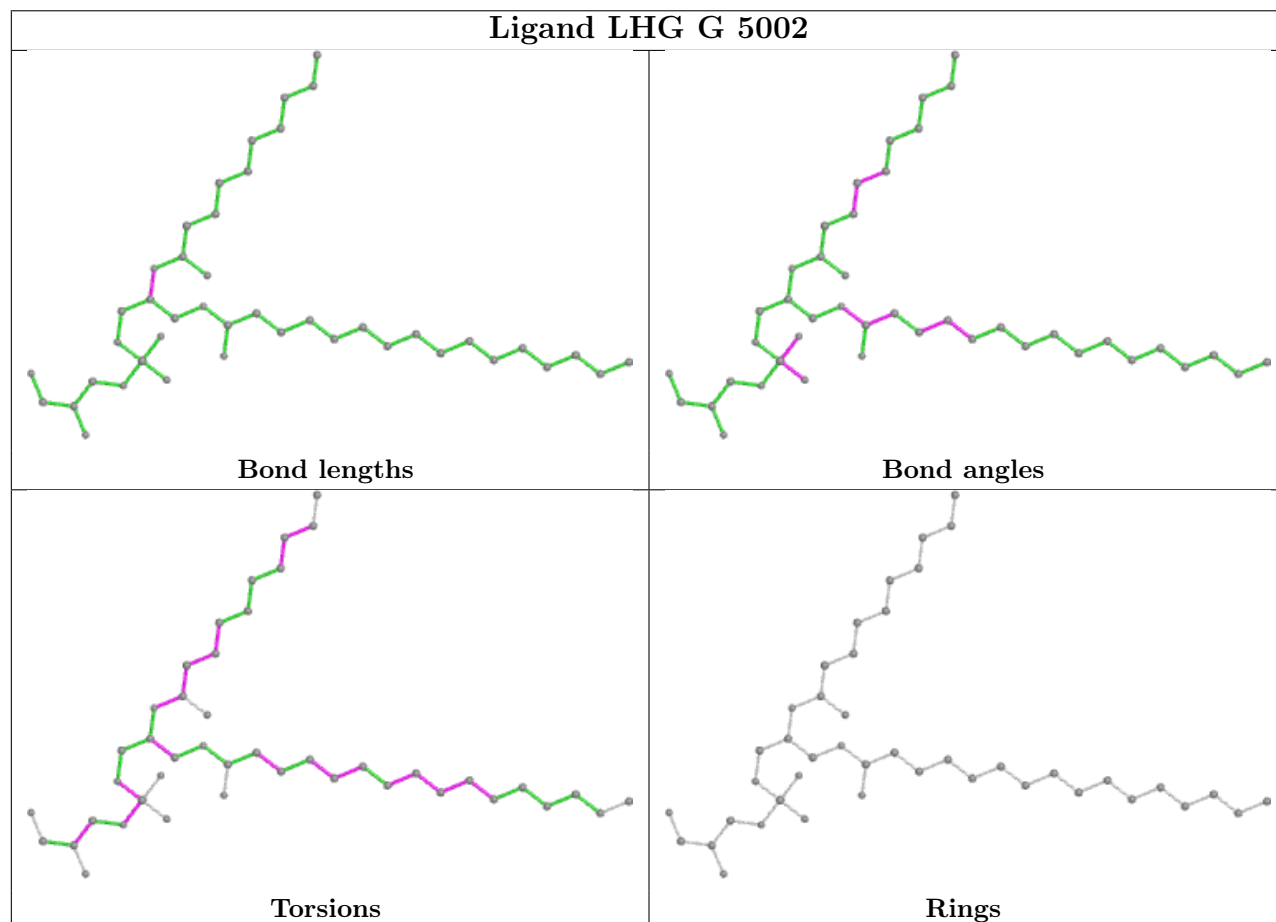
Ligand CLA Y 501



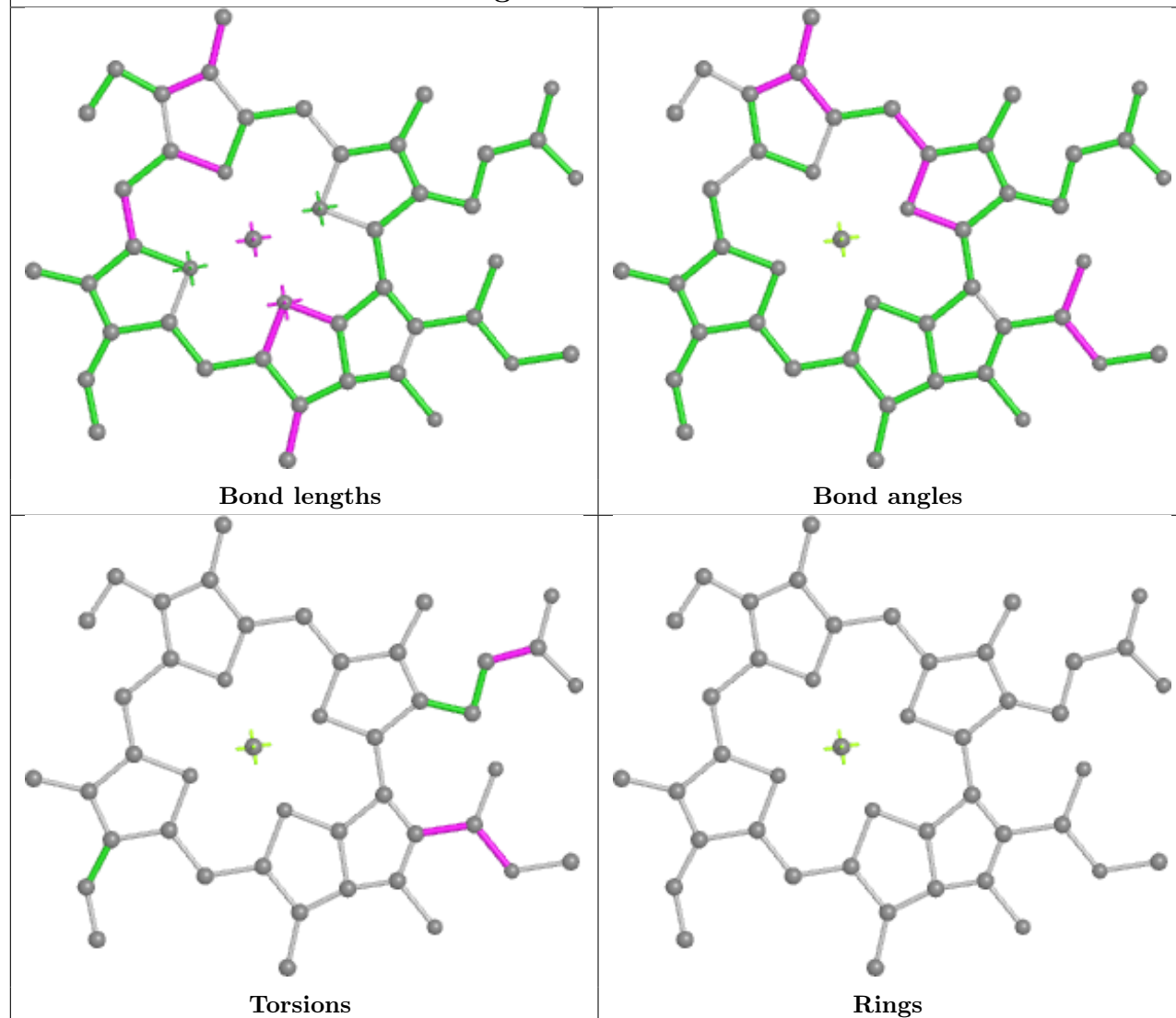
Ligand SQD 2 822



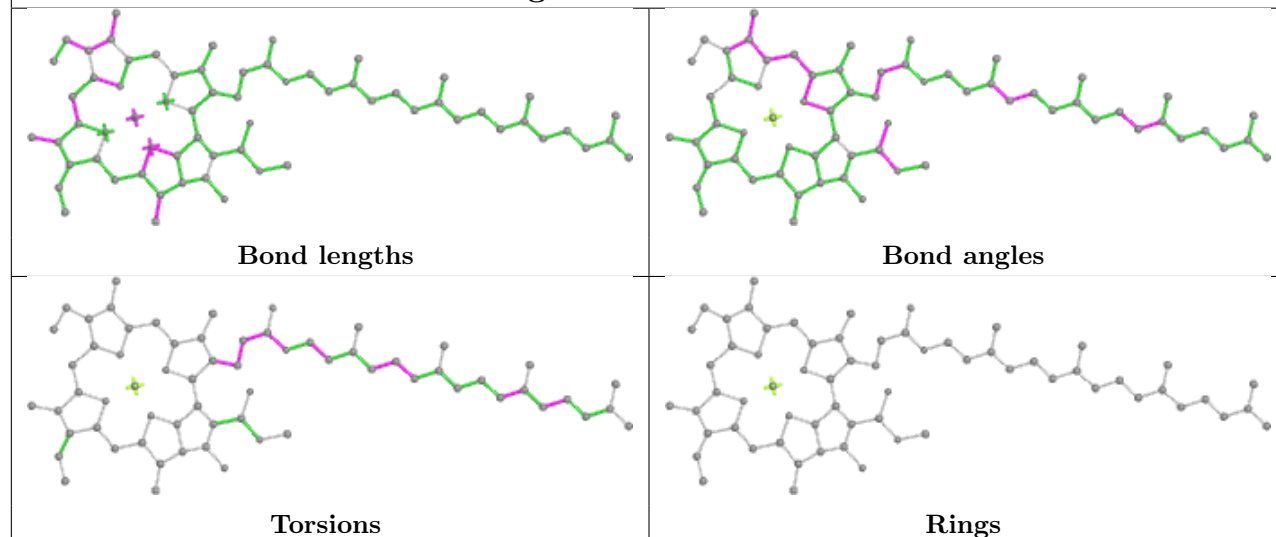
Ligand LHG G 5002

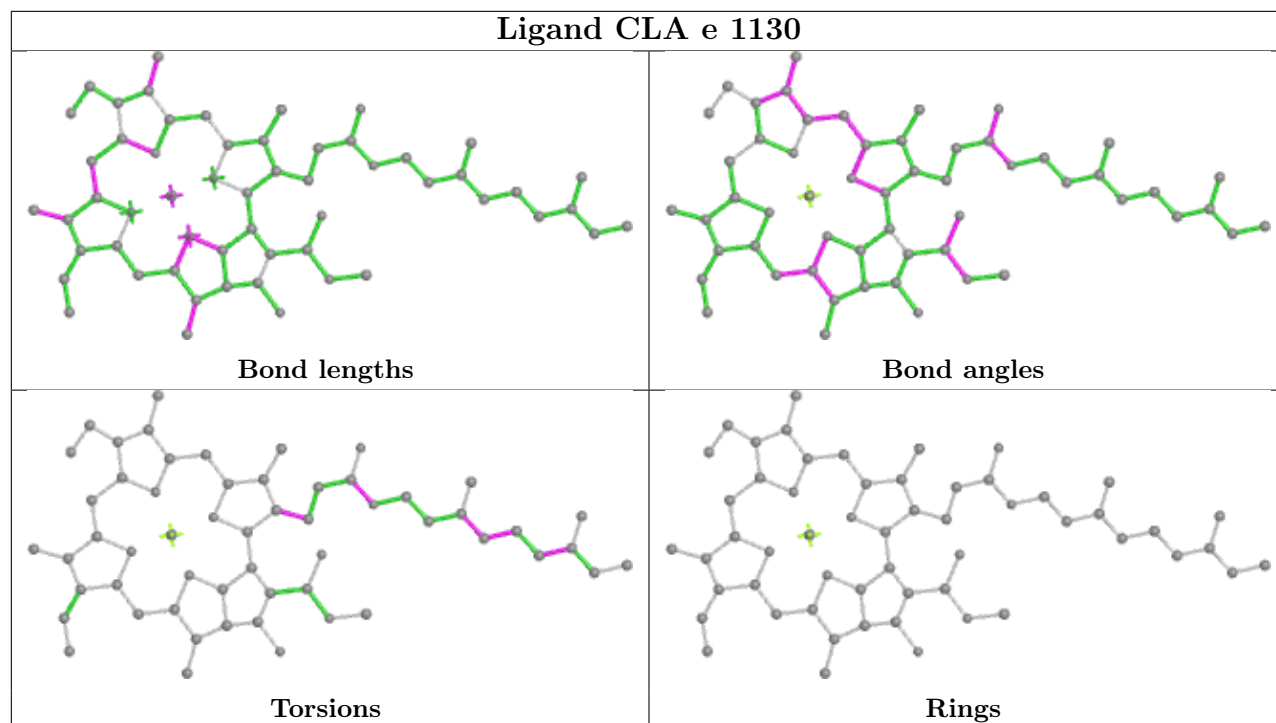


Ligand CLA 1 512

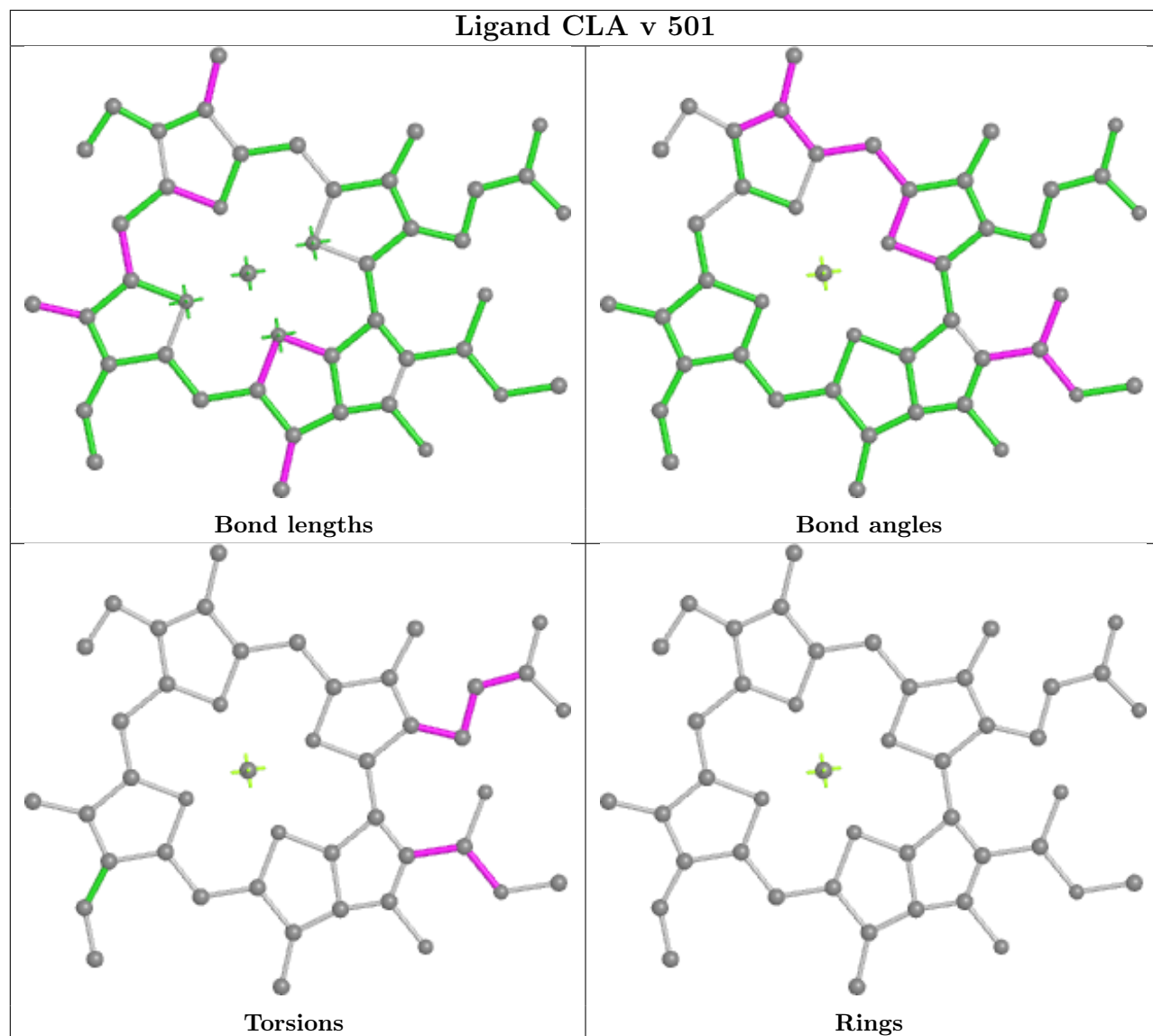


Ligand CLA e 1125

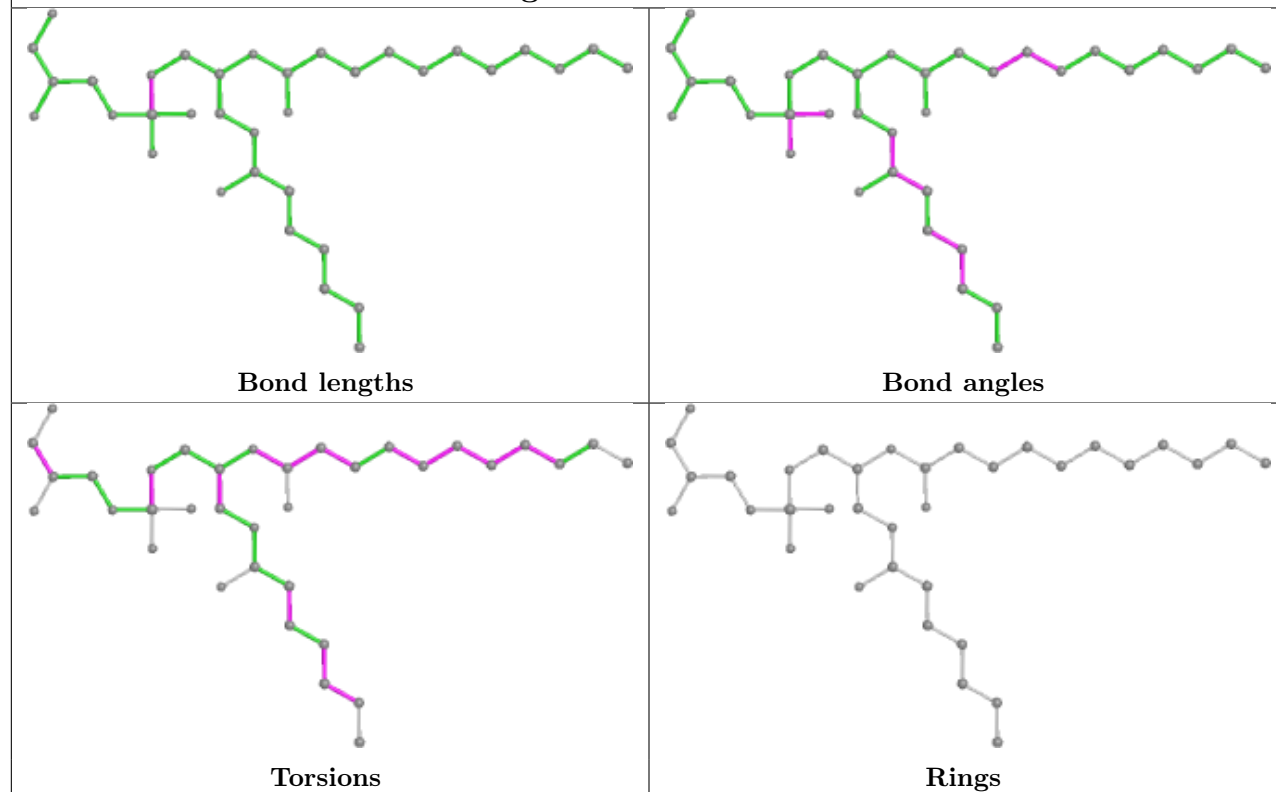




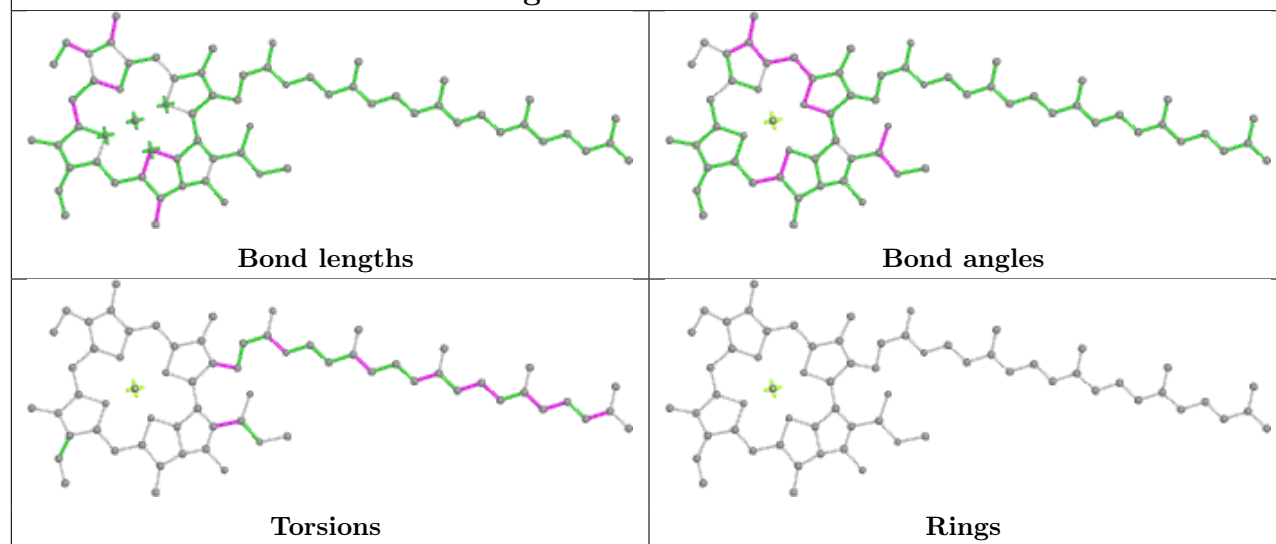
Ligand CLA v 501



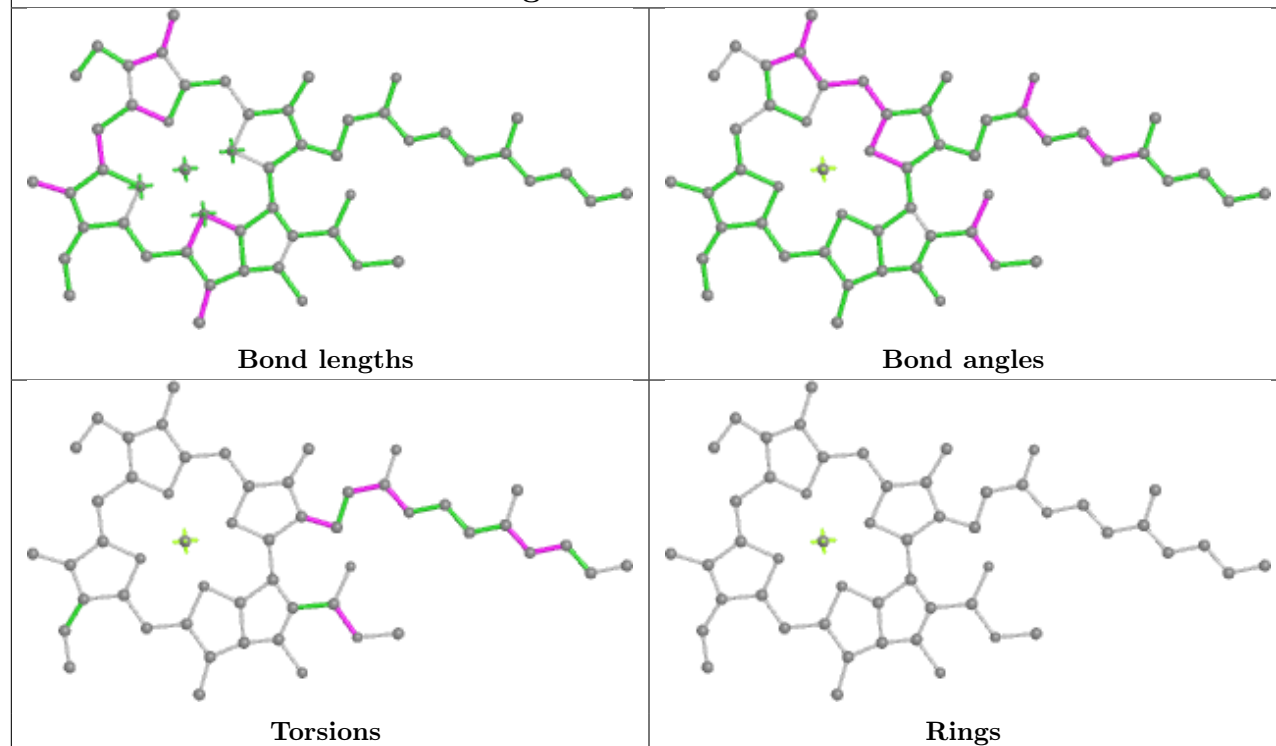
Ligand LHG A 5008



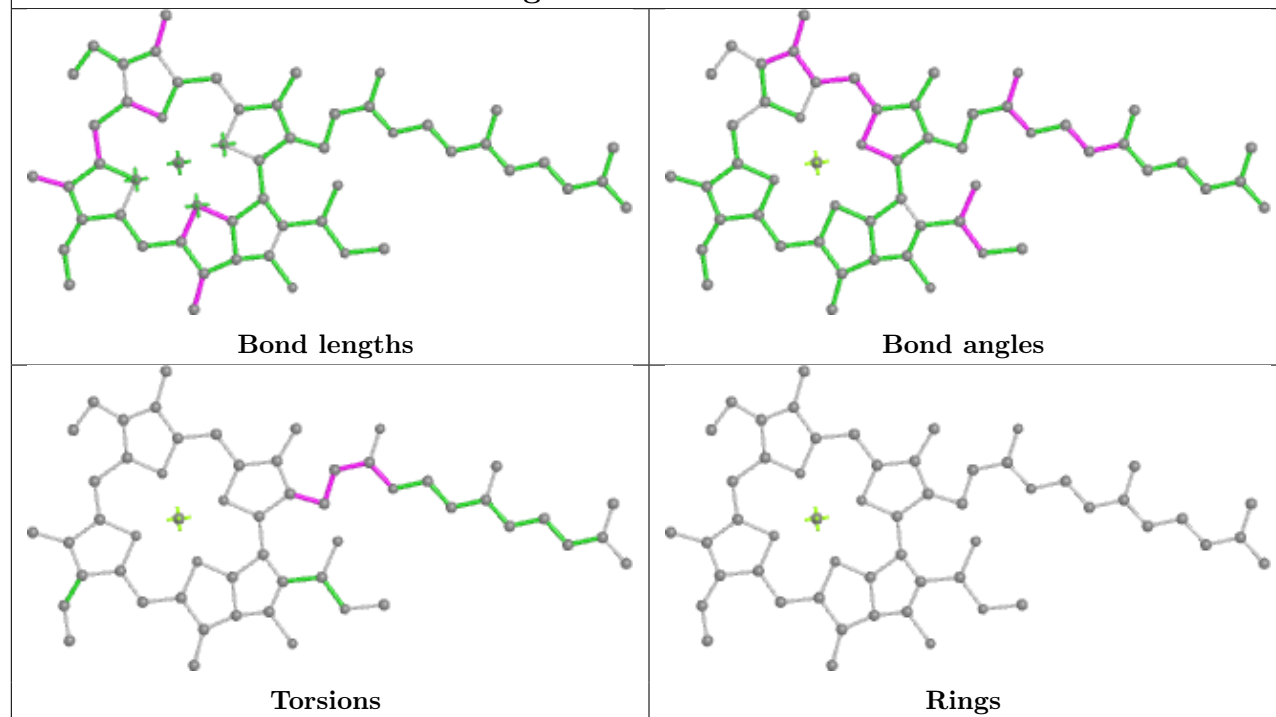
Ligand CLA B 1208

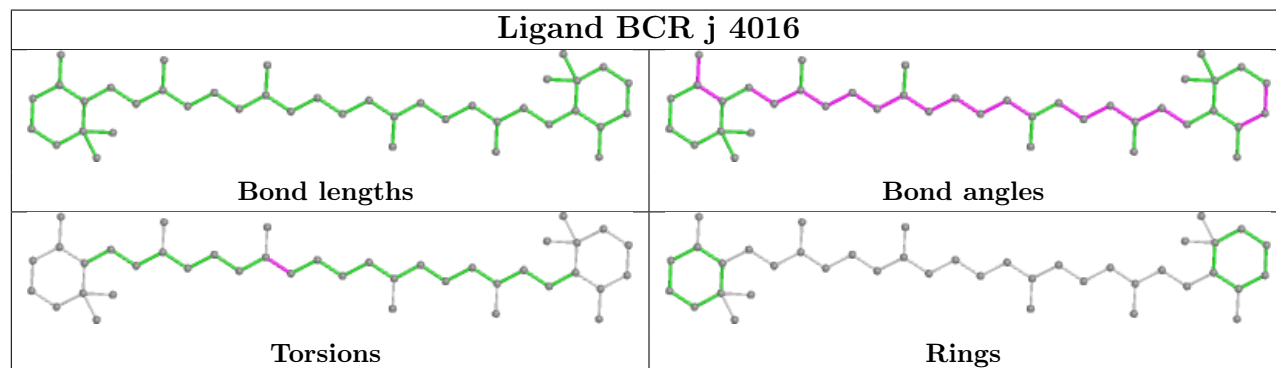
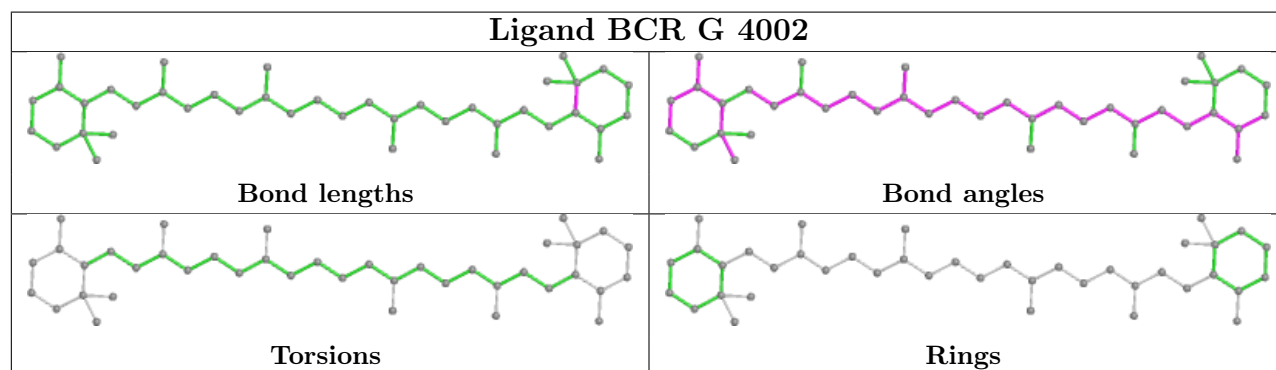
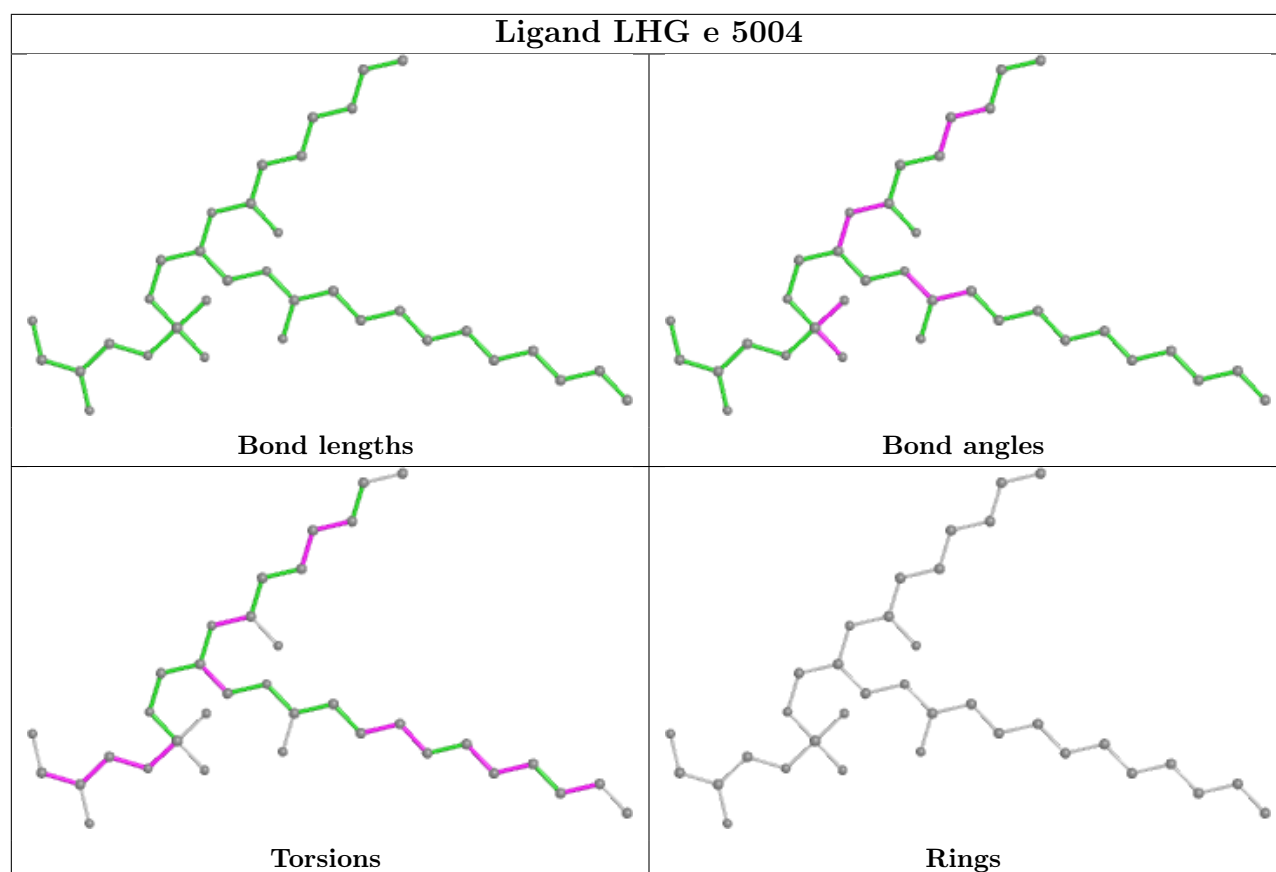


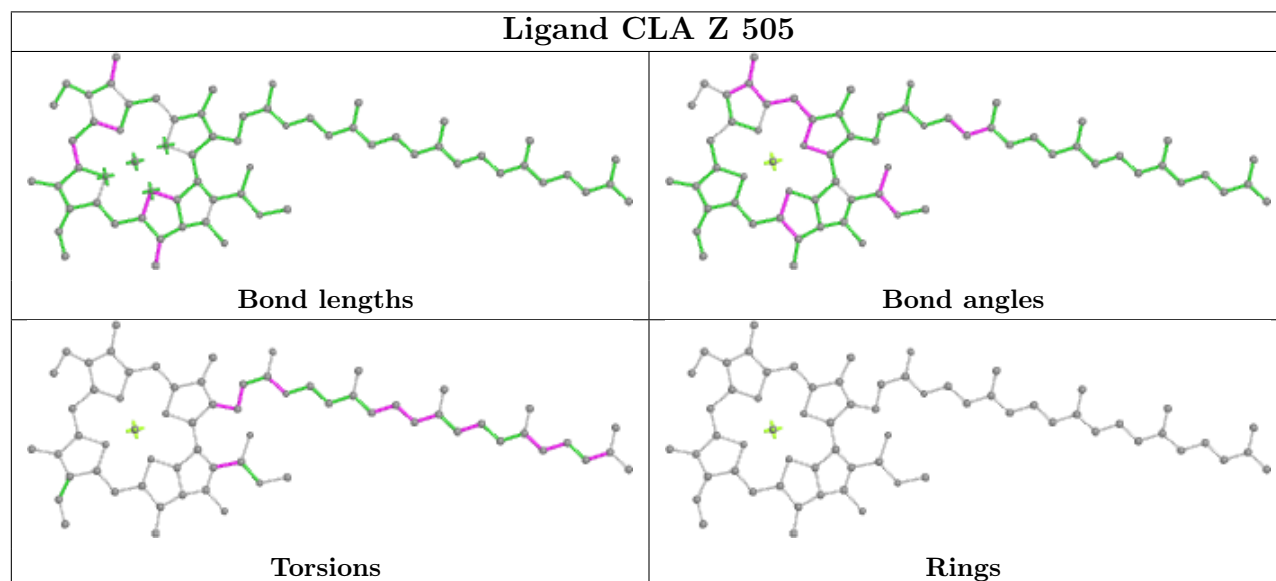
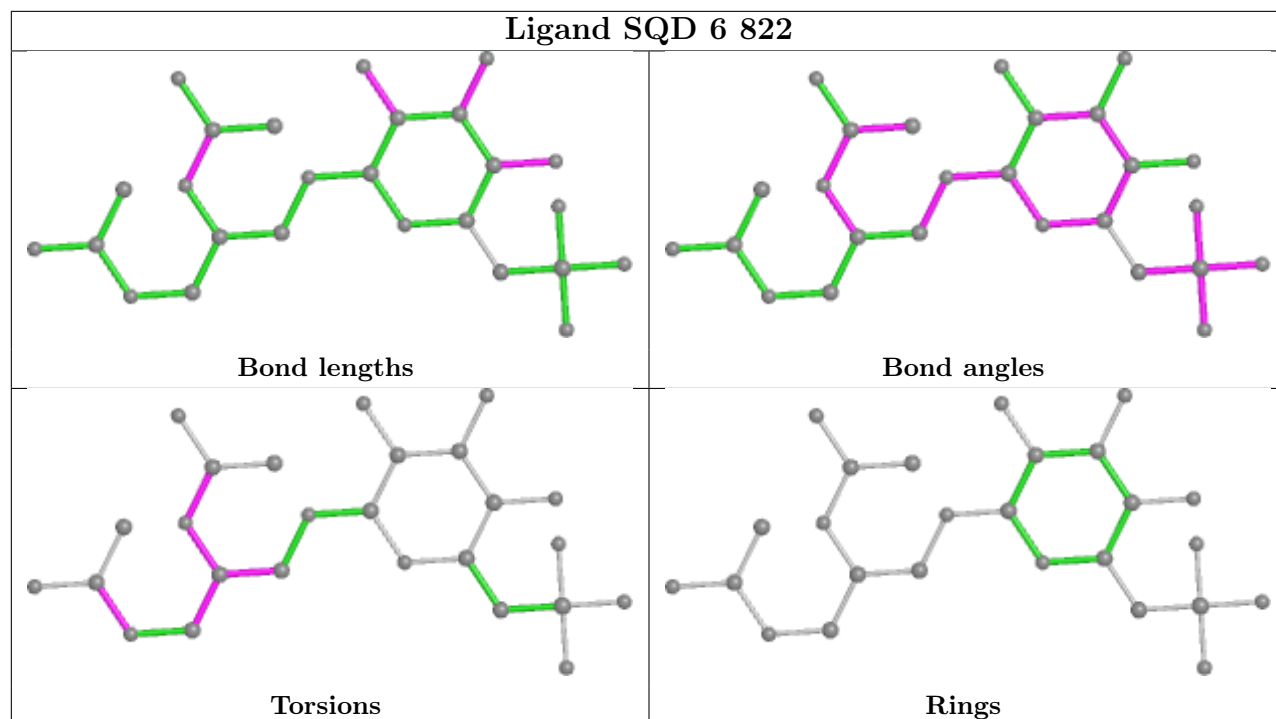
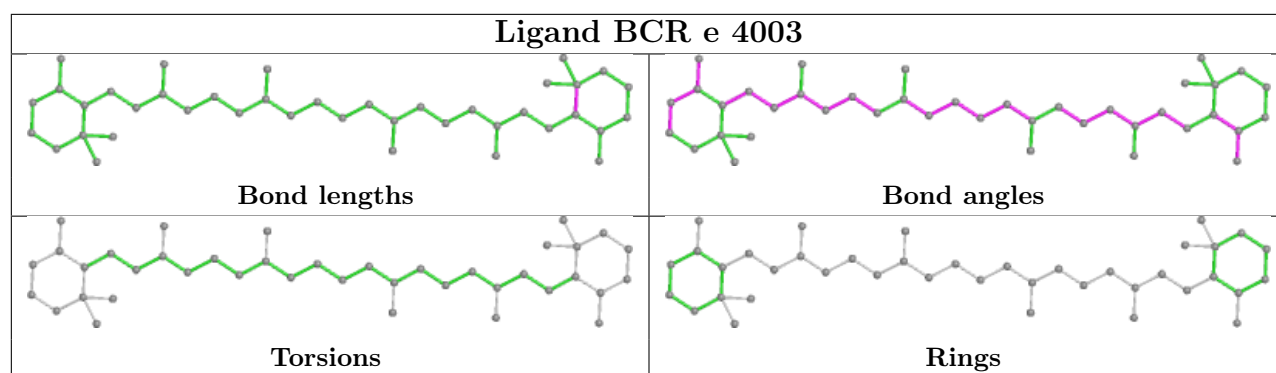
Ligand CLA A 1110



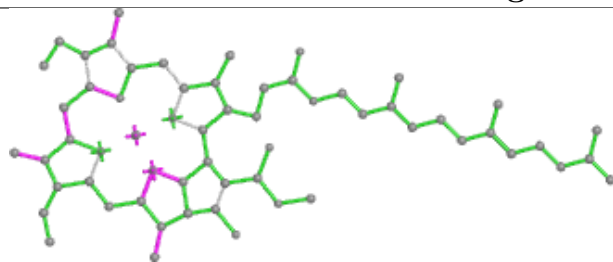
Ligand CLA B 1228



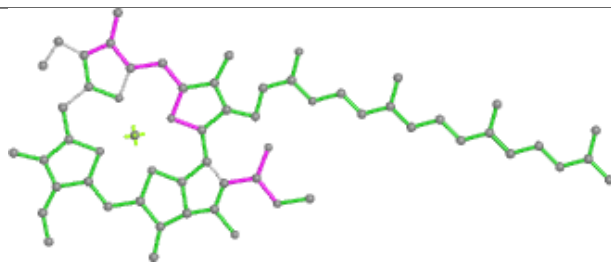




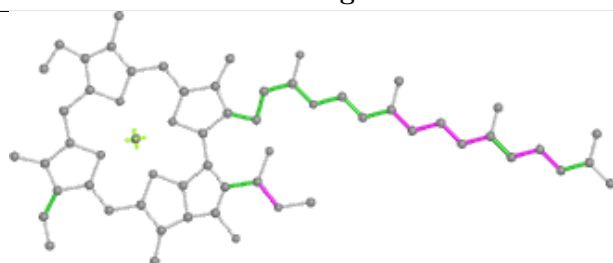
Ligand CLA L 1503



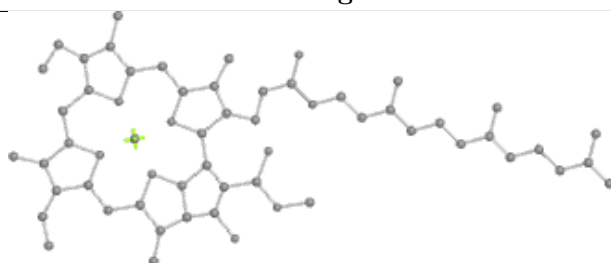
Bond lengths



Bond angles

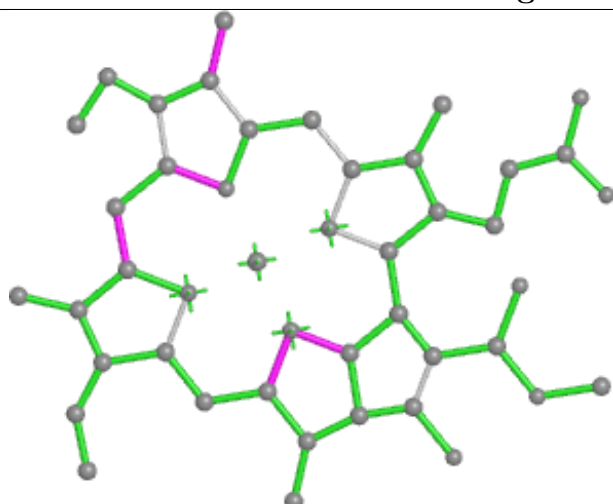


Torsions

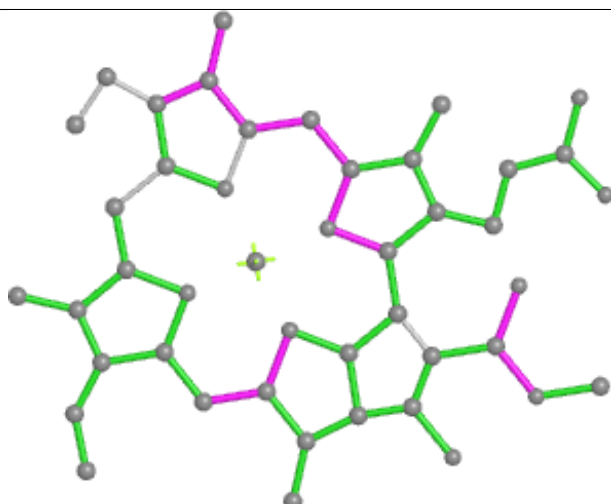


Rings

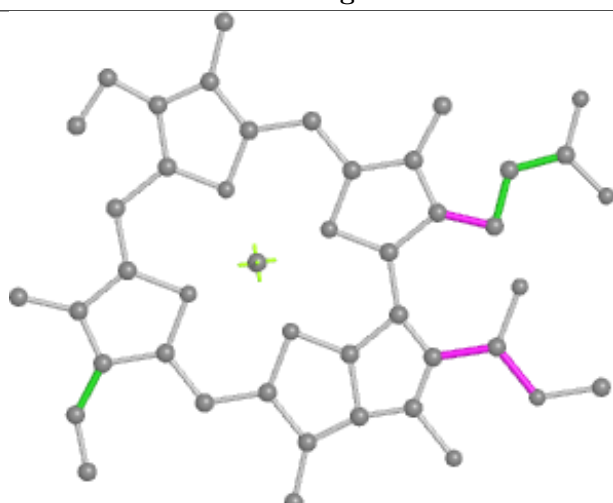
Ligand CLA b 504



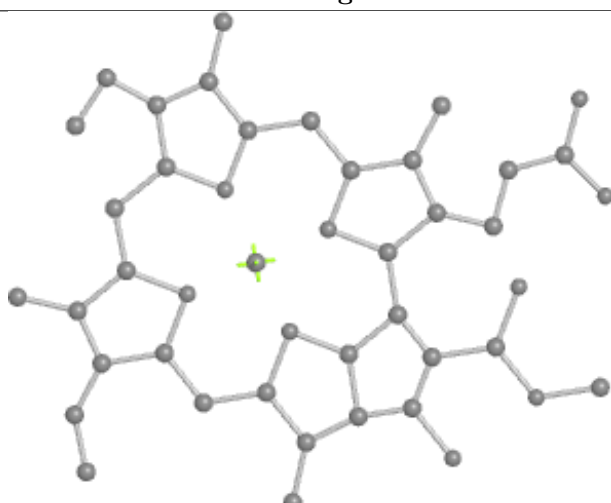
Bond lengths



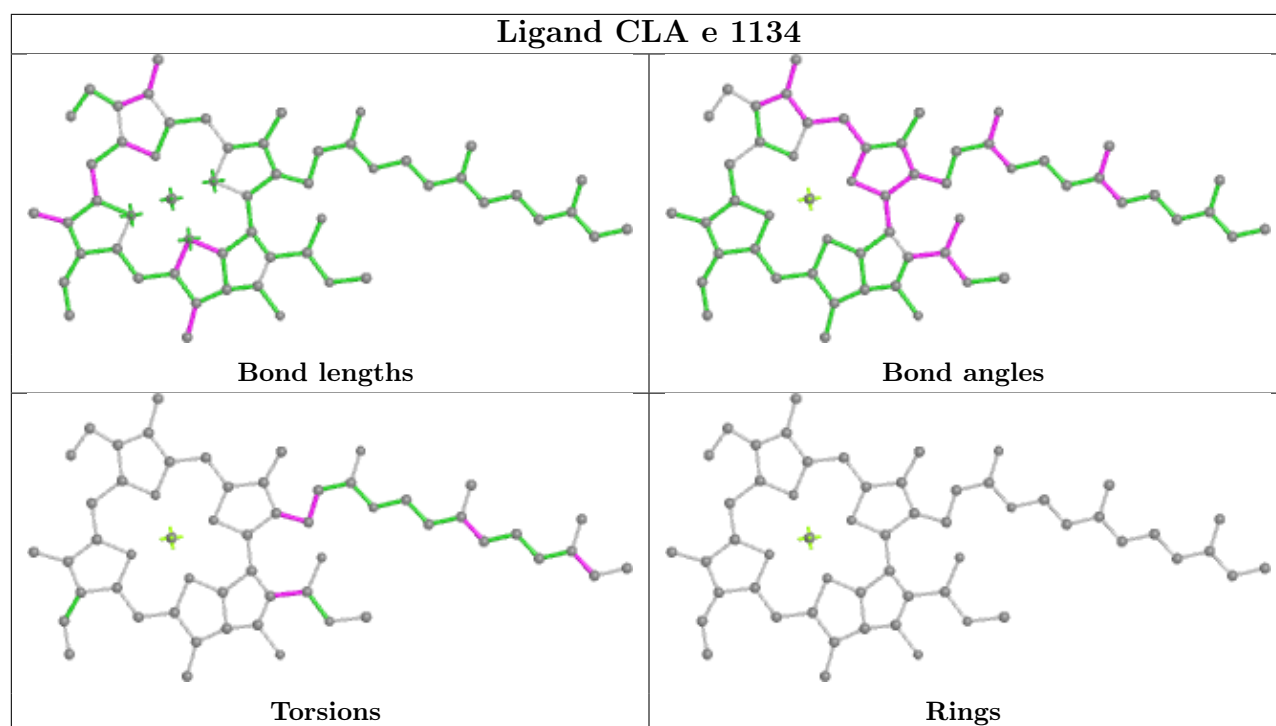
Bond angles



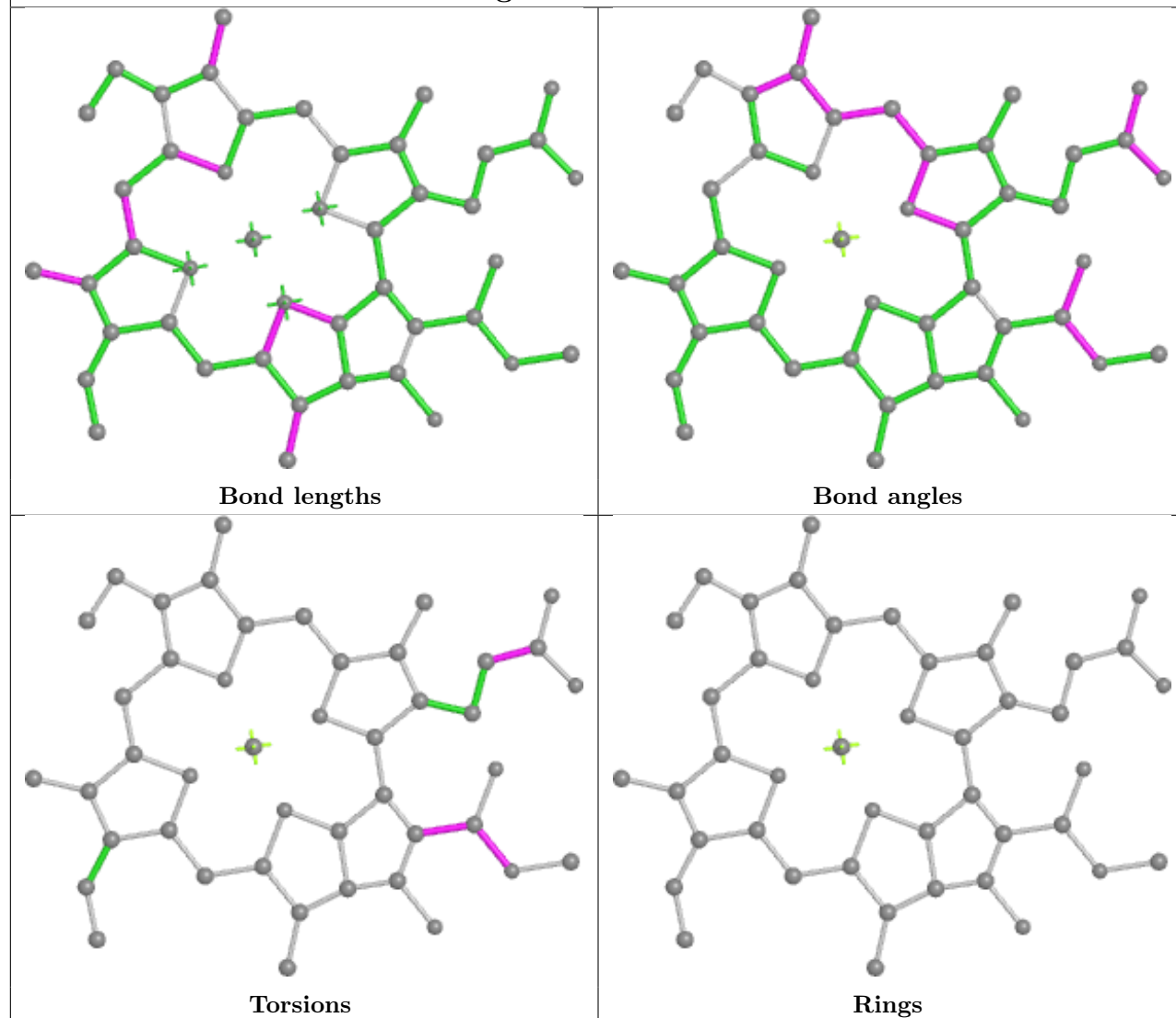
Torsions



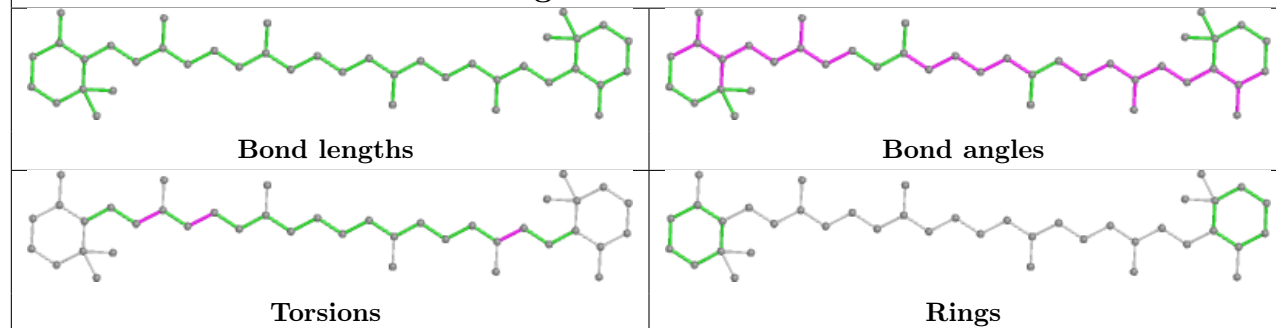
Rings

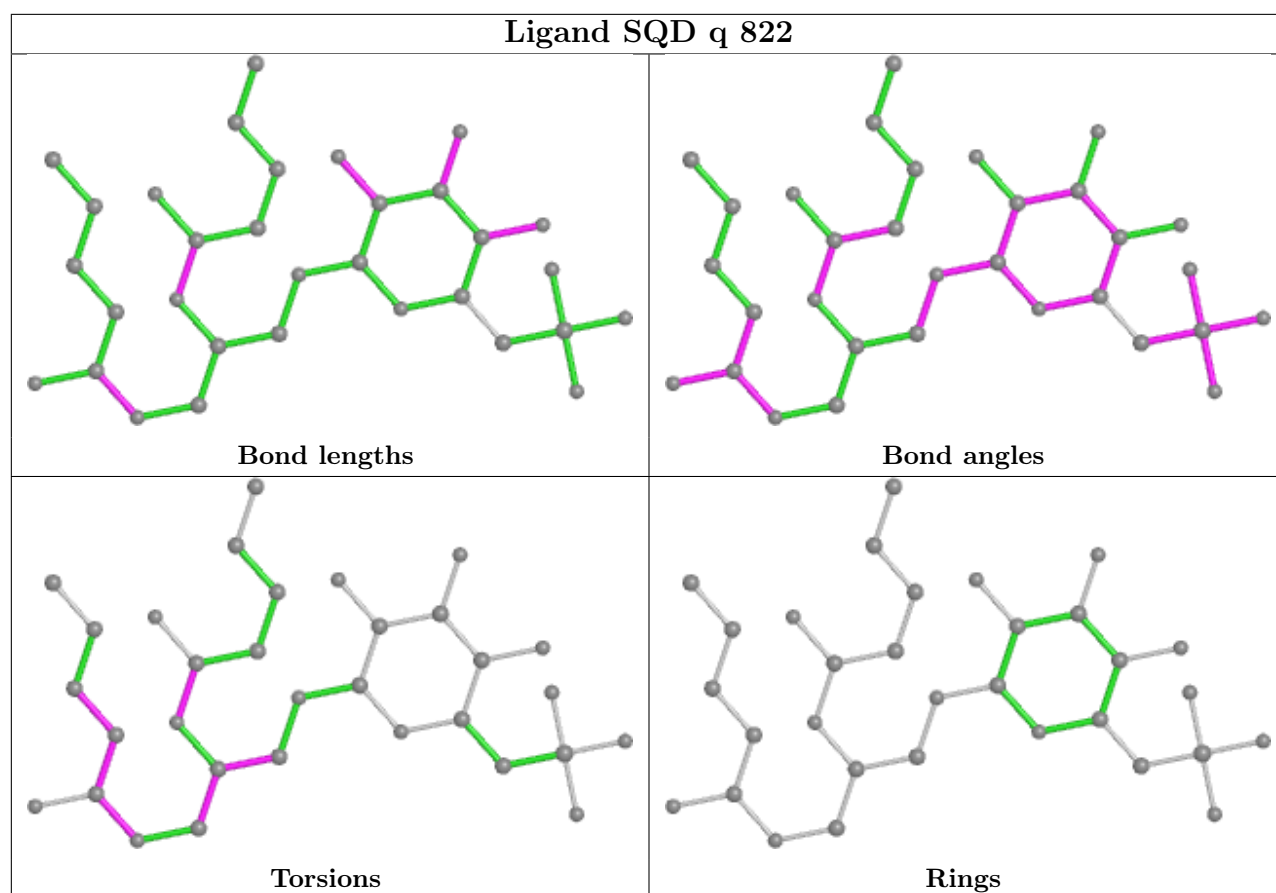


Ligand CLA t 519

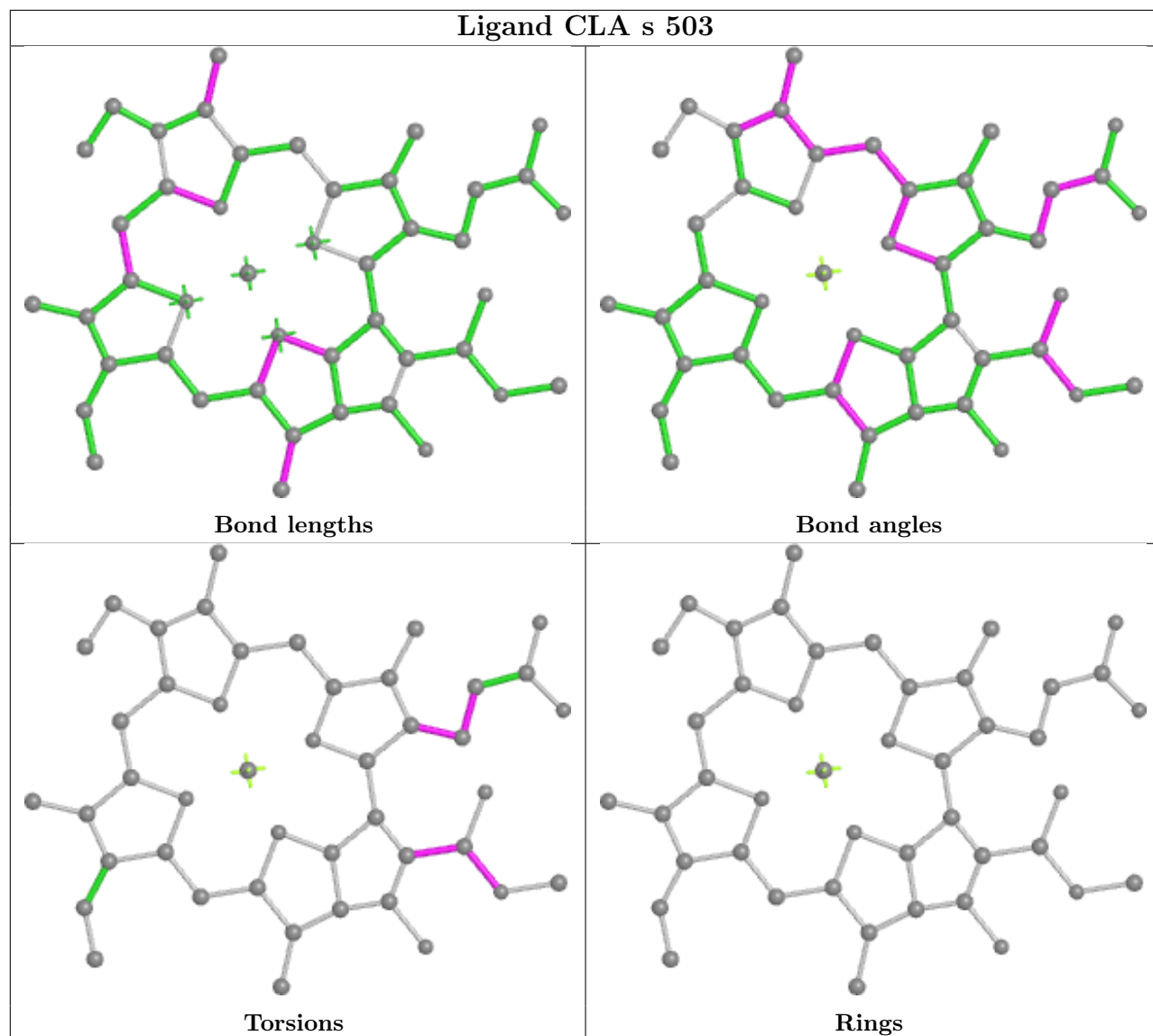


Ligand BCR 3 524

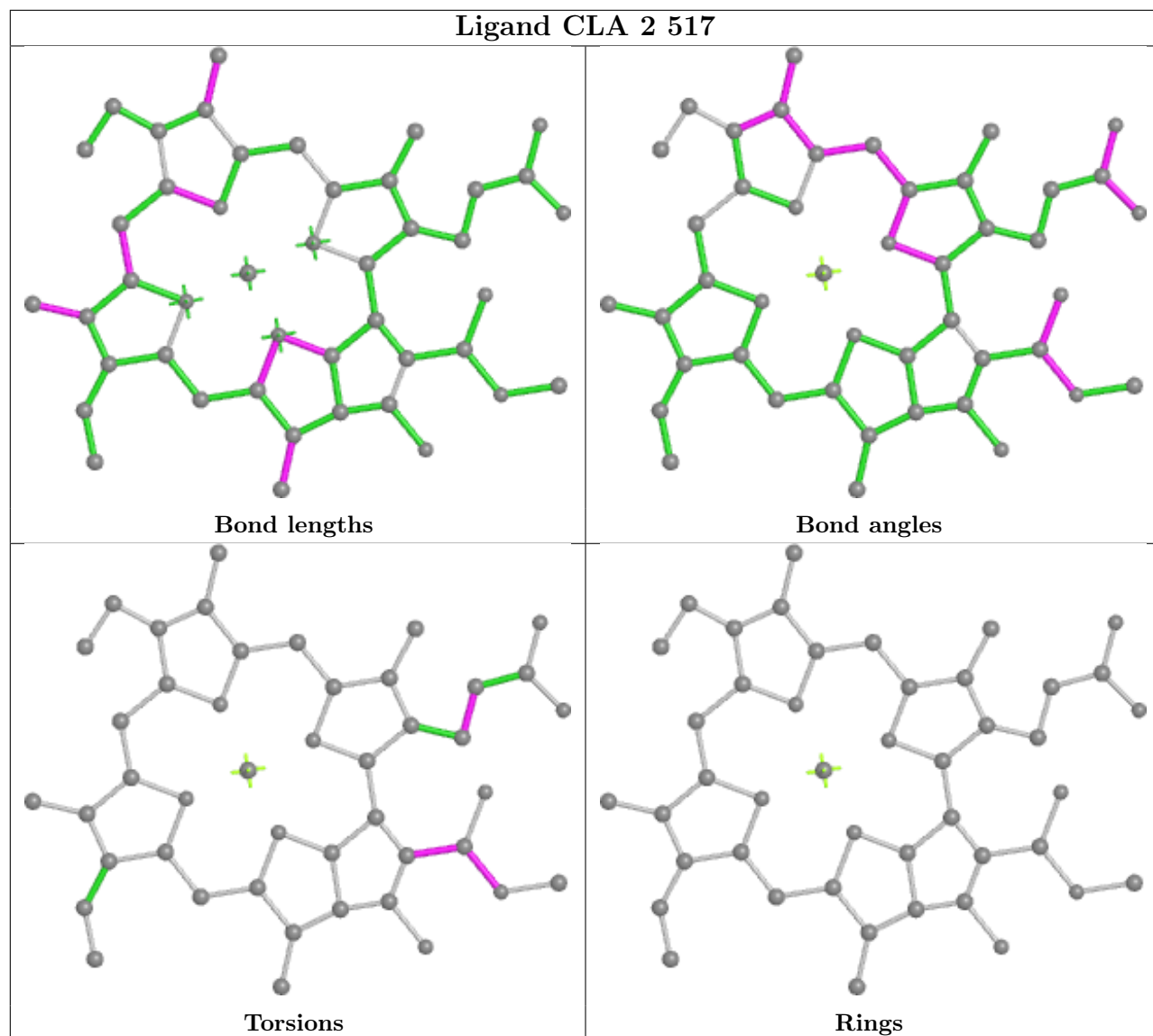




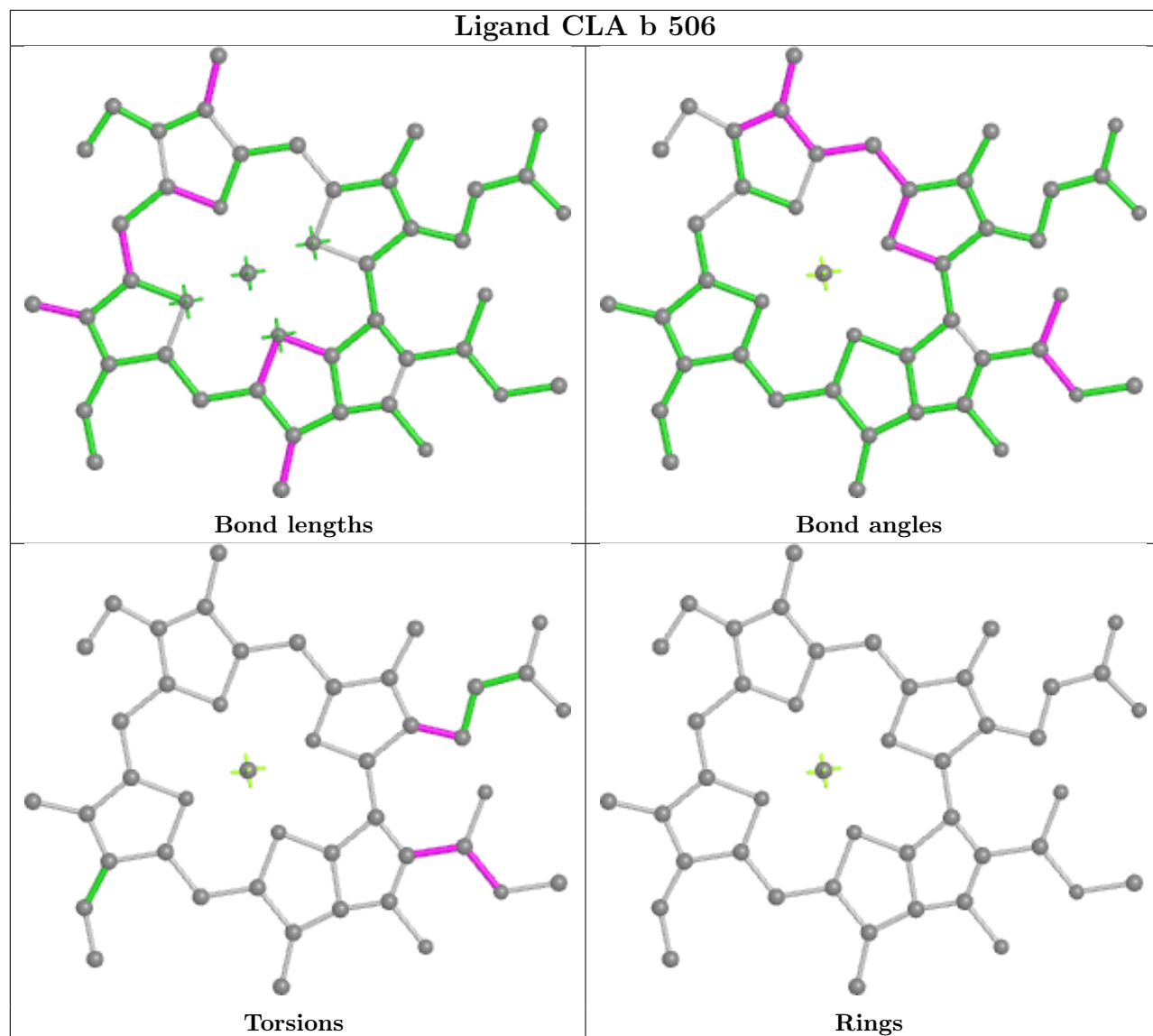
Ligand CLA s 503



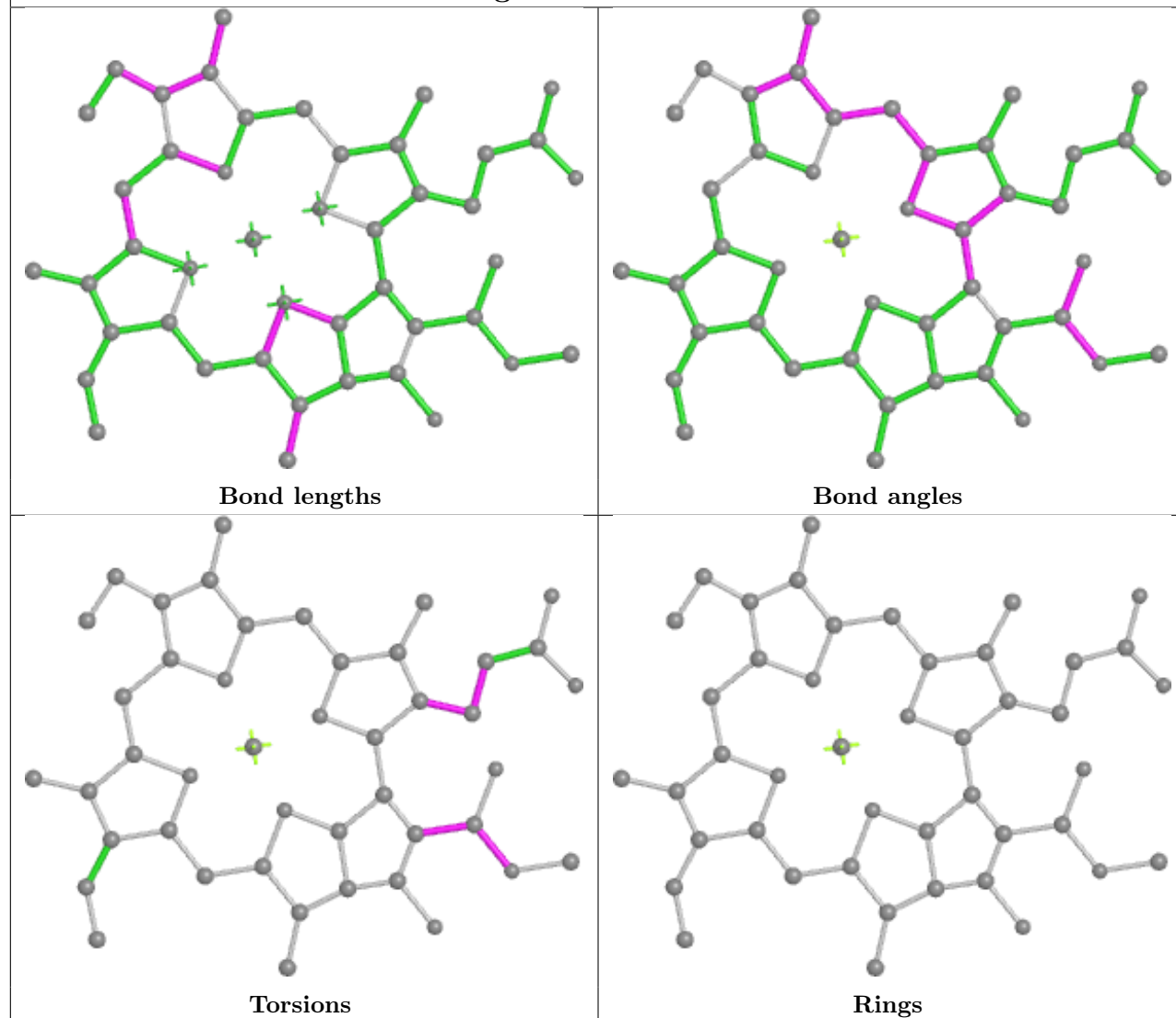
Ligand CLA 2 517



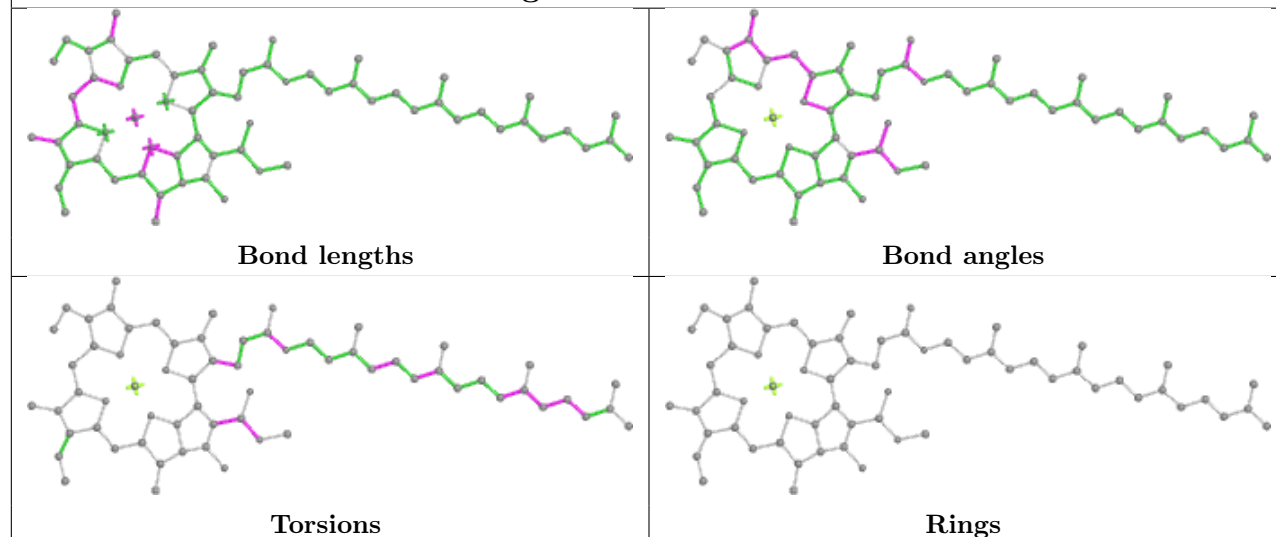
Ligand CLA b 506



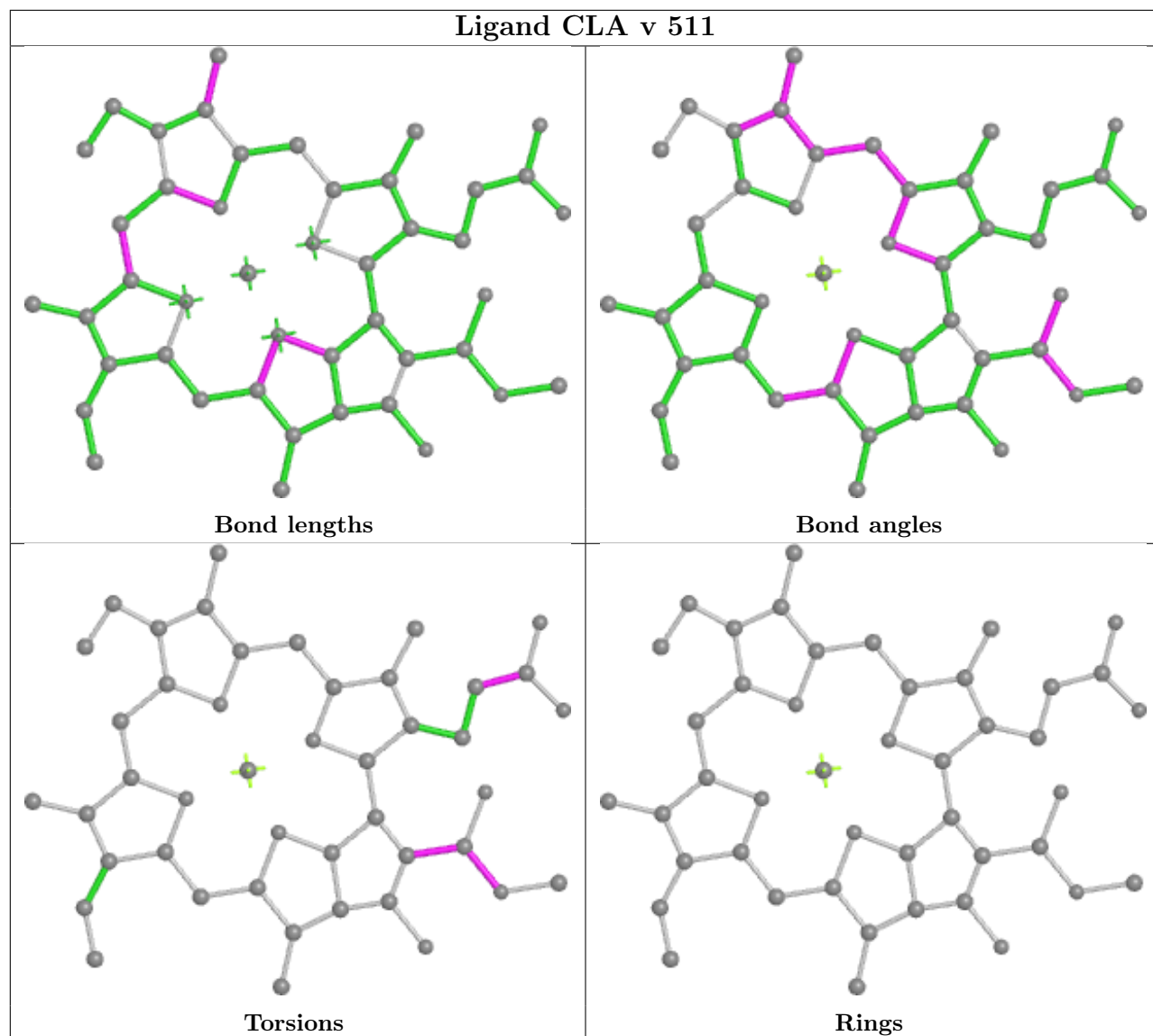
Ligand CLA 1 503



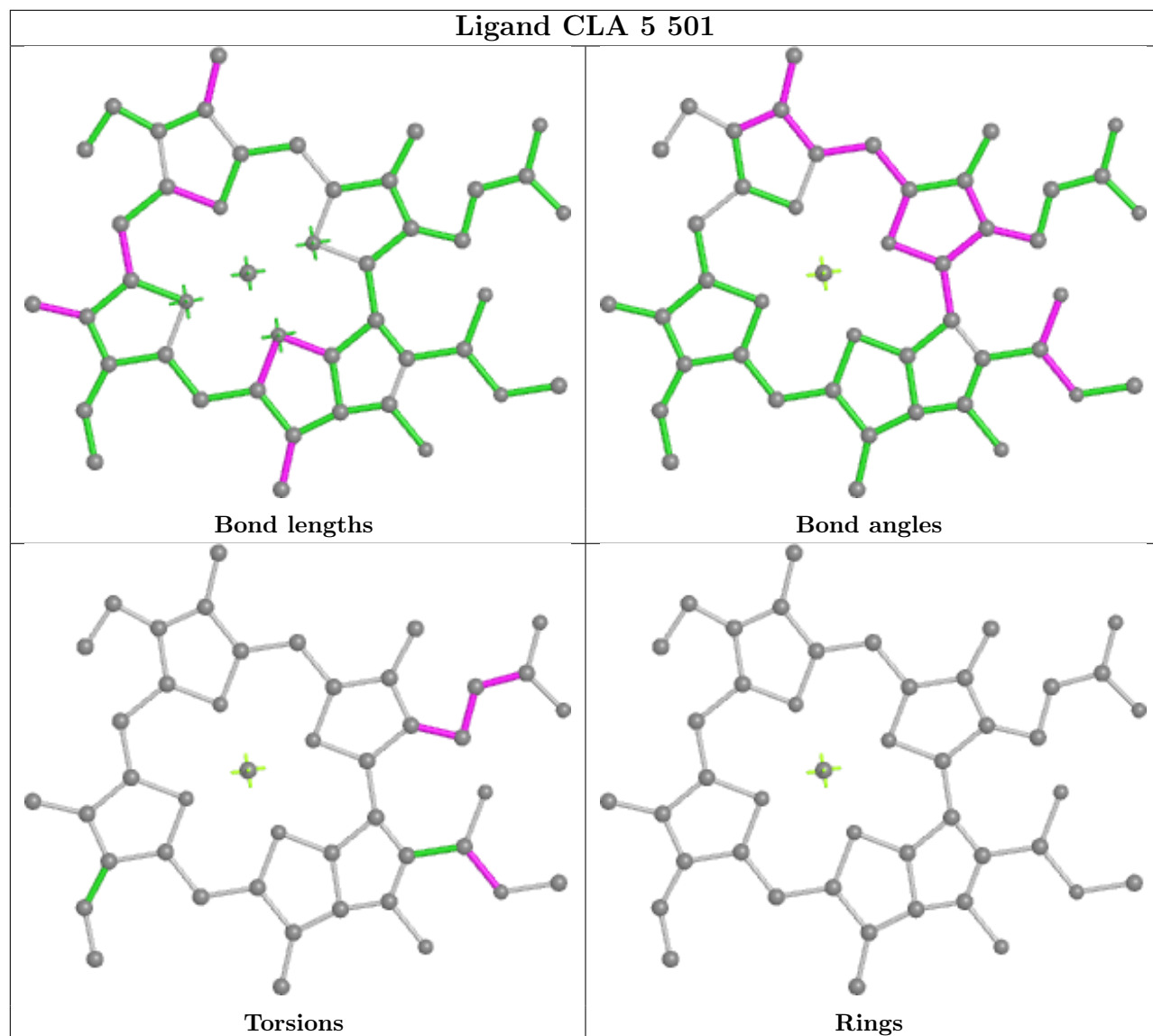
Ligand CLA G 1109



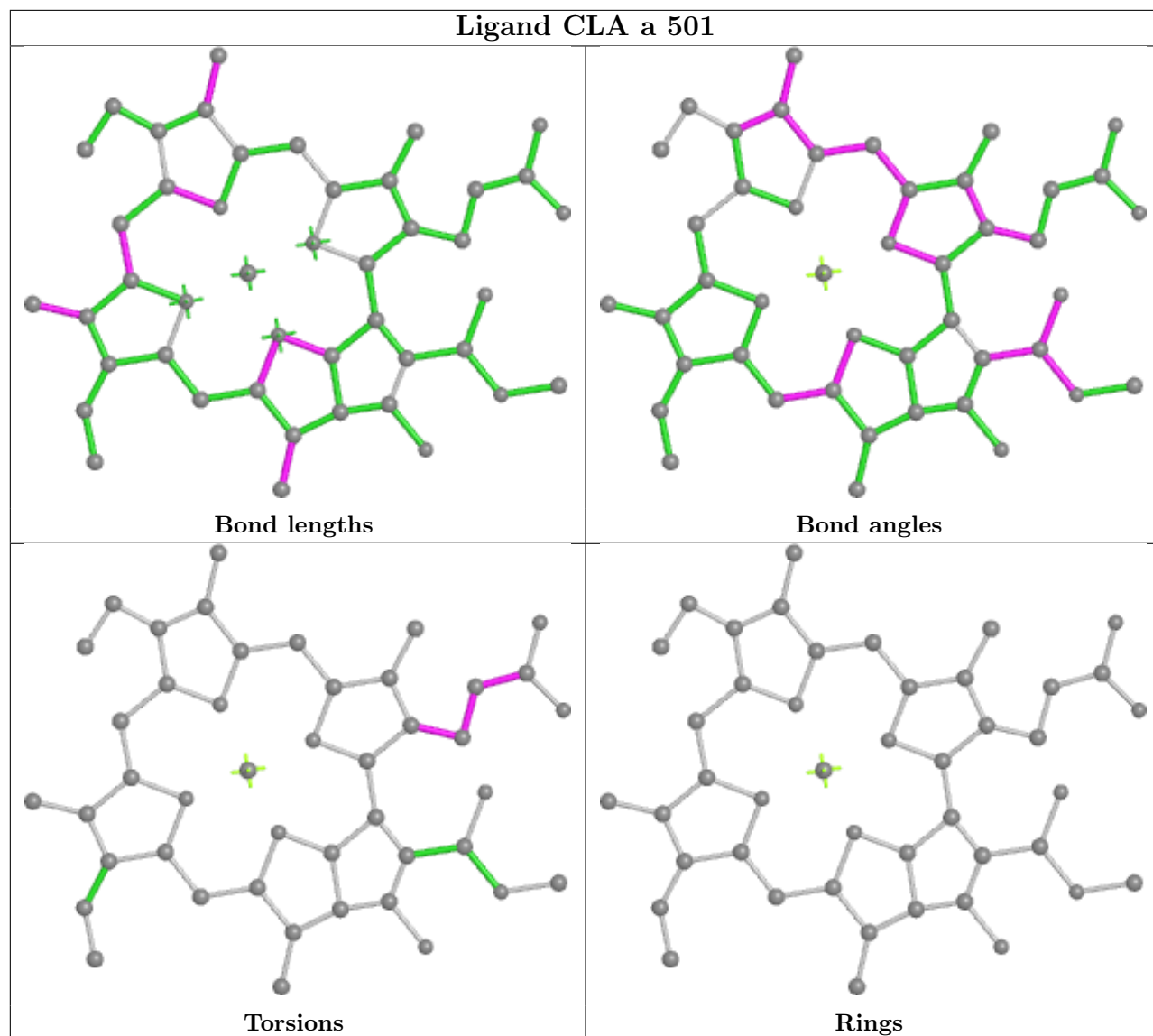
Ligand CLA v 511



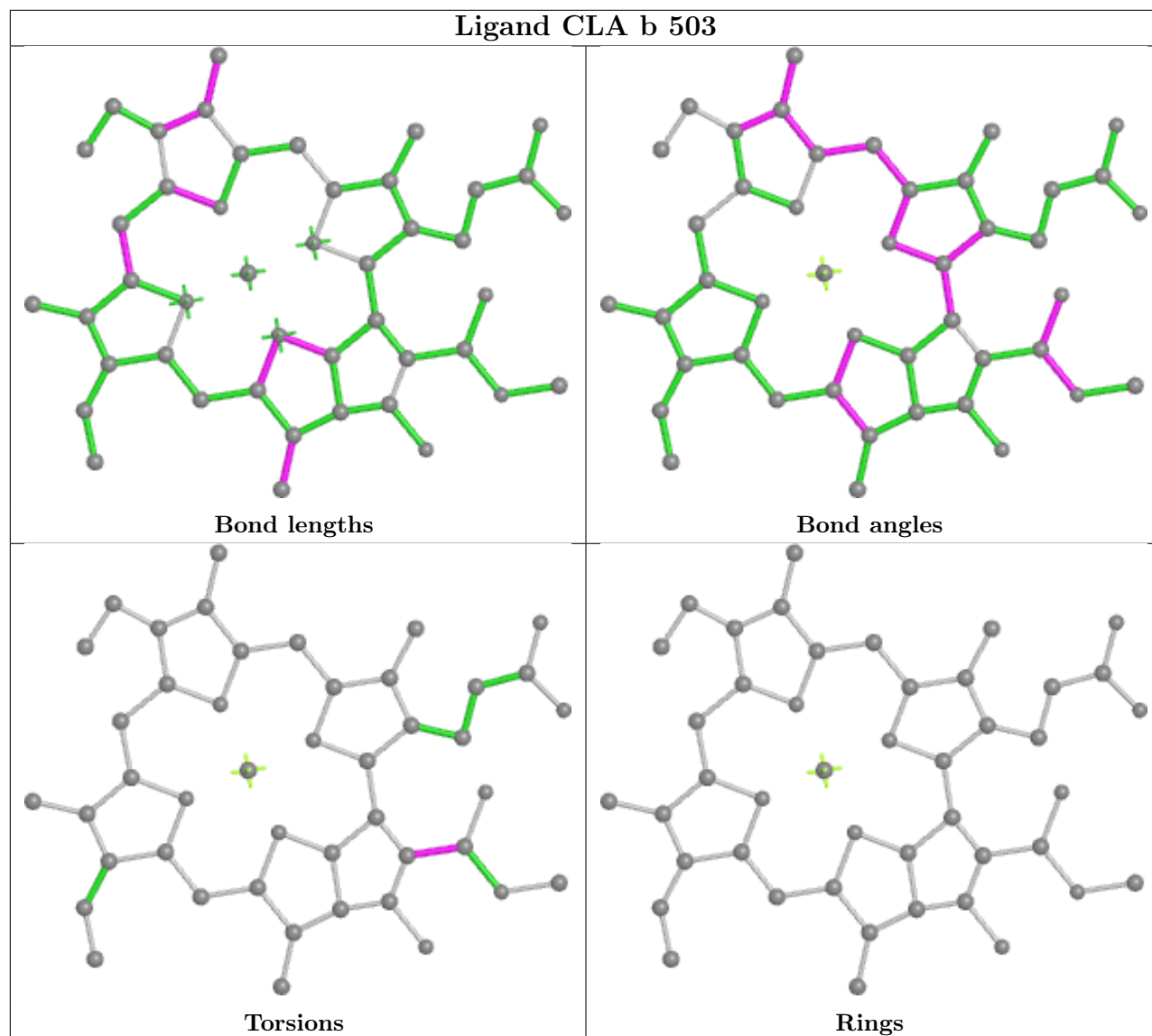
Ligand CLA 5 501



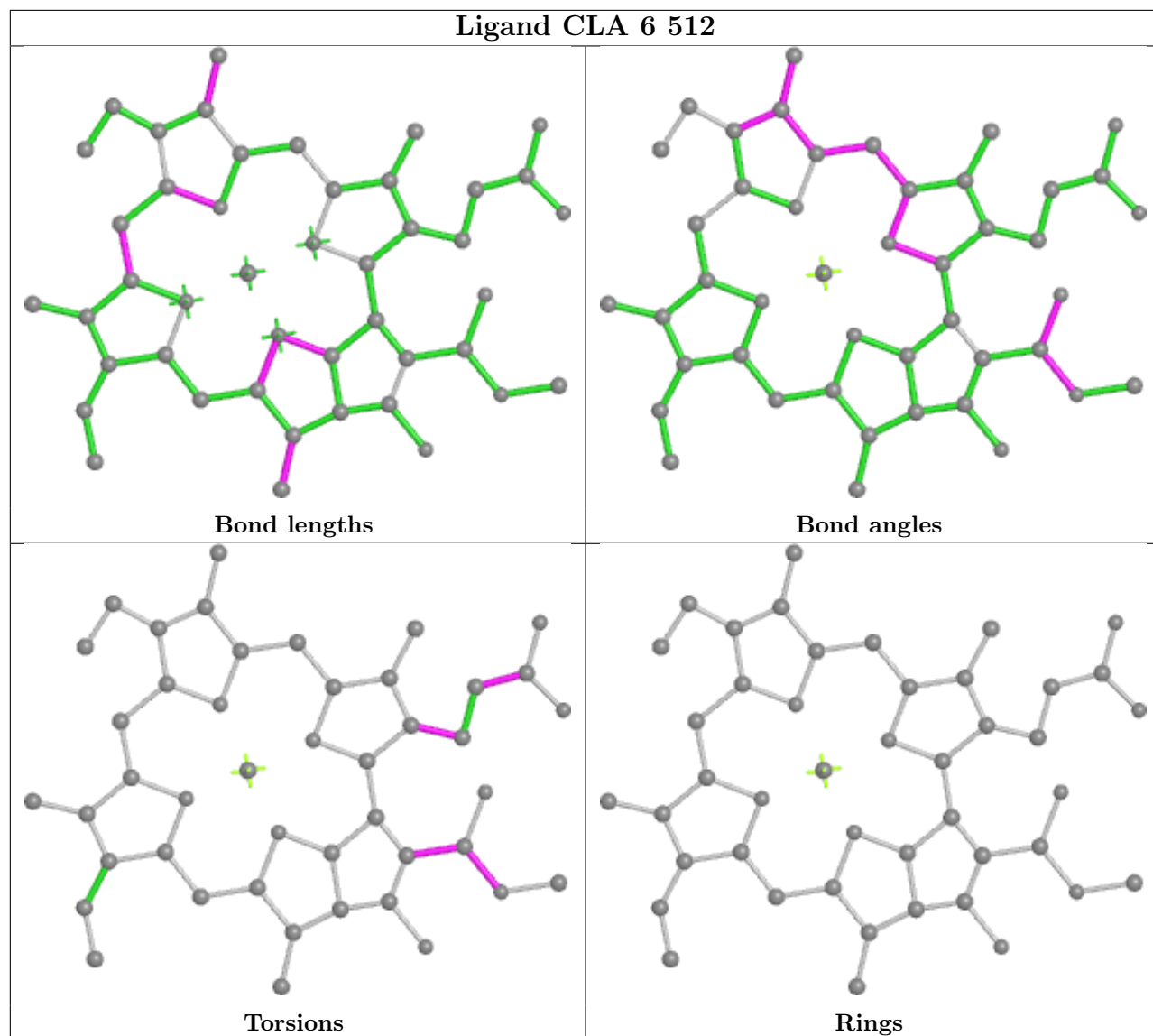
Ligand CLA a 501



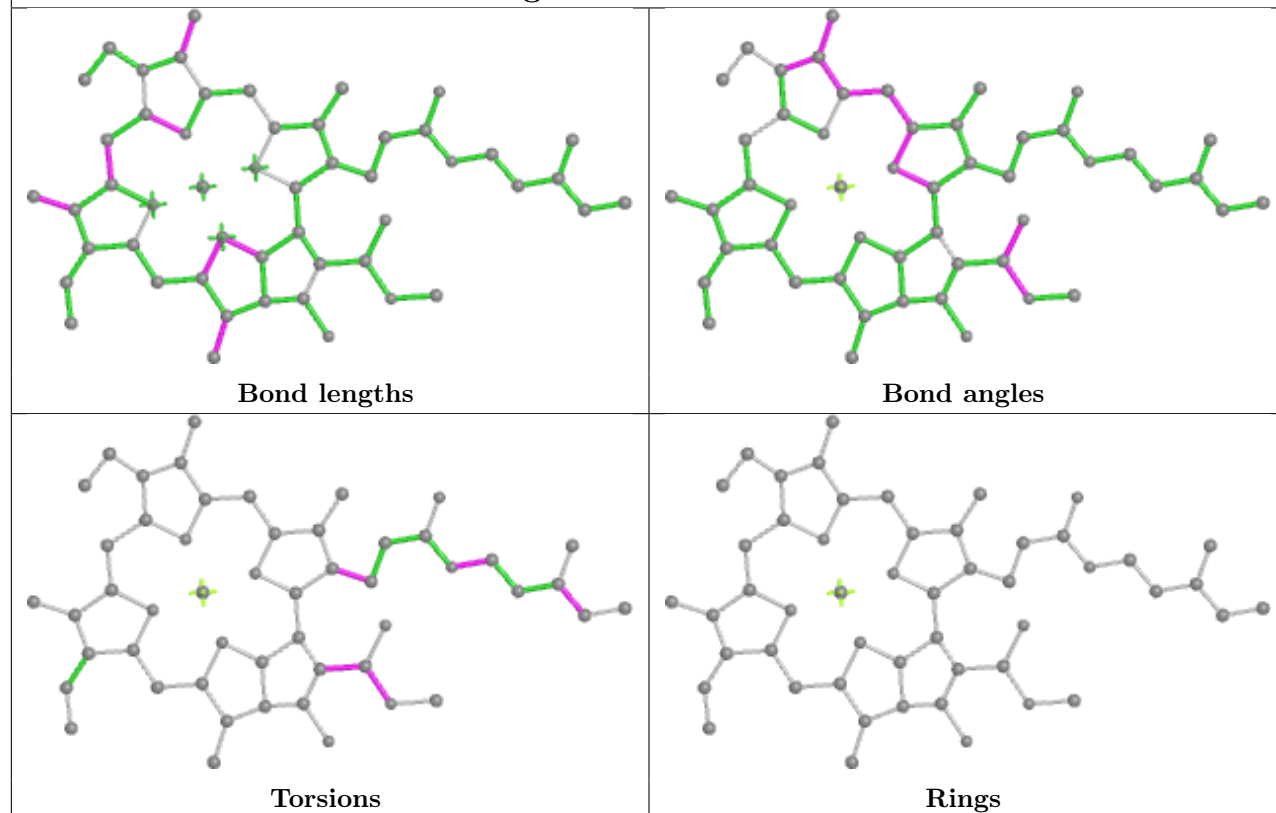
Ligand CLA b 503



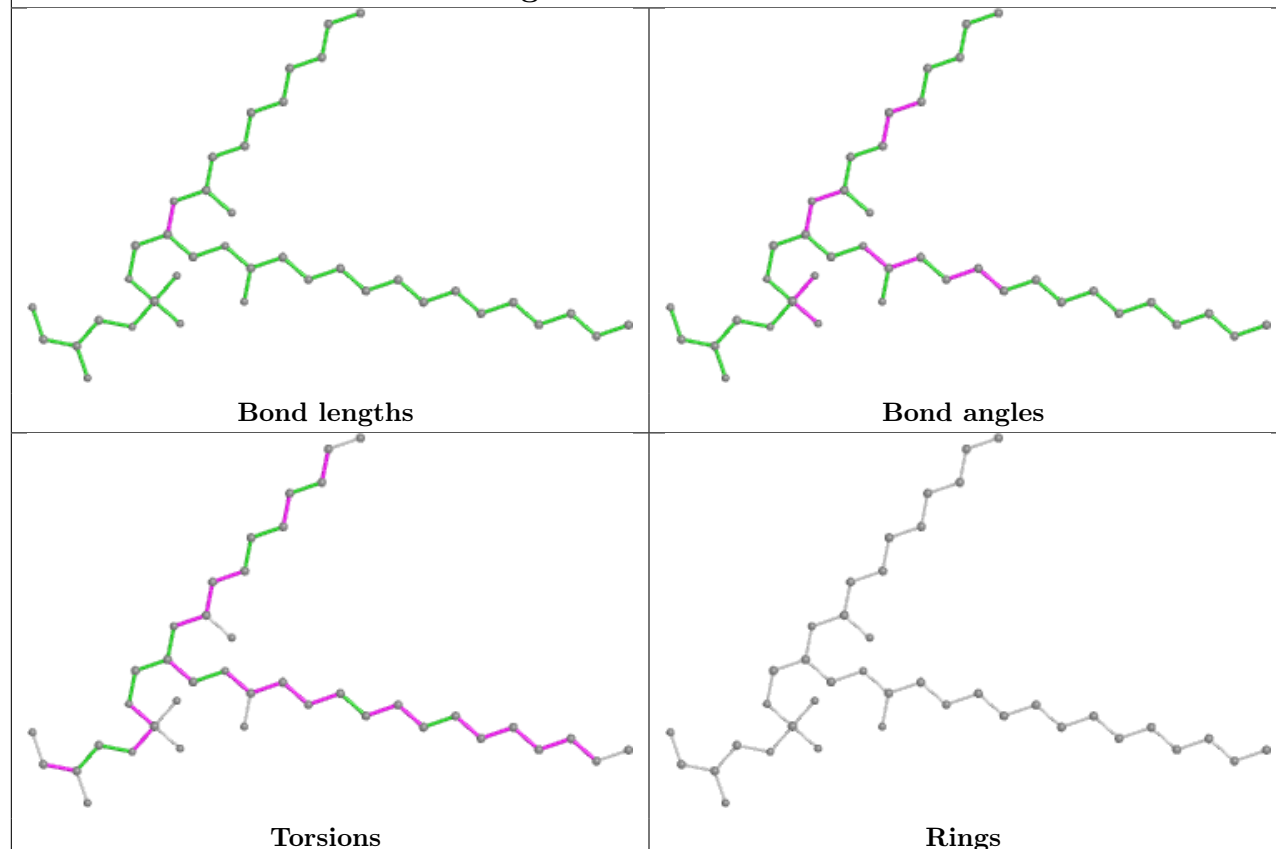
Ligand CLA 6 512



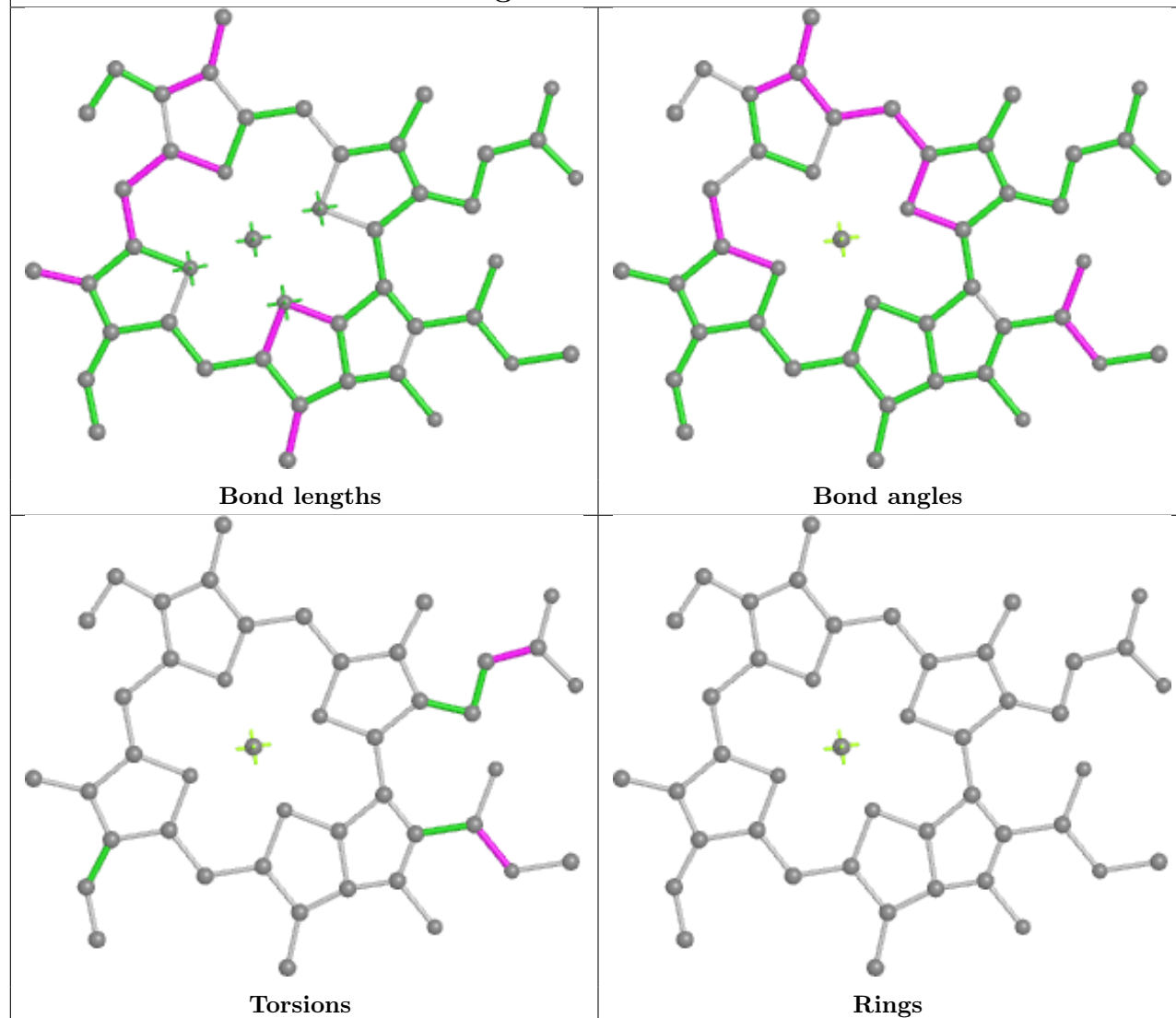
Ligand CLA B 1212



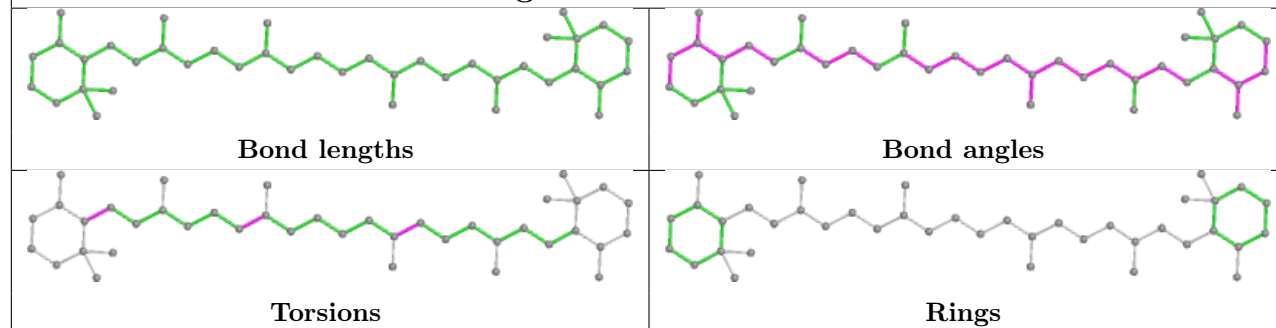
Ligand LHG A 5006

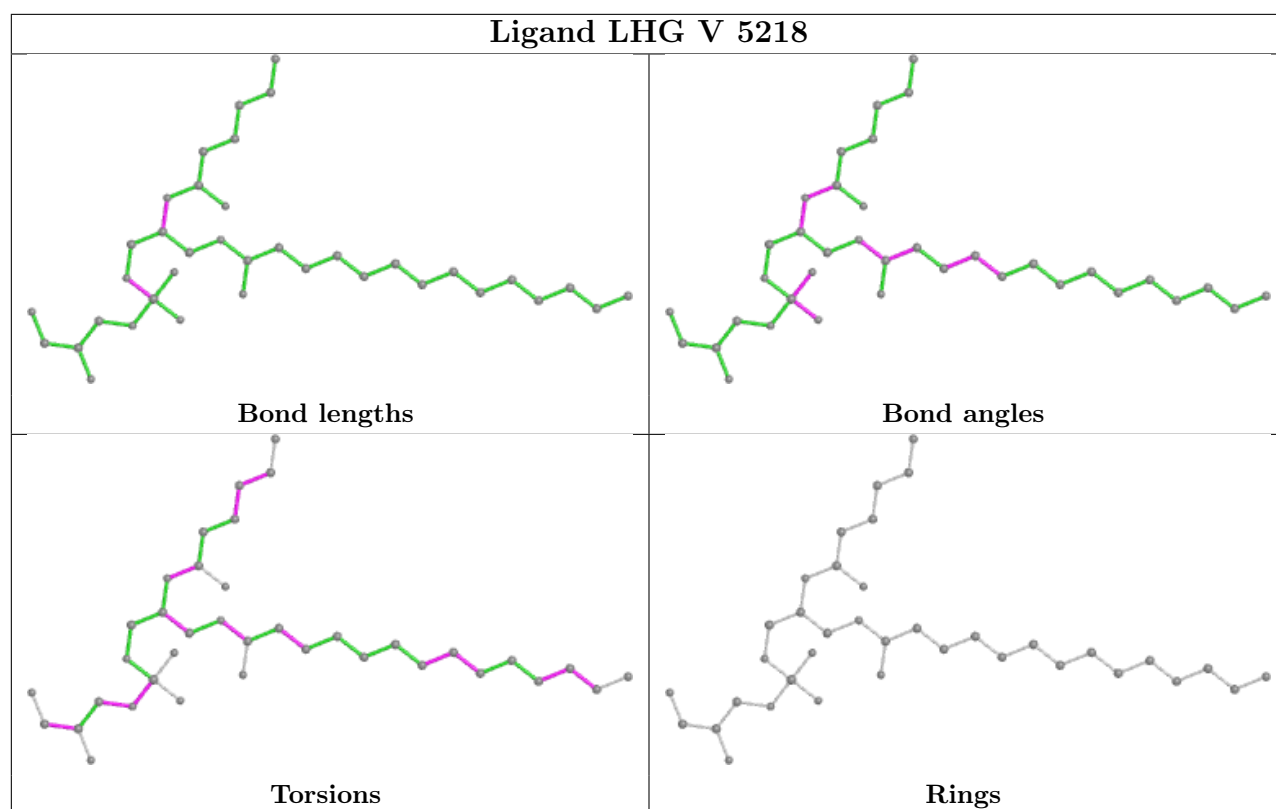


Ligand CLA c 508

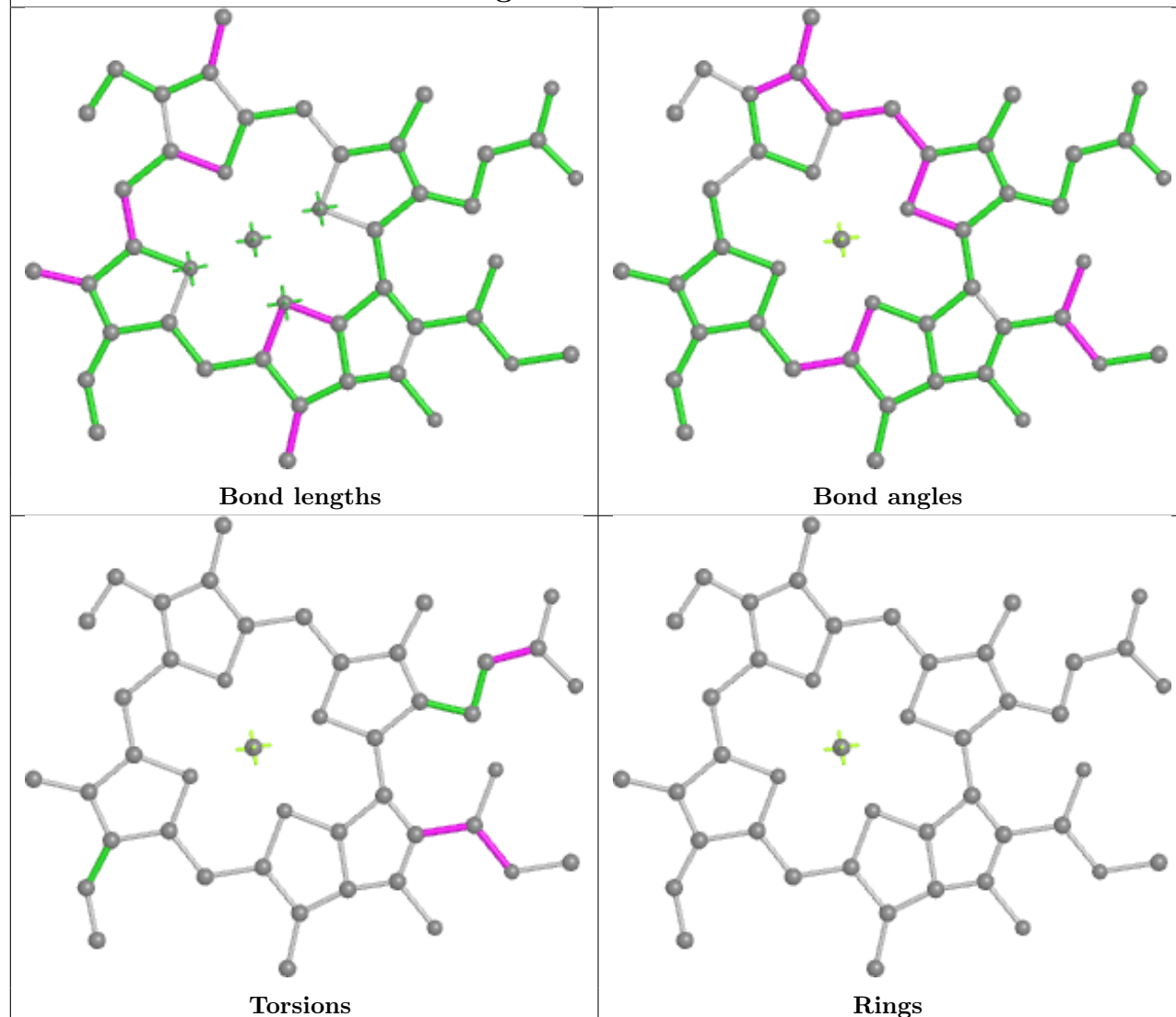


Ligand BCR W 4021

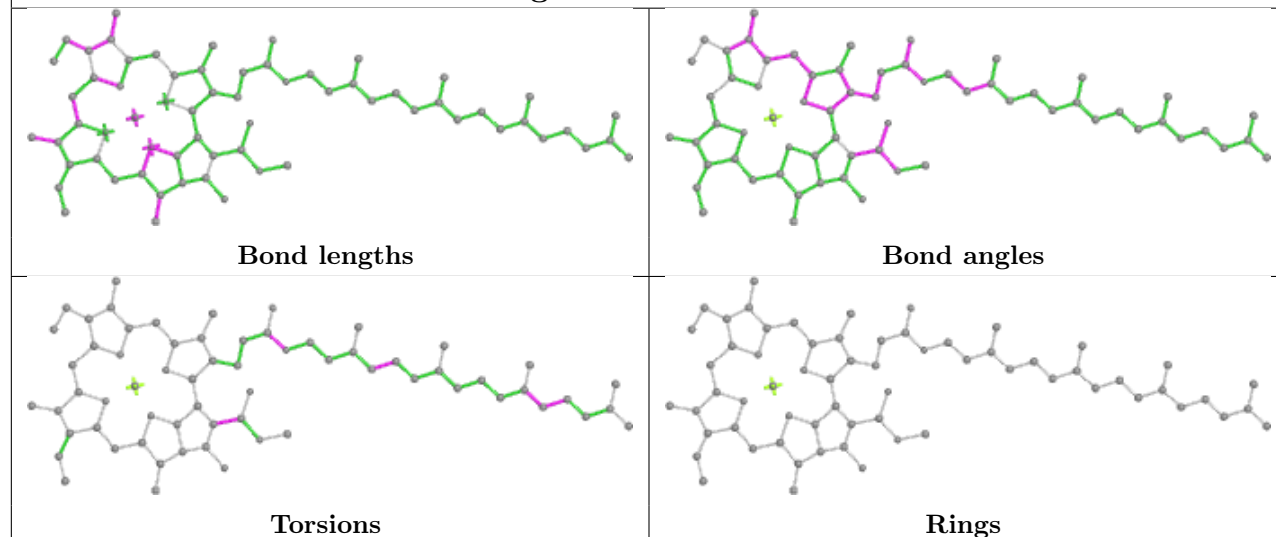




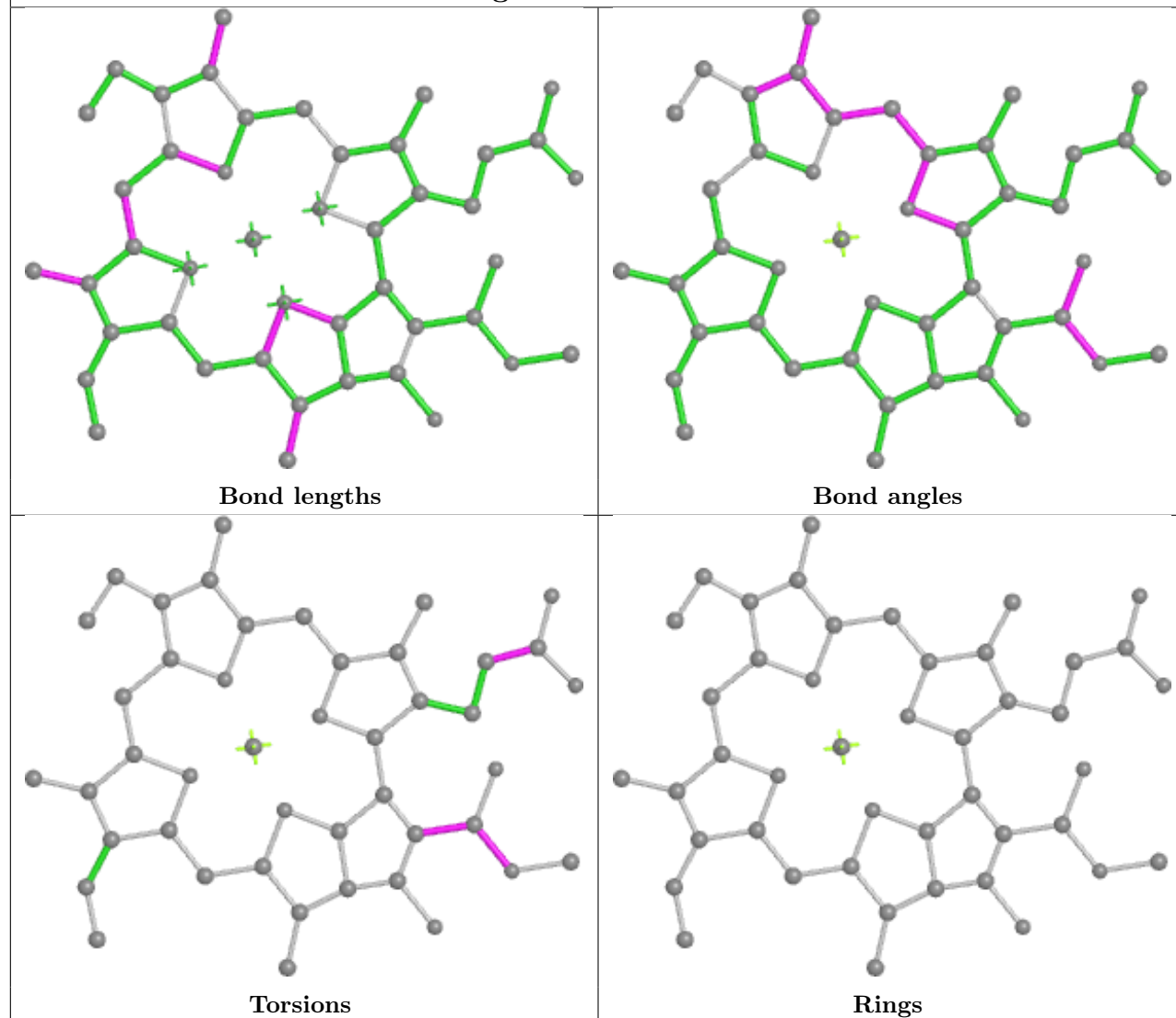
Ligand CLA r 510



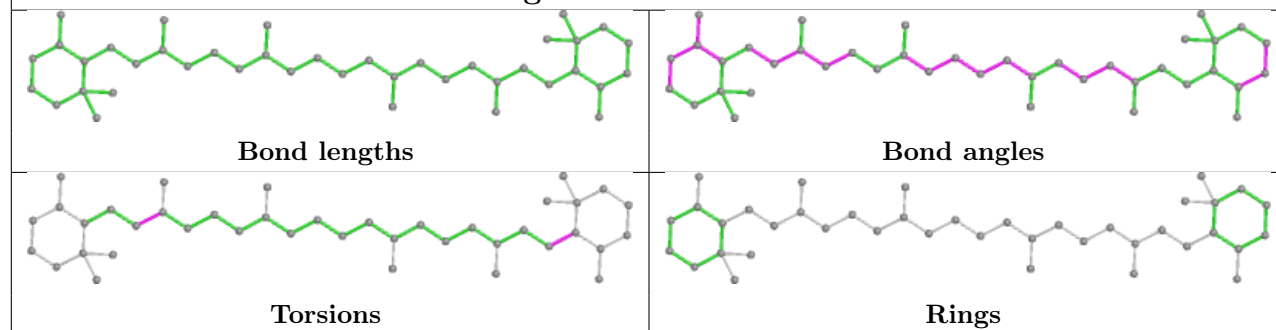
Ligand CLA f 1205

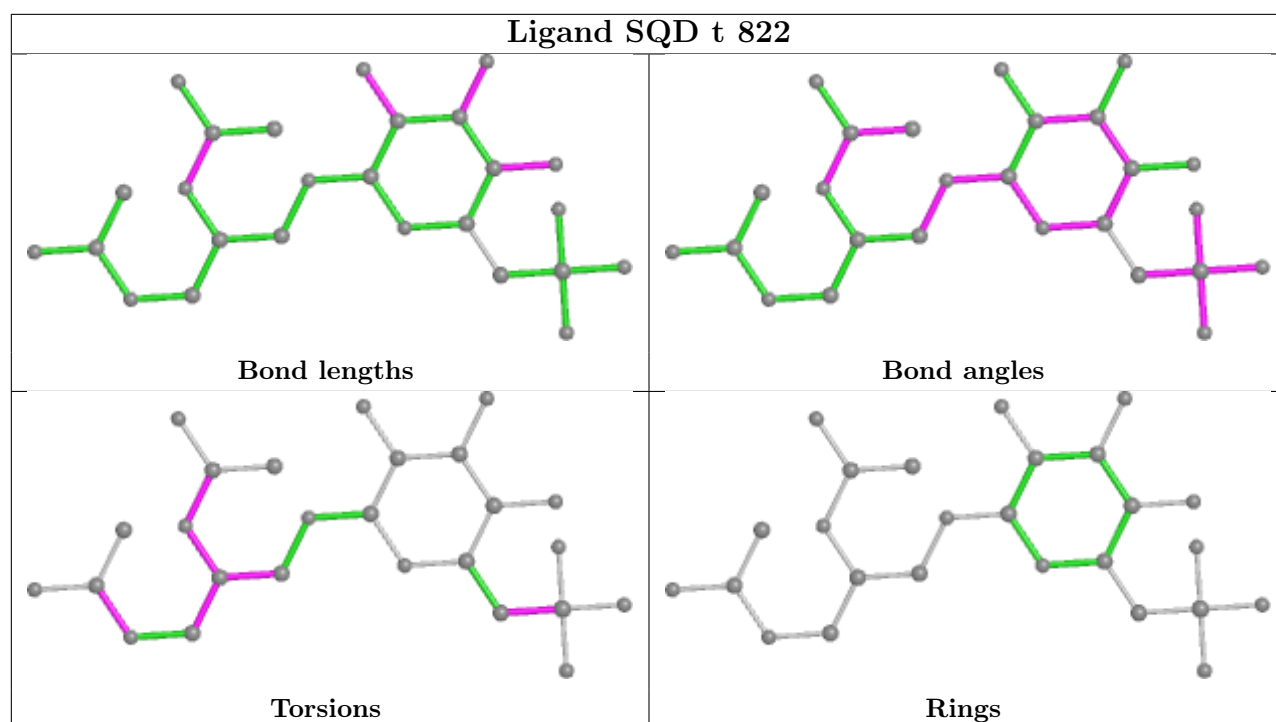


Ligand CLA Z 510

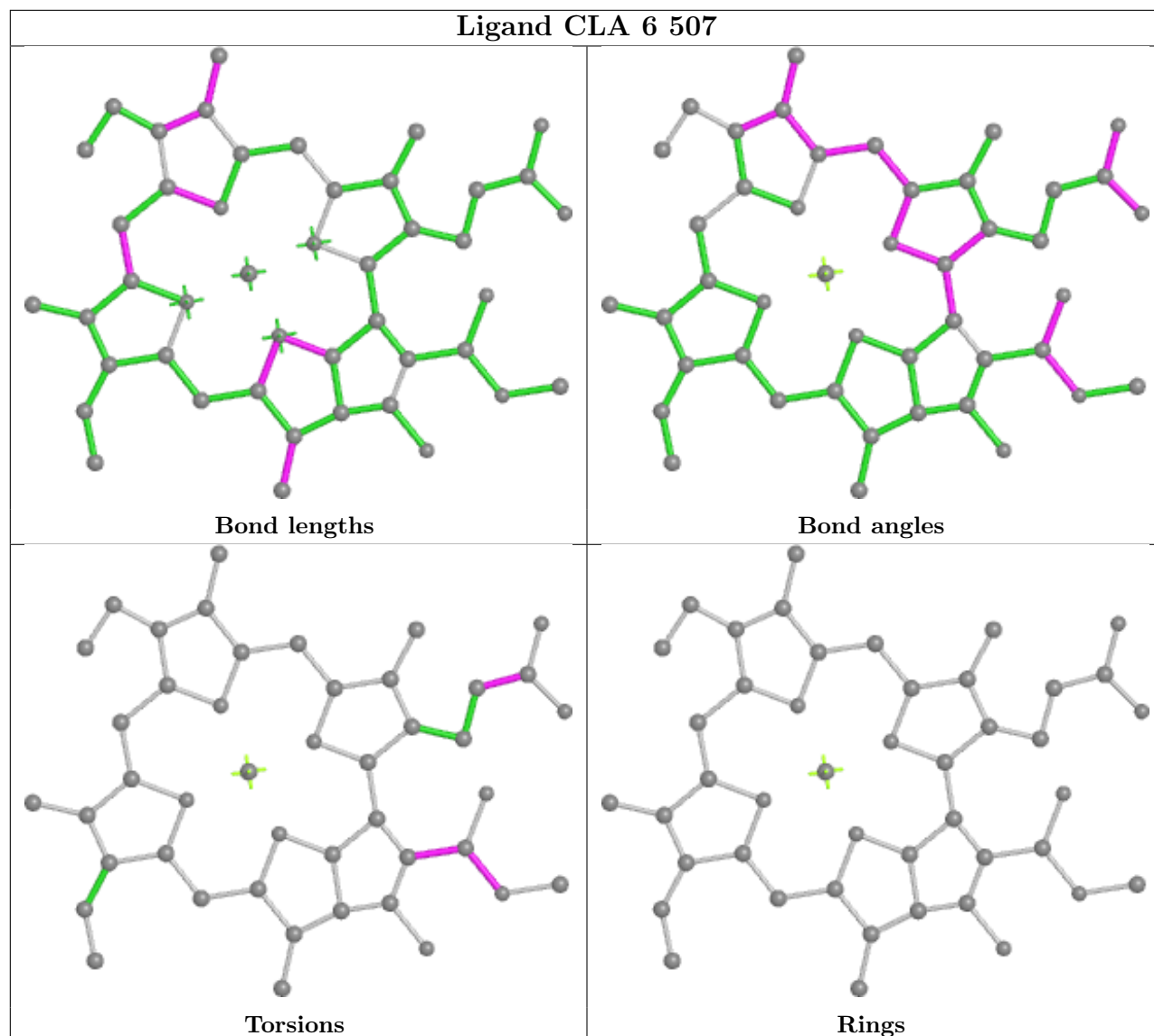


Ligand BCR L 4022

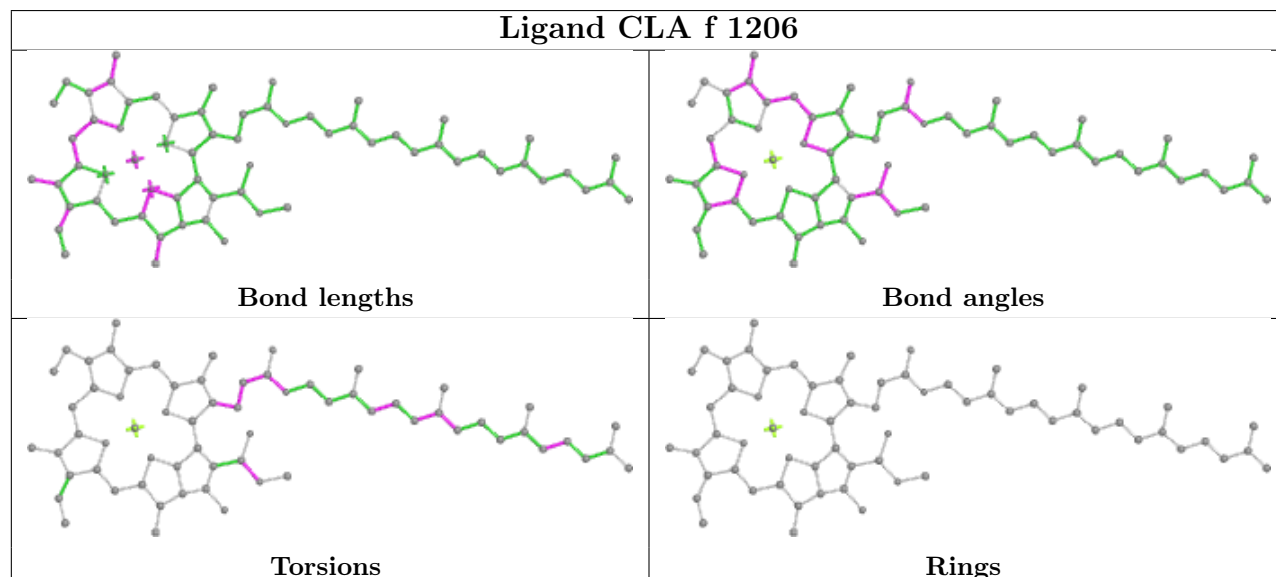




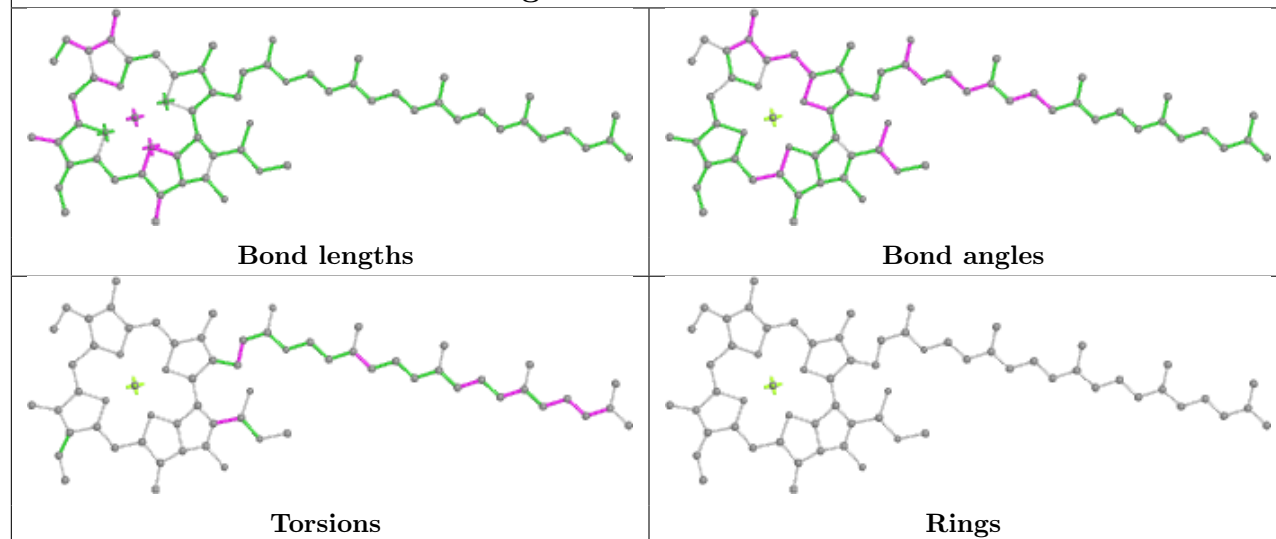
Ligand CLA 6 507



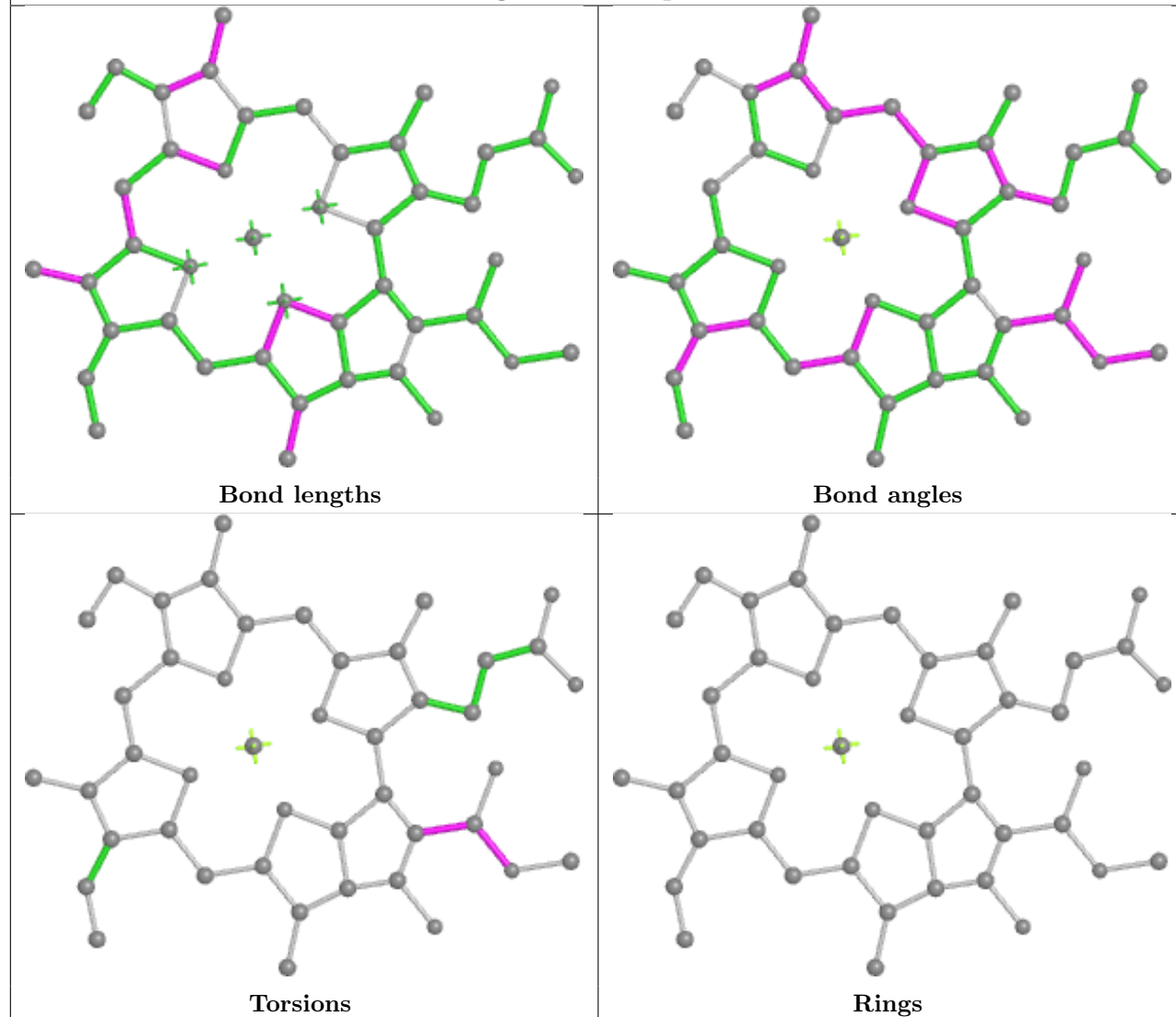
Ligand CLA f 1206

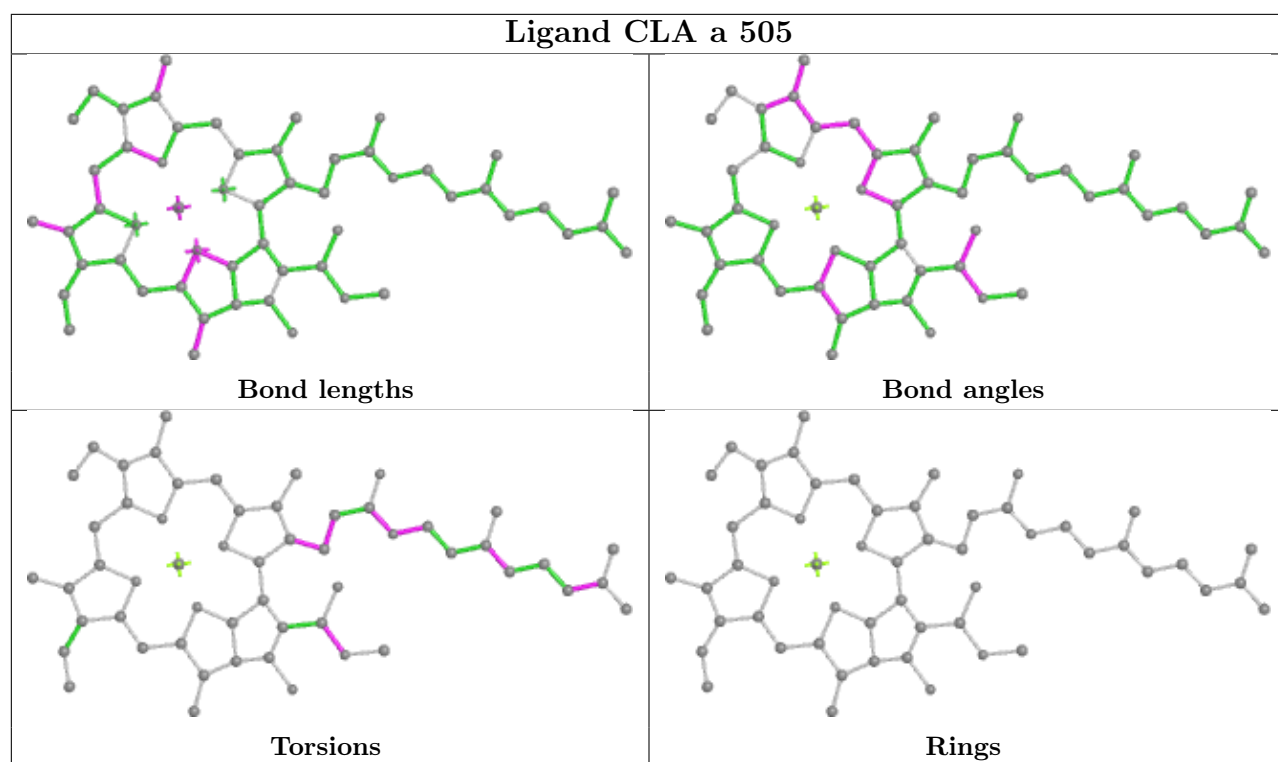


Ligand CLA G 1117

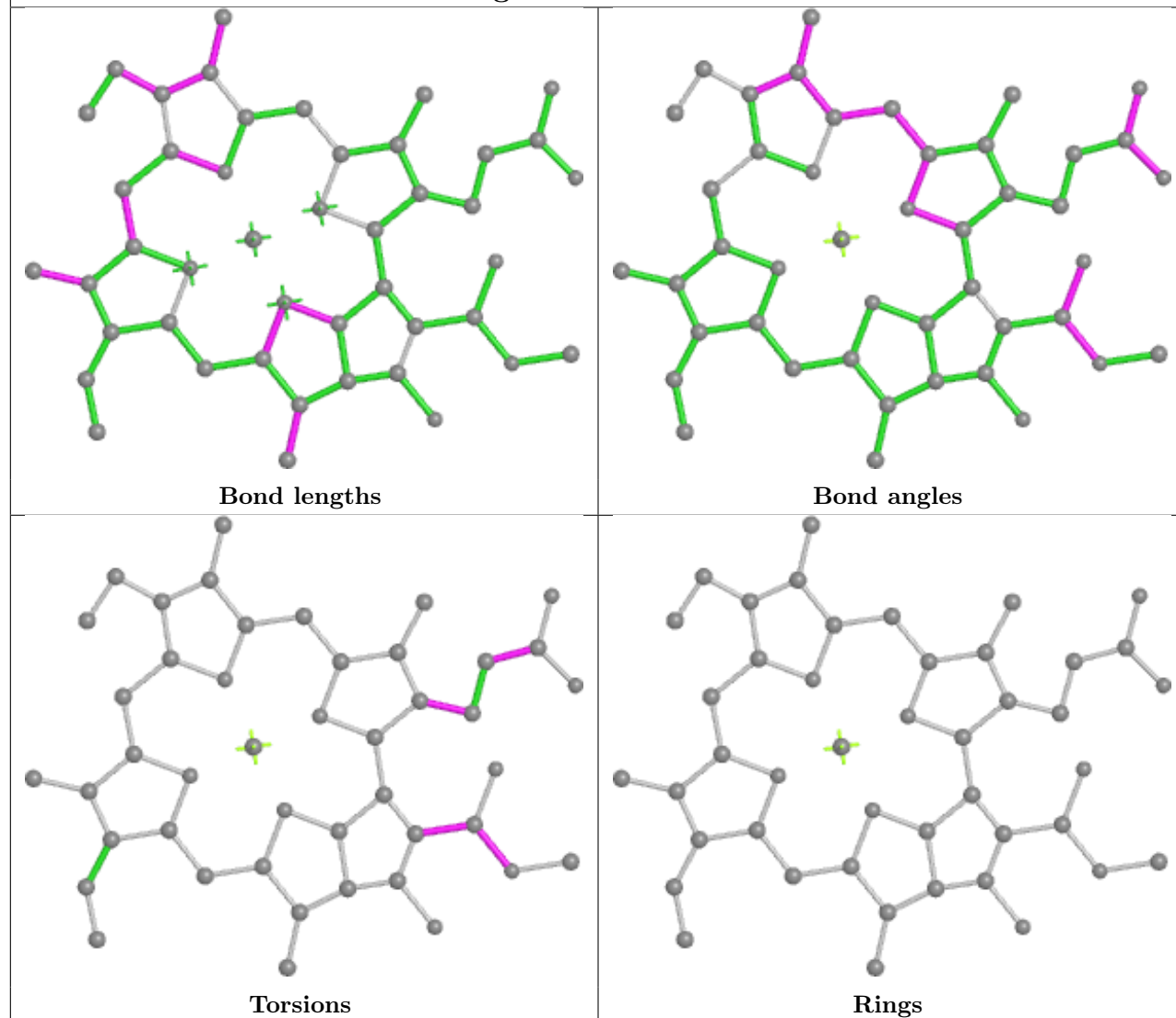


Ligand CLA q 504

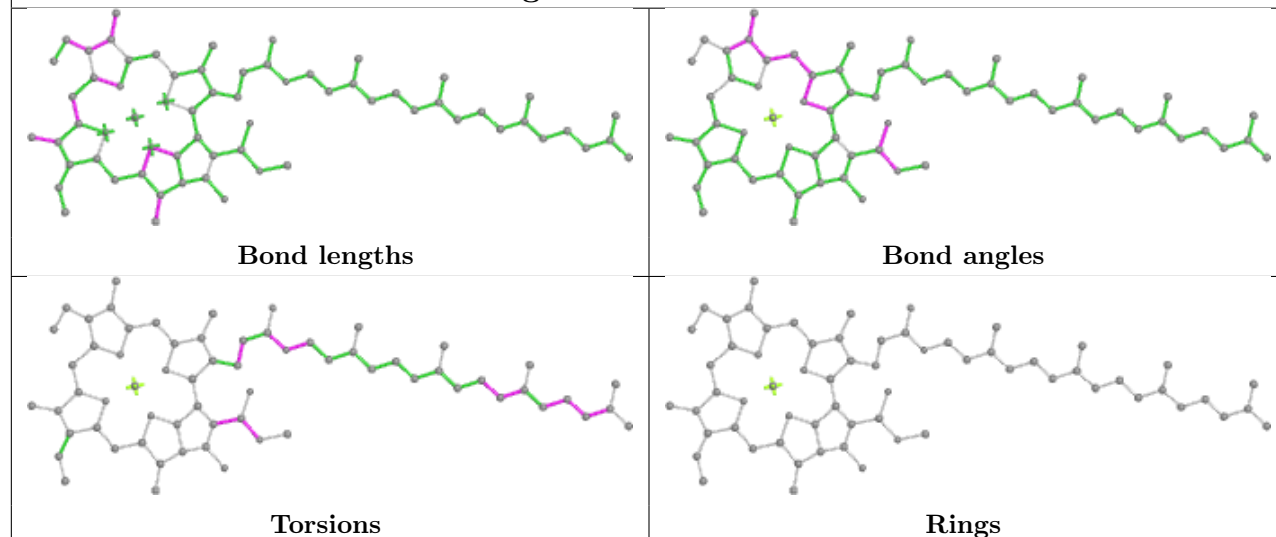




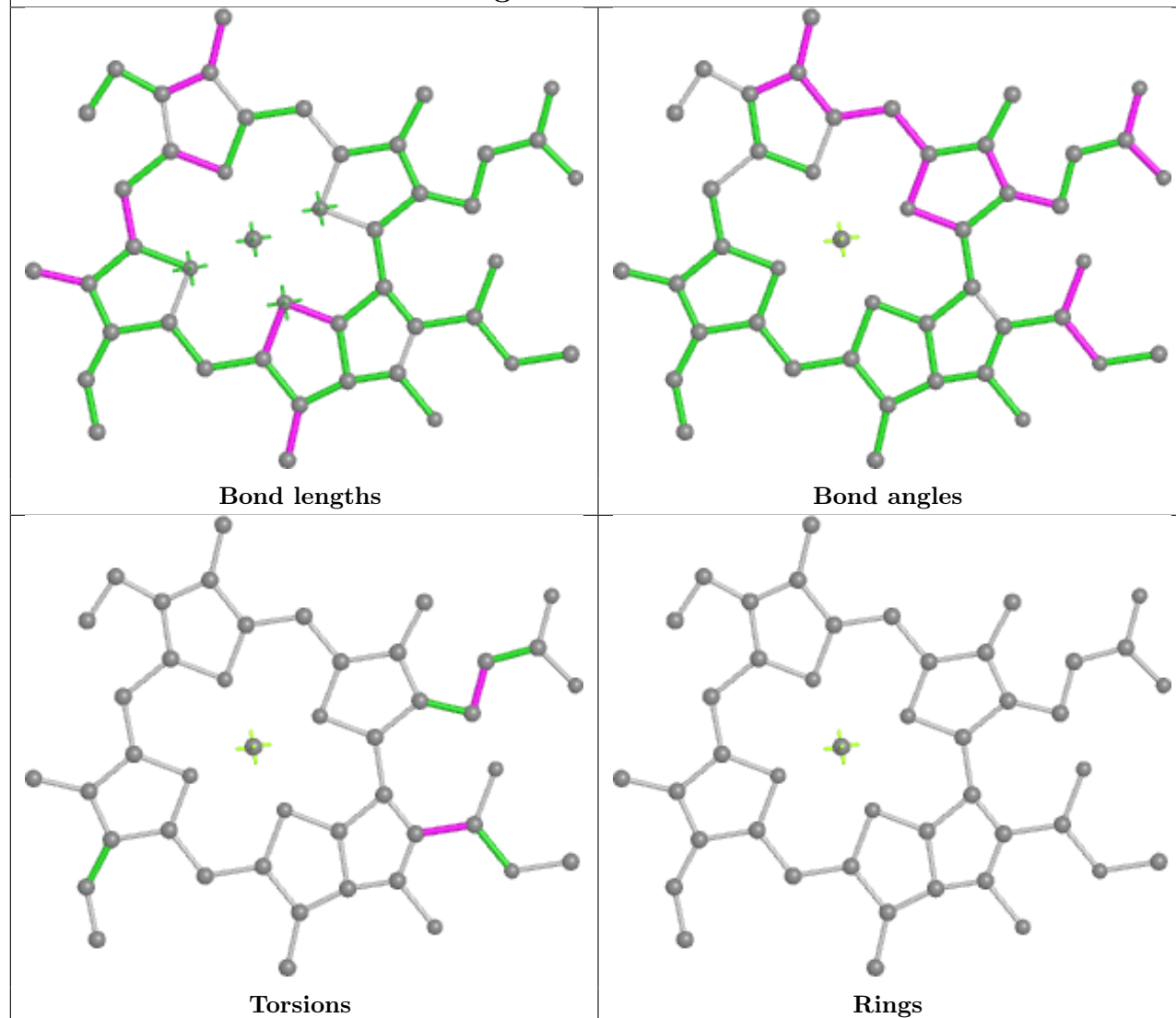
Ligand CLA d 519



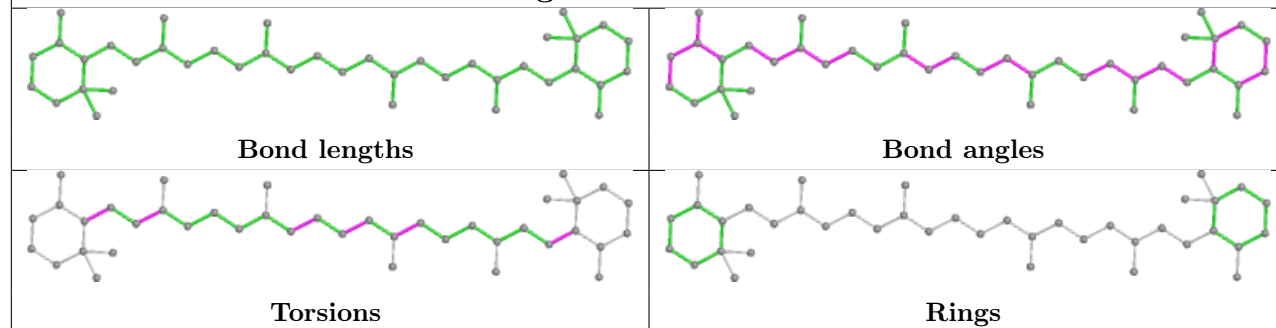
Ligand CLA H 1207

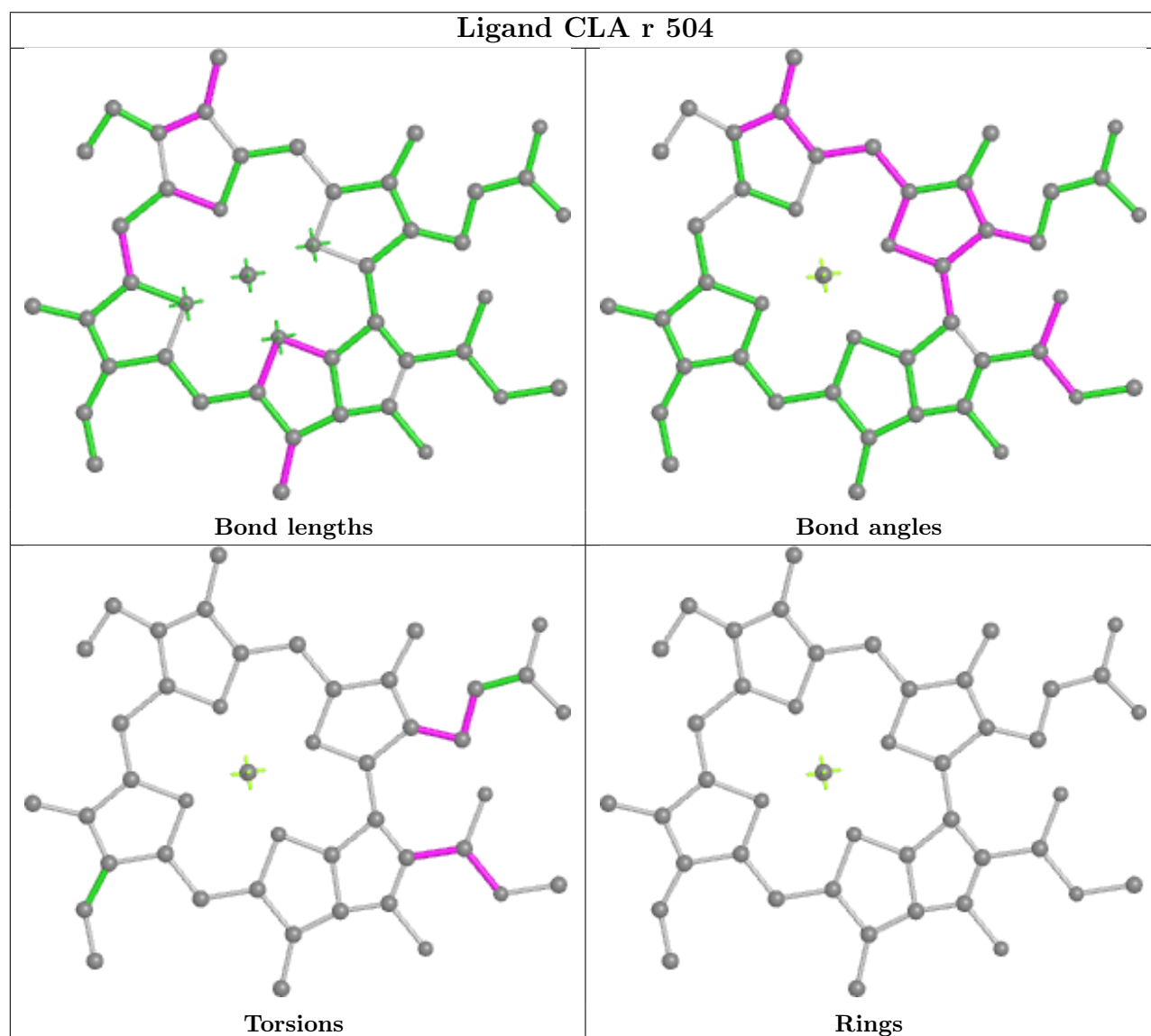
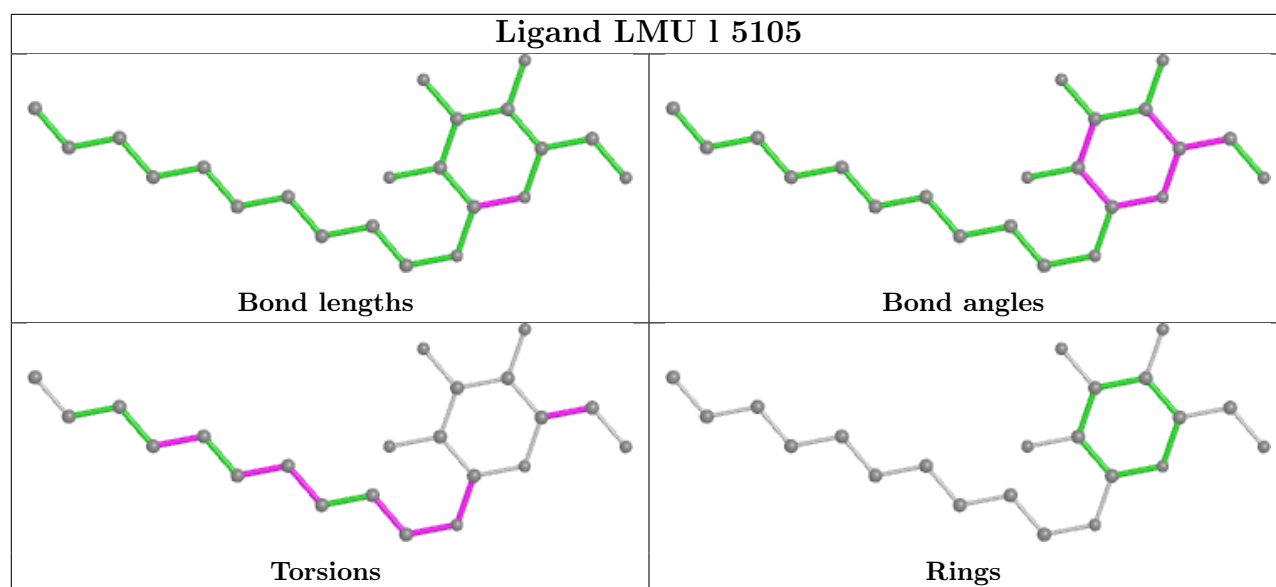


Ligand CLA 1 502

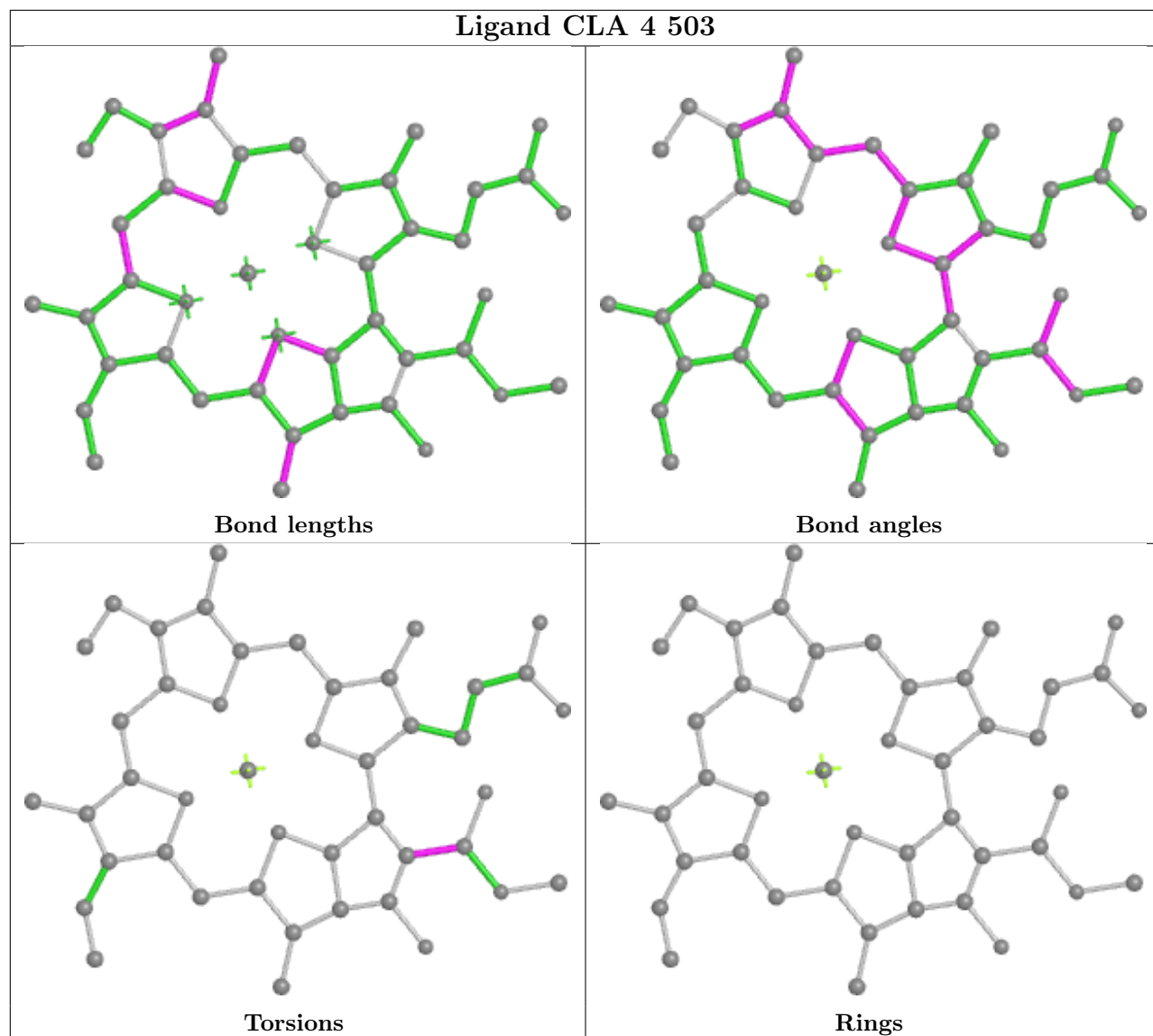


Ligand BCR t 521

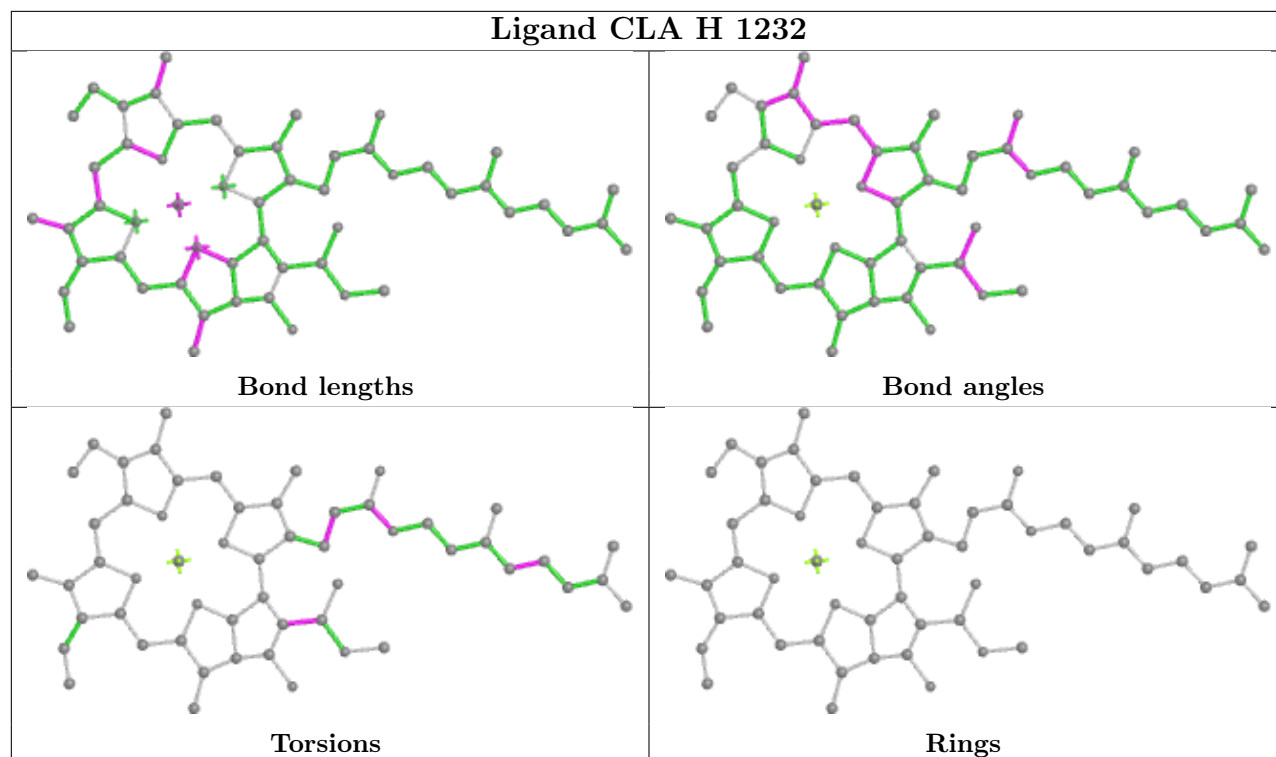




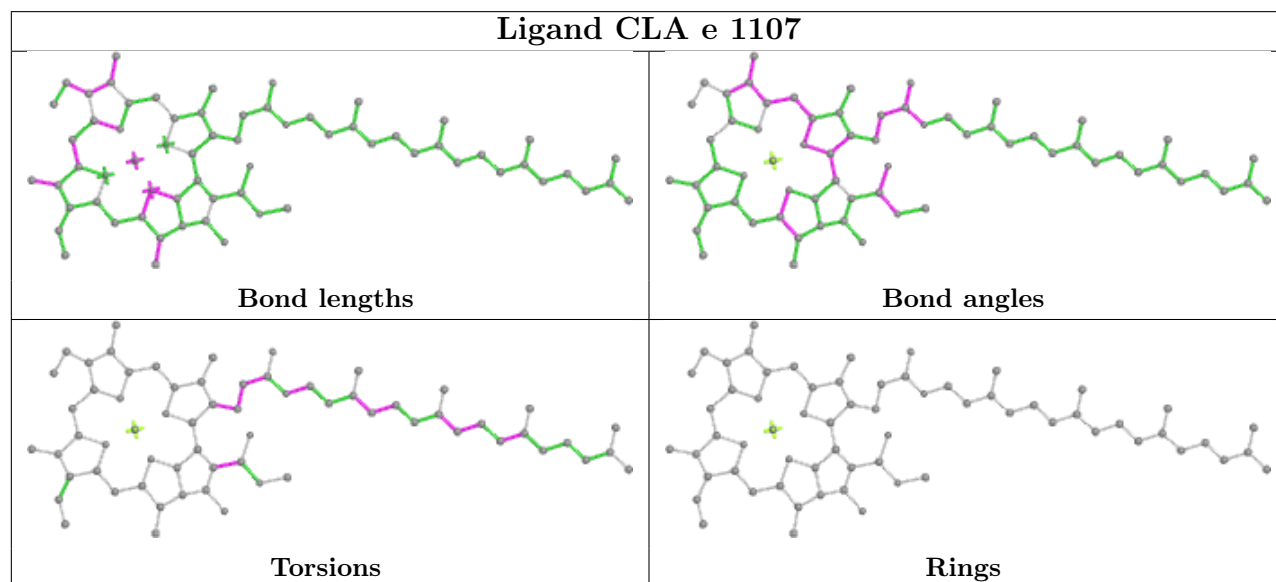
Ligand CLA 4 503

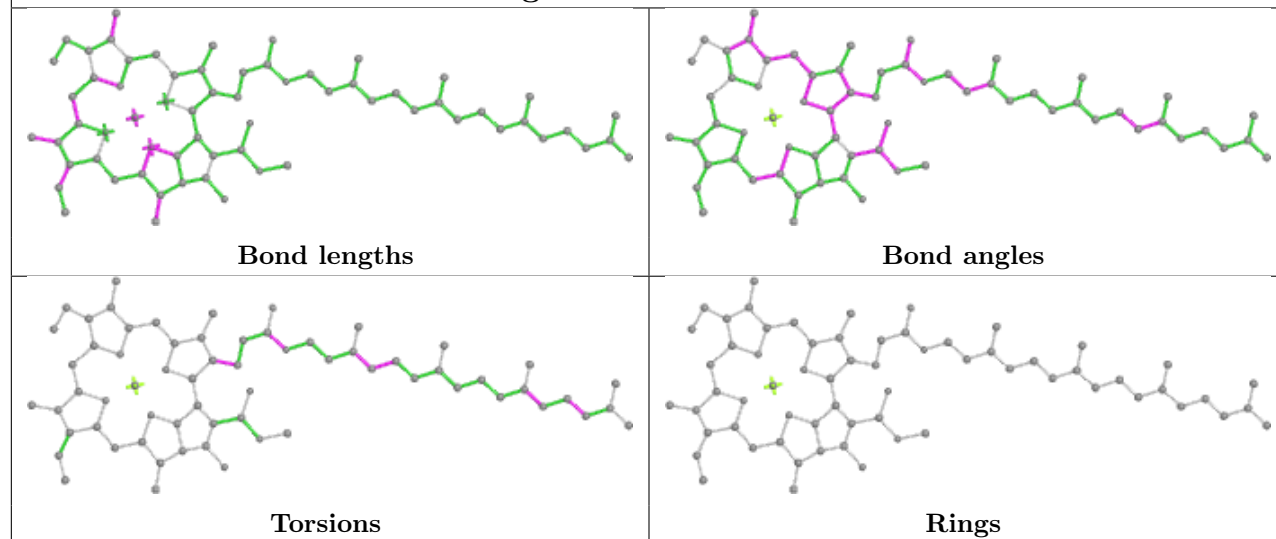
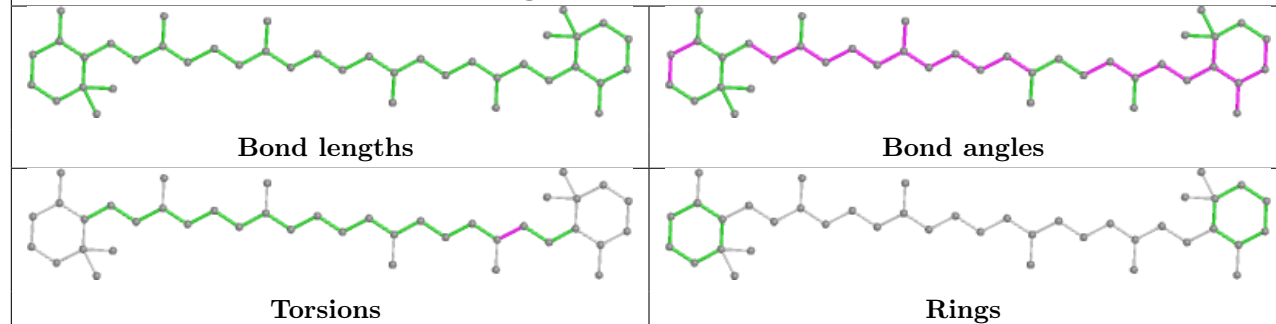


Ligand CLA H 1232

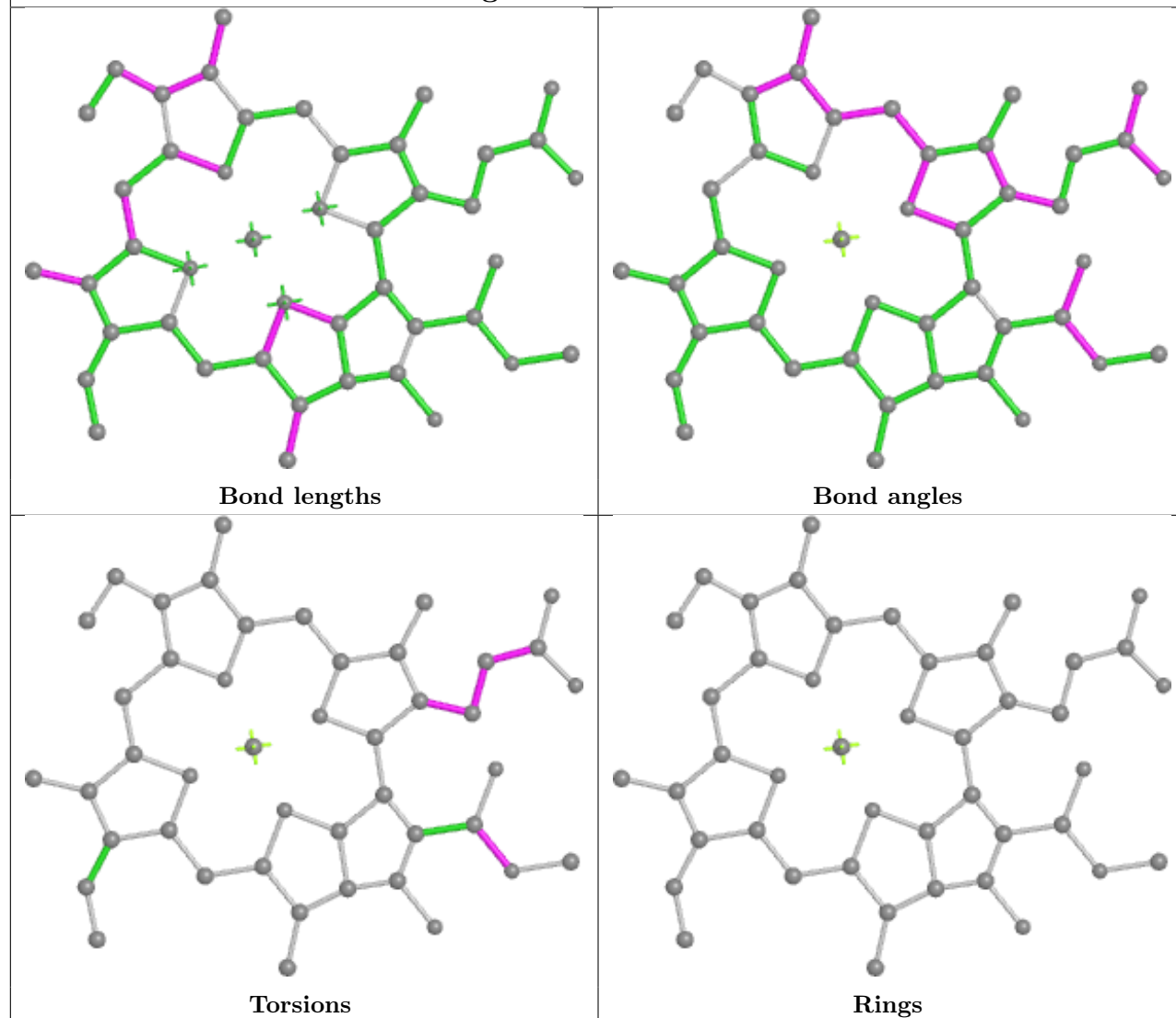


Ligand CLA e 1107

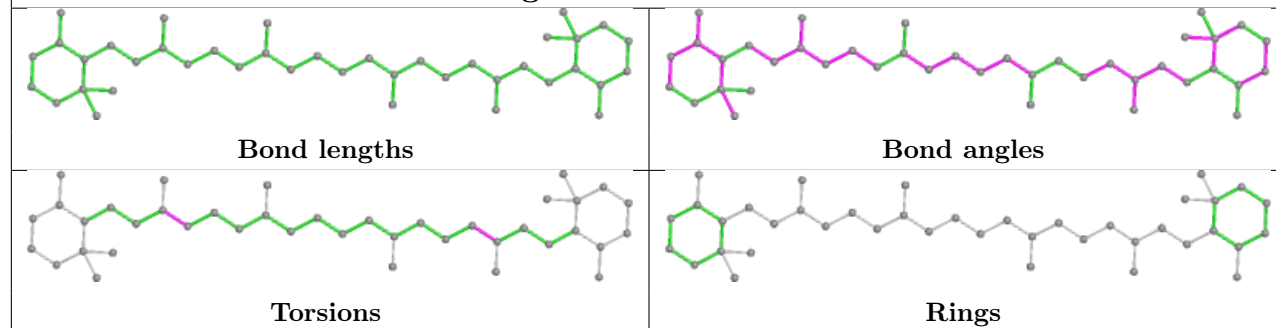


Ligand CLA G 1104**Ligand BCR U 4104**

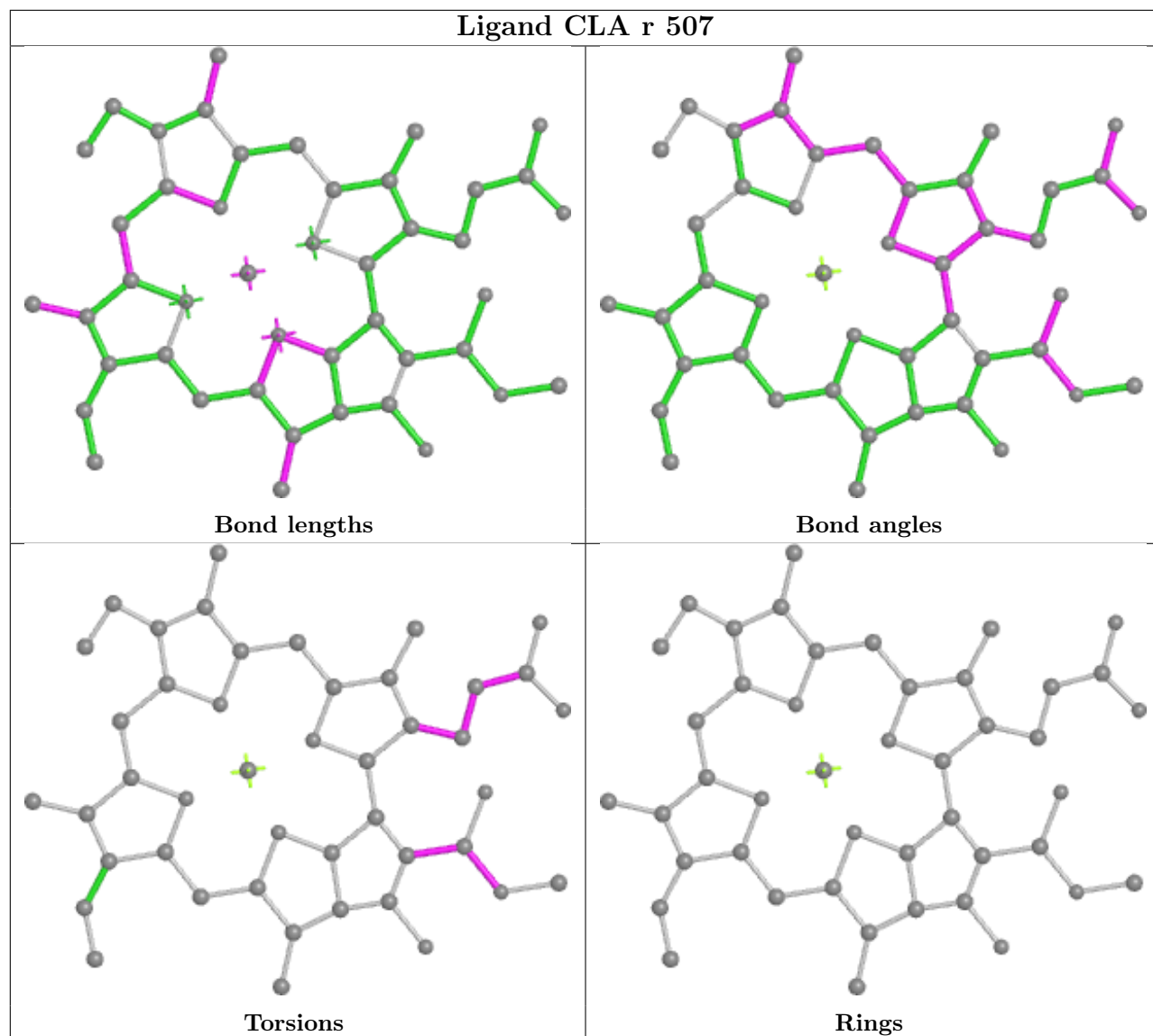
Ligand CLA R 1302

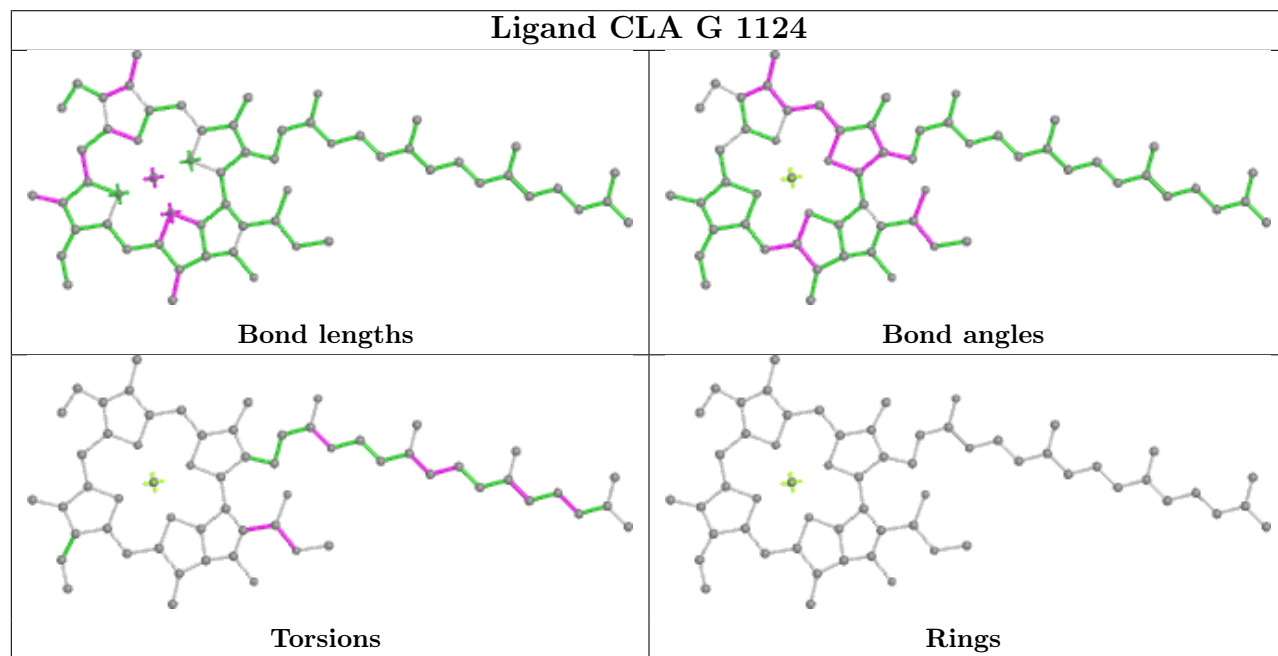
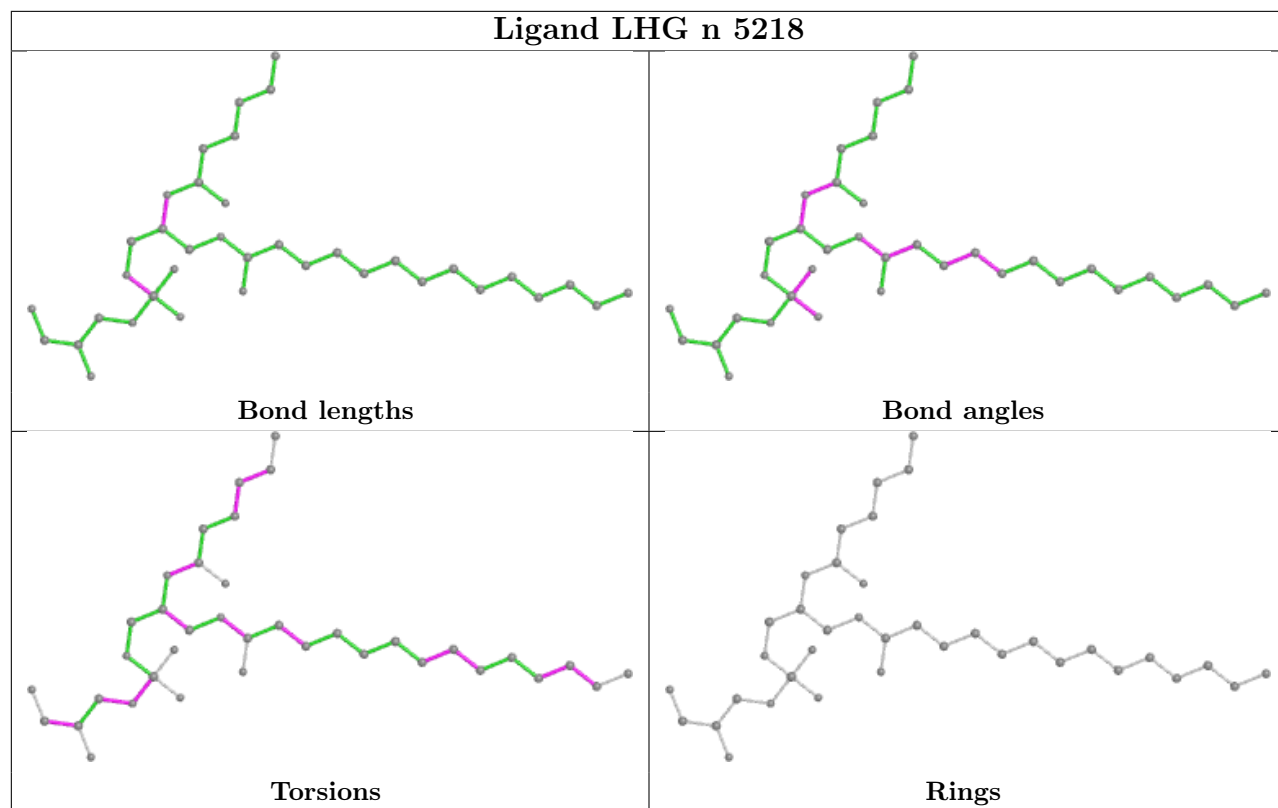


Ligand BCR B 4006

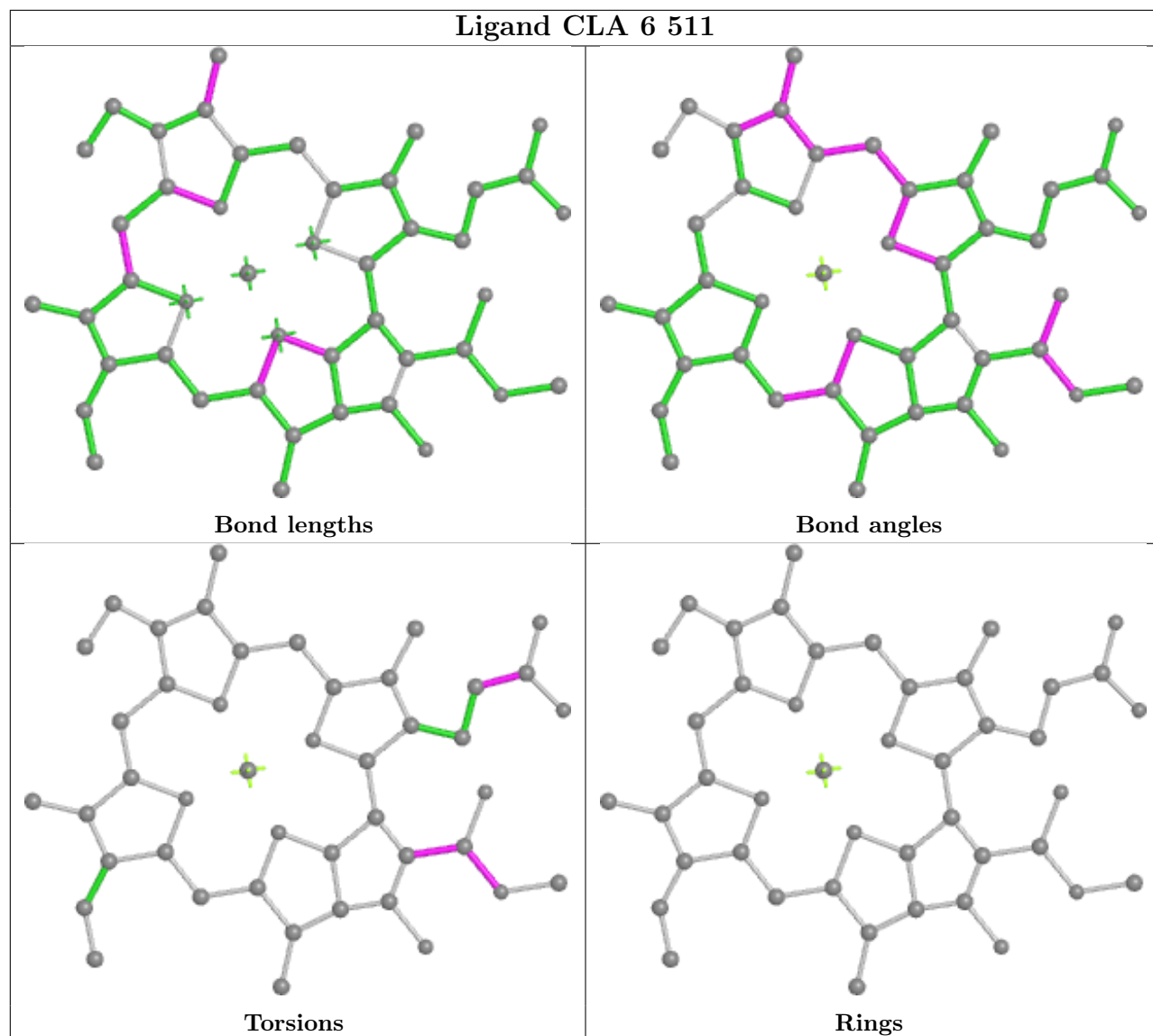


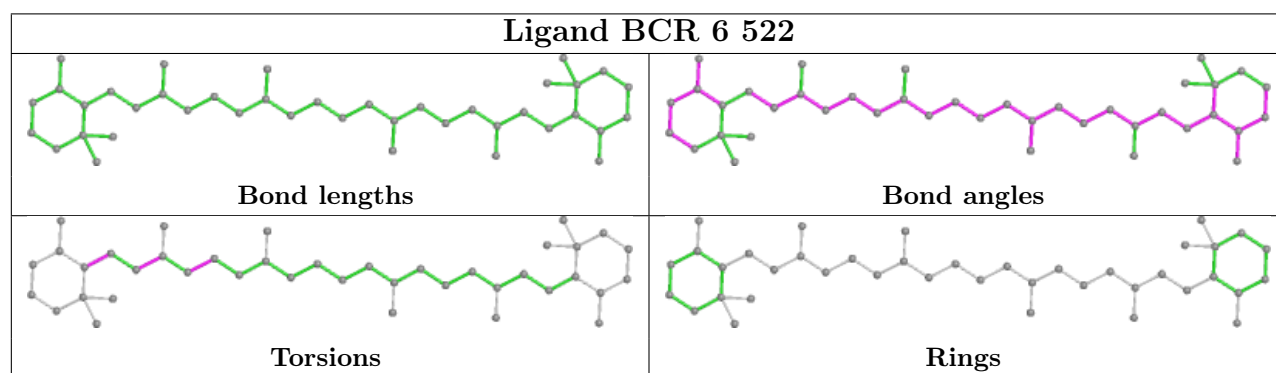
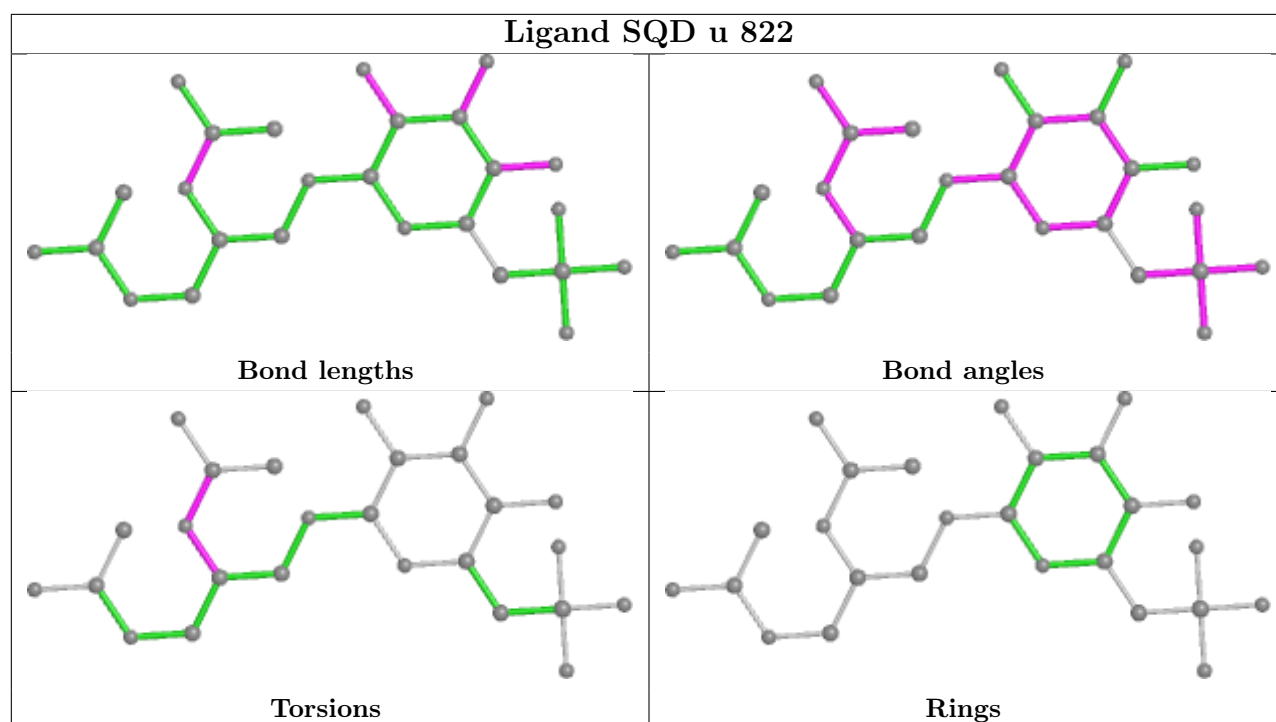
Ligand CLA r 507



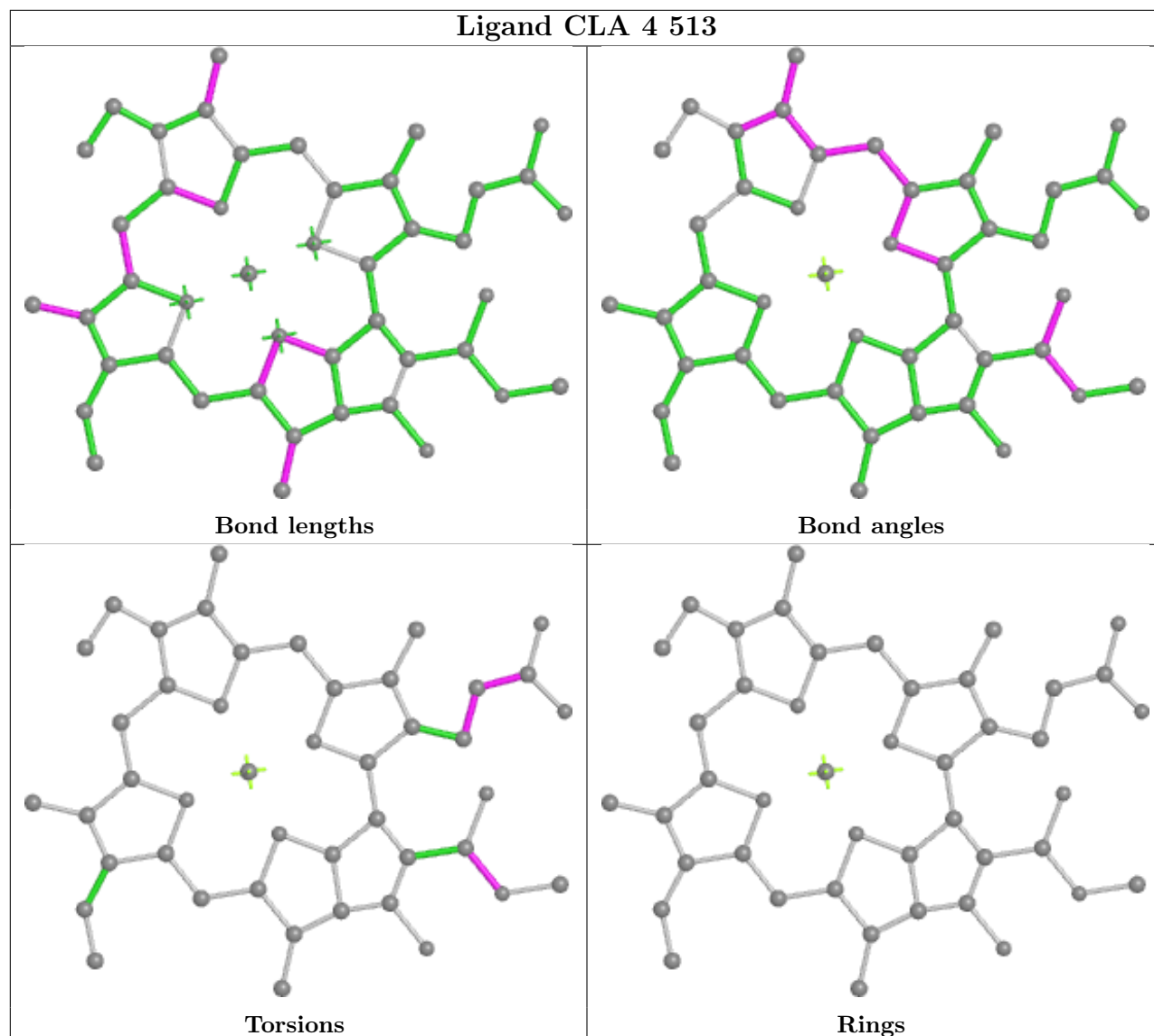


Ligand CLA 6 511

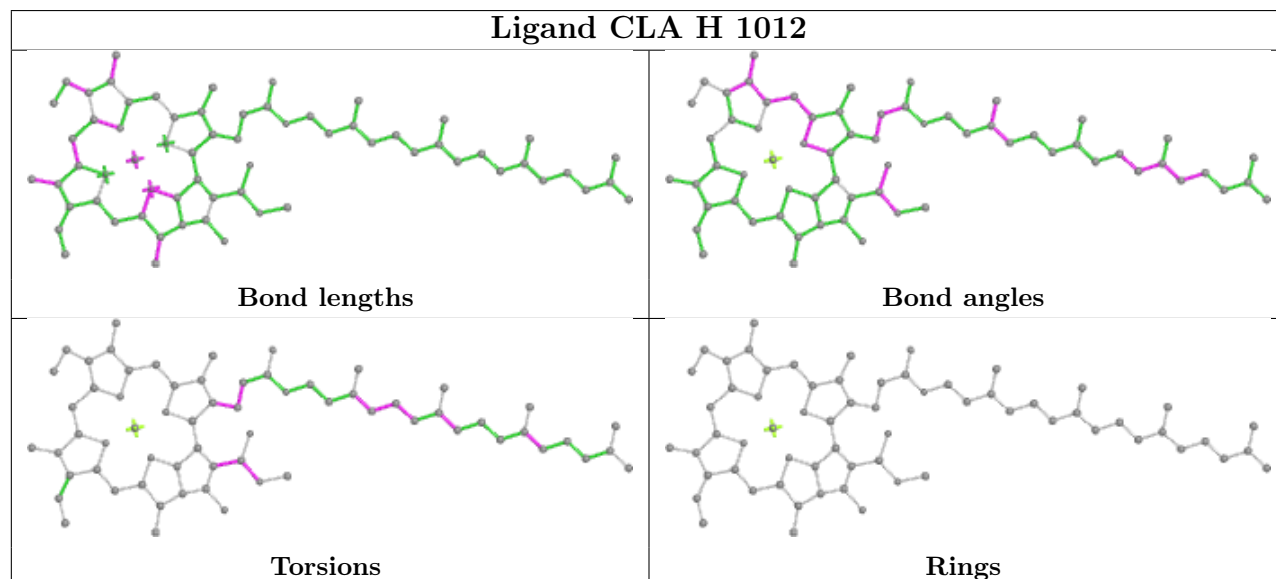




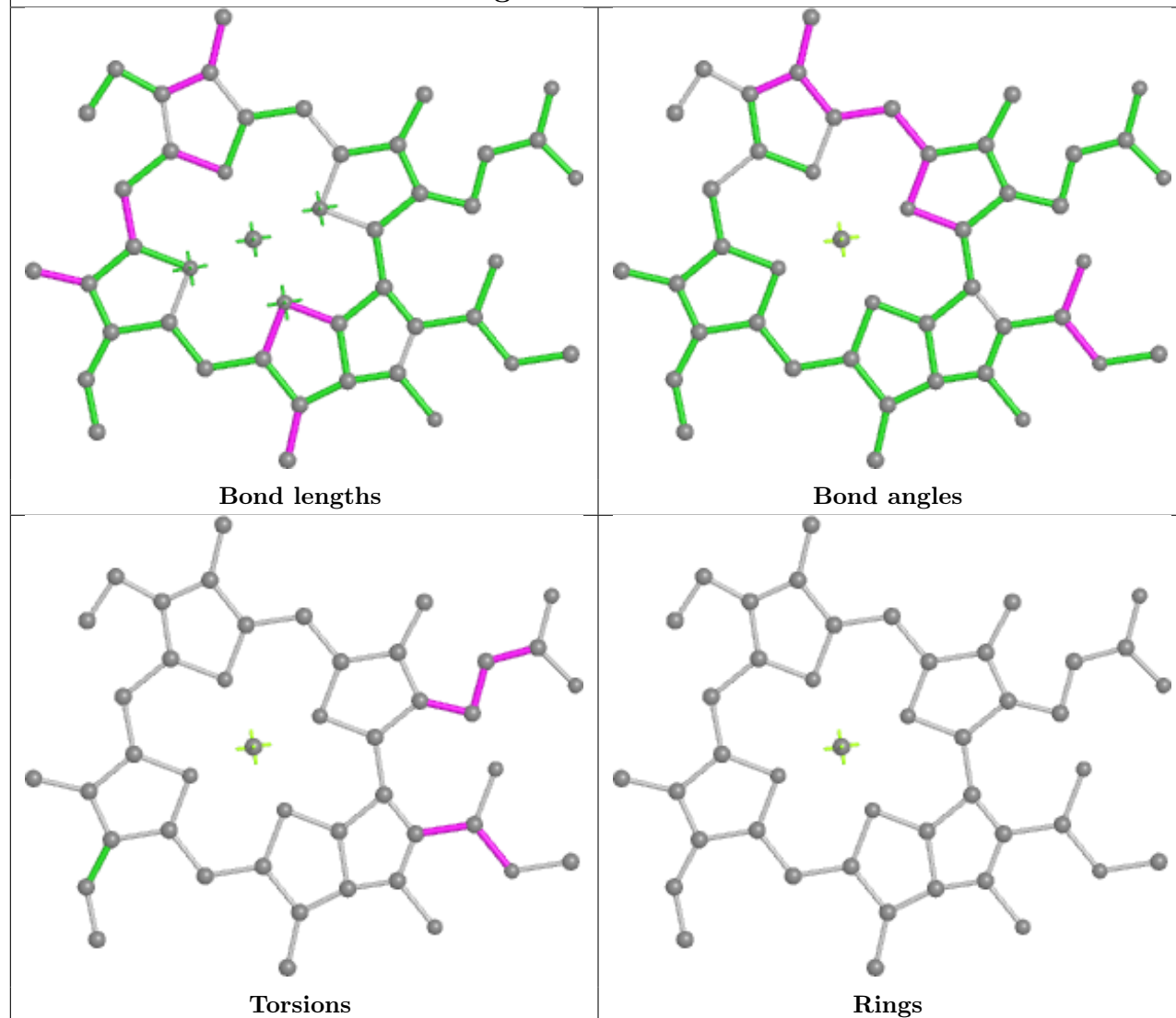
Ligand CLA 4 513



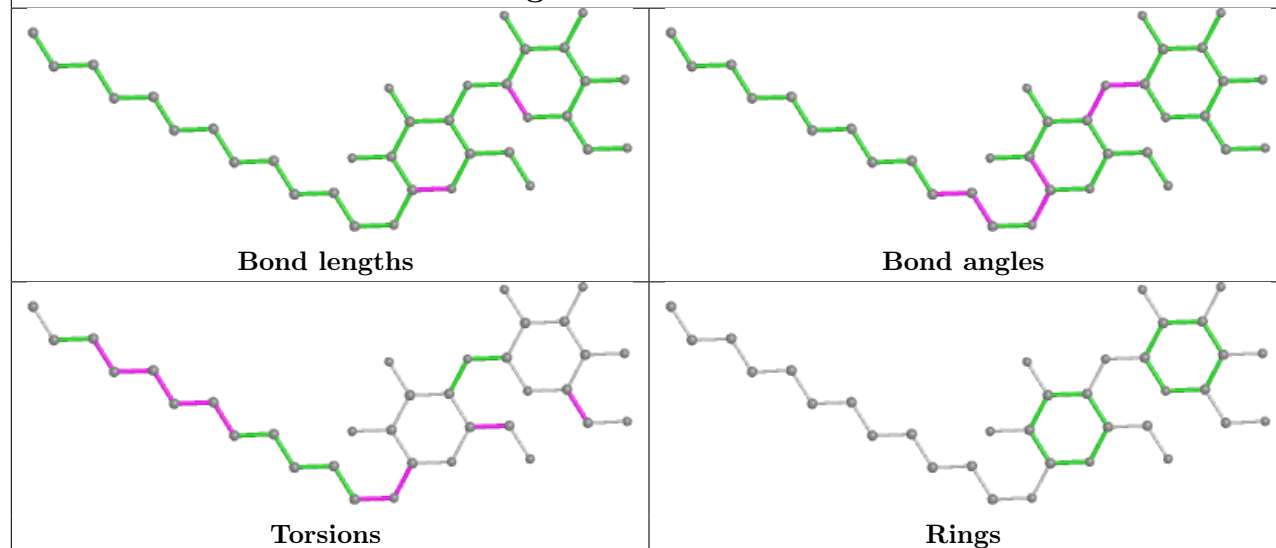
Ligand CLA H 1012

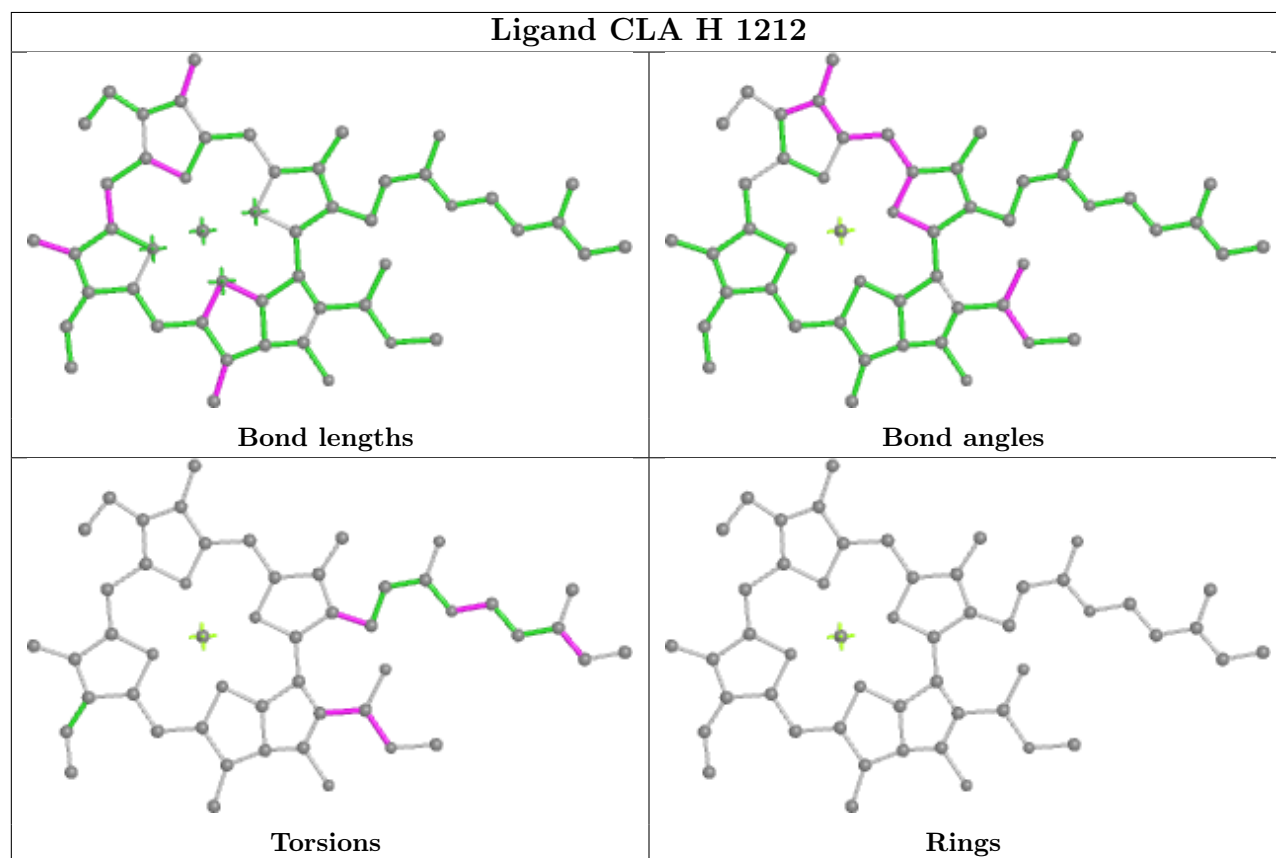
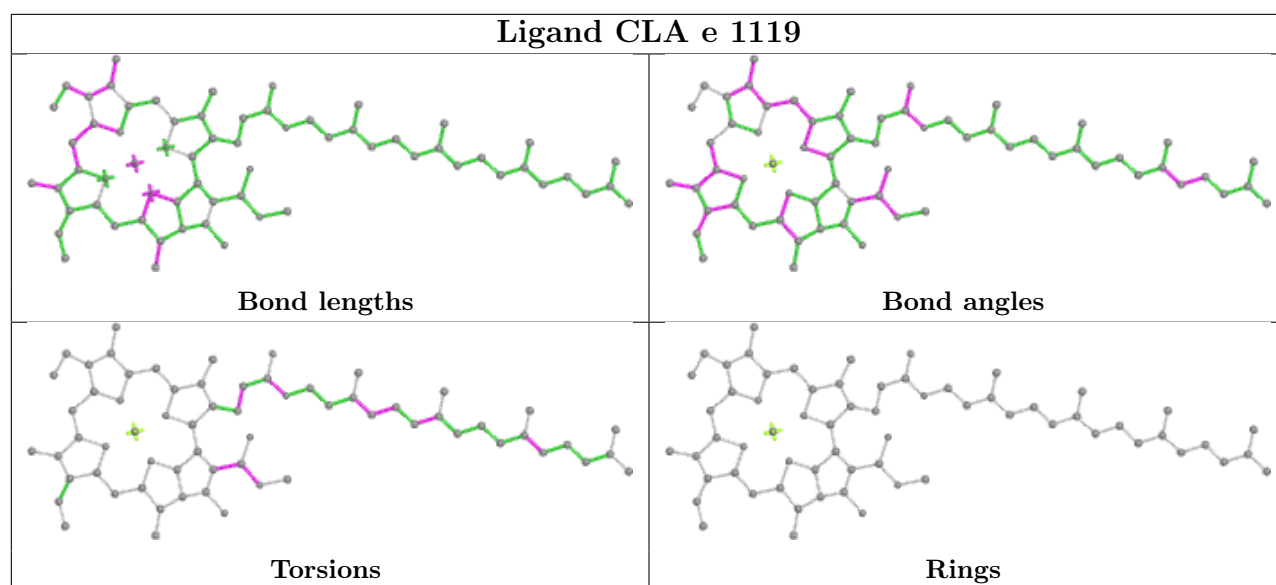


Ligand CLA 5 517

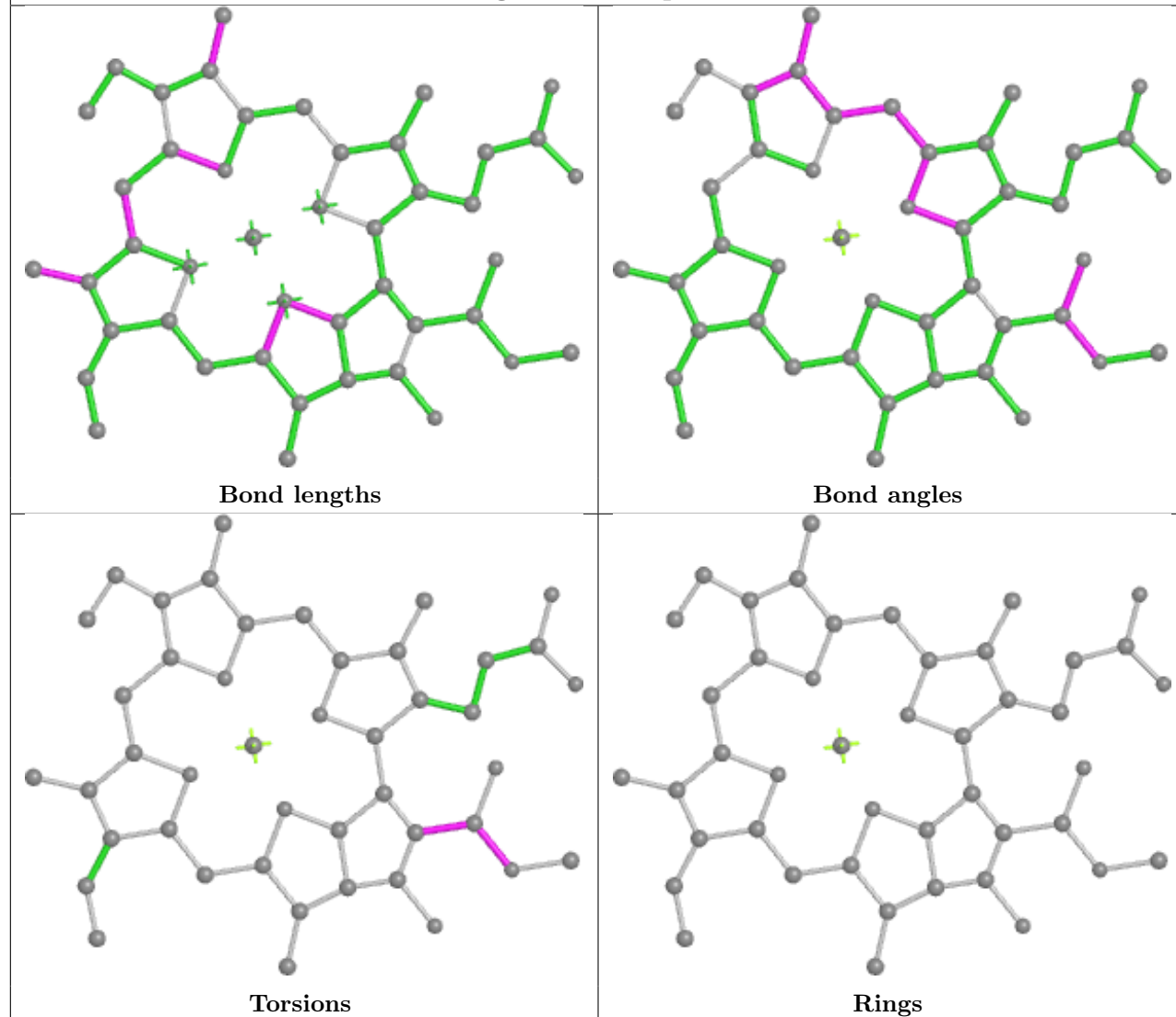


Ligand LMU f 1843

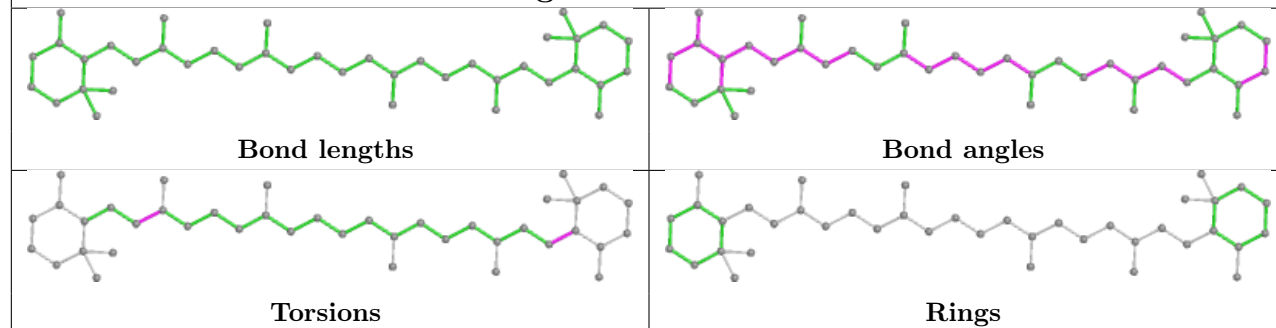


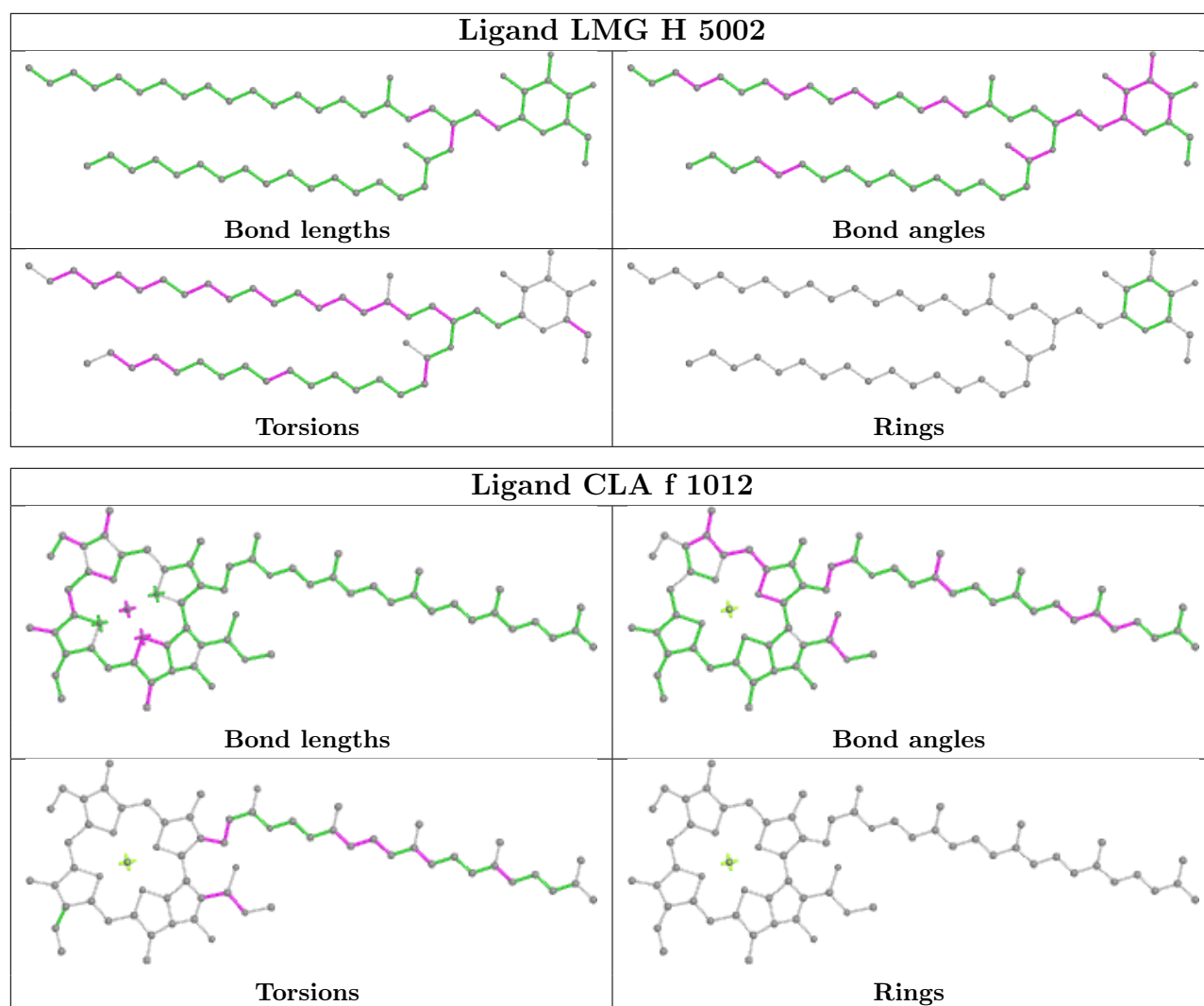


Ligand CLA q 506

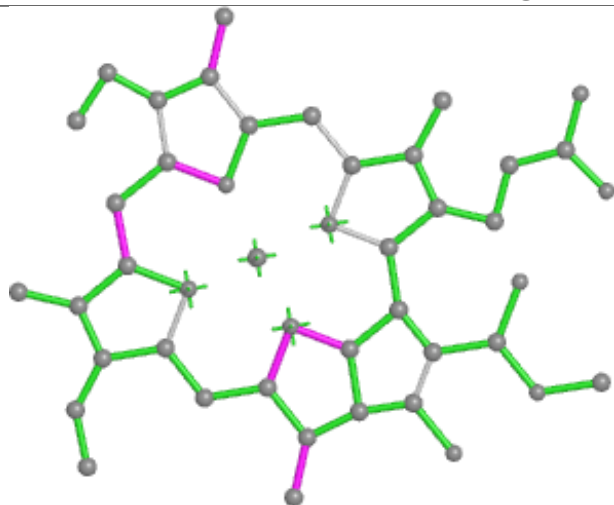


Ligand BCR t 524

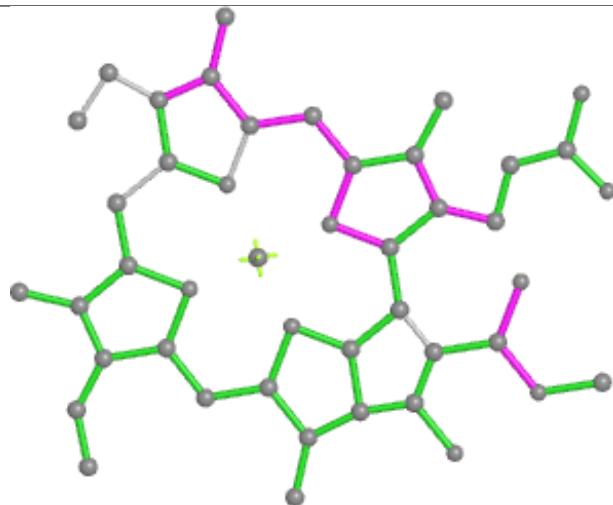




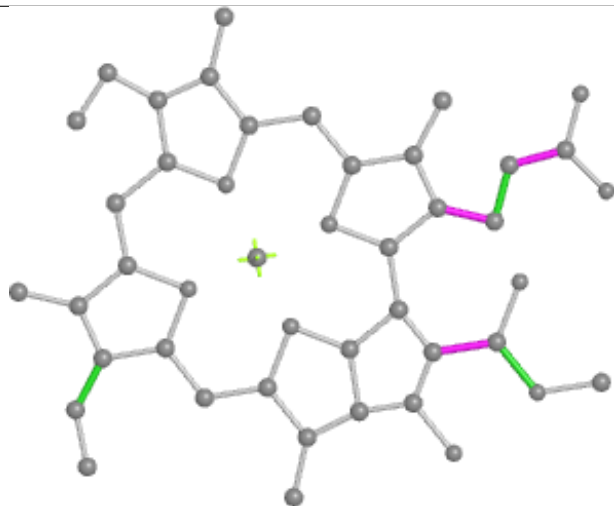
Ligand CLA b 516



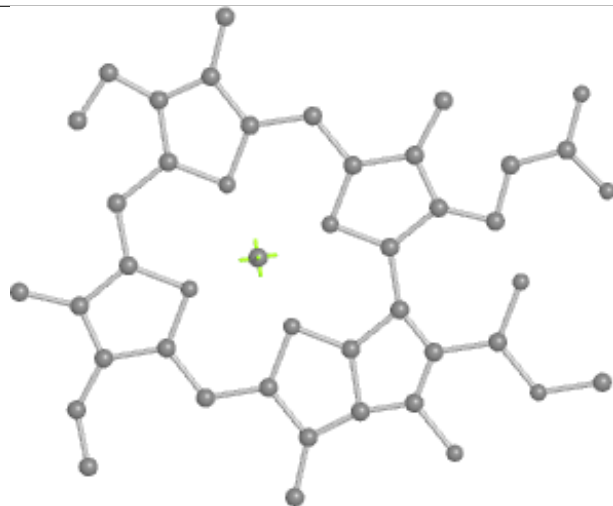
Bond lengths



Bond angles

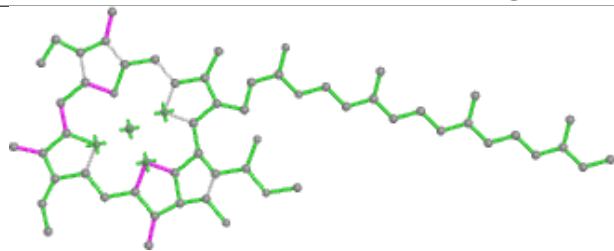


Torsions

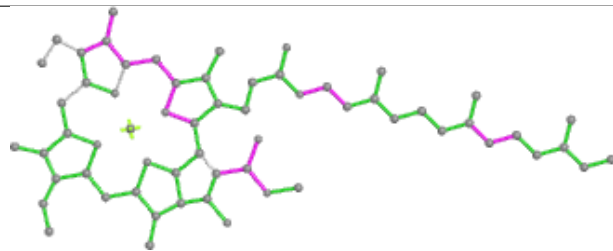


Rings

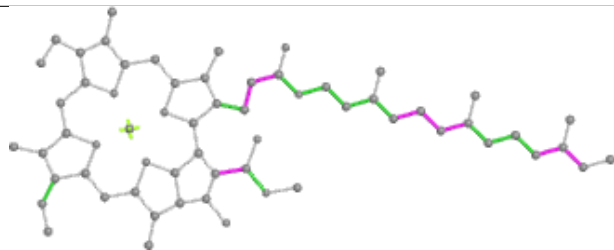
Ligand CLA B 1213



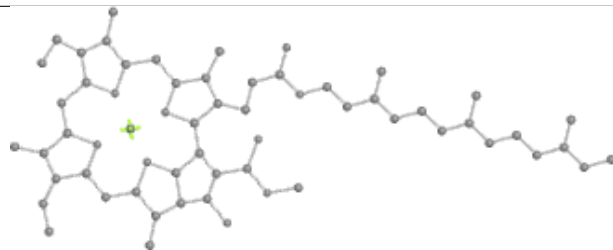
Bond lengths



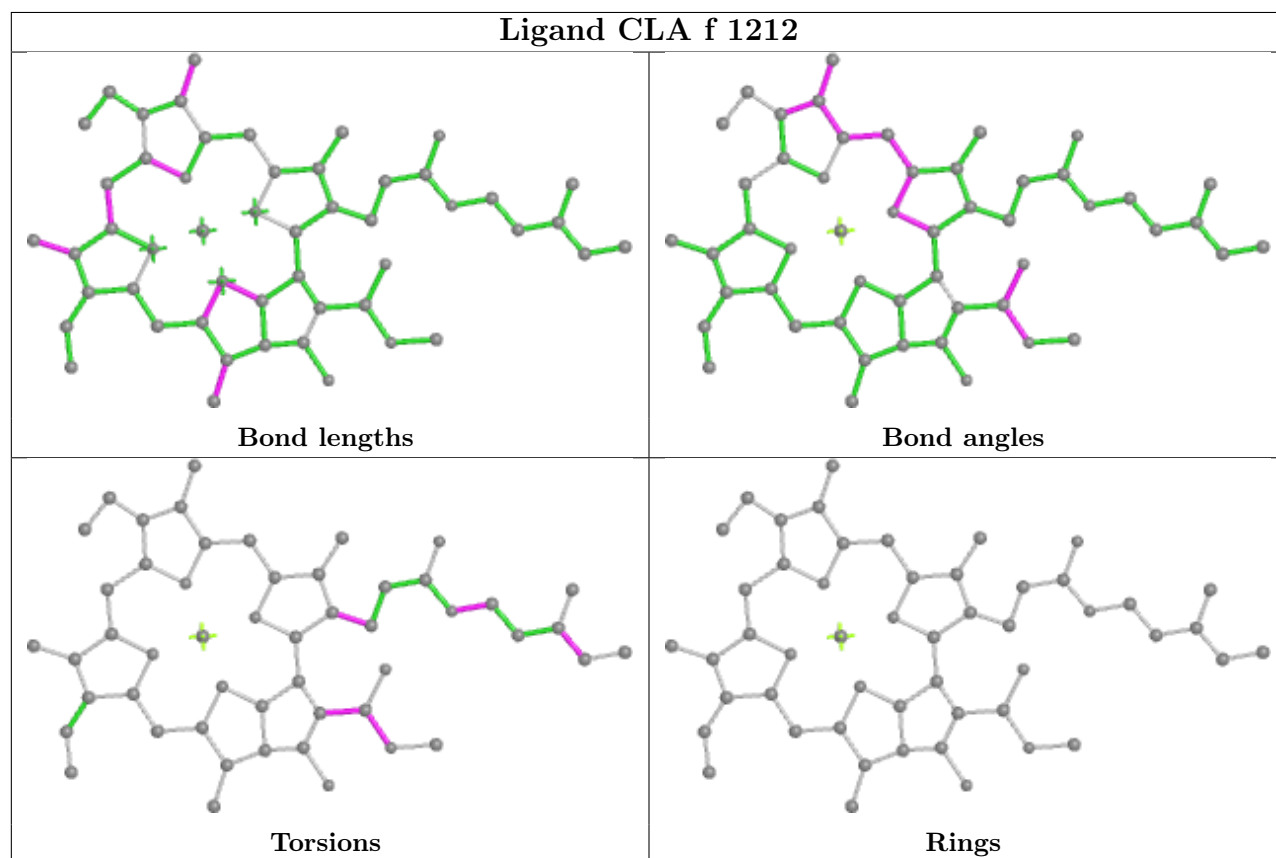
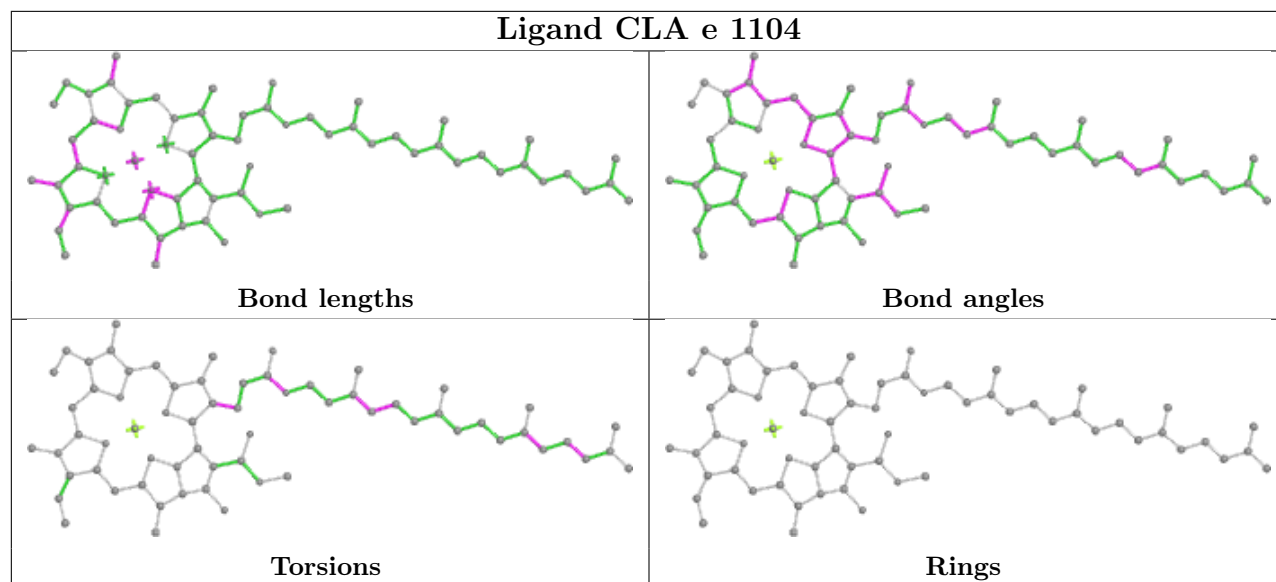
Bond angles

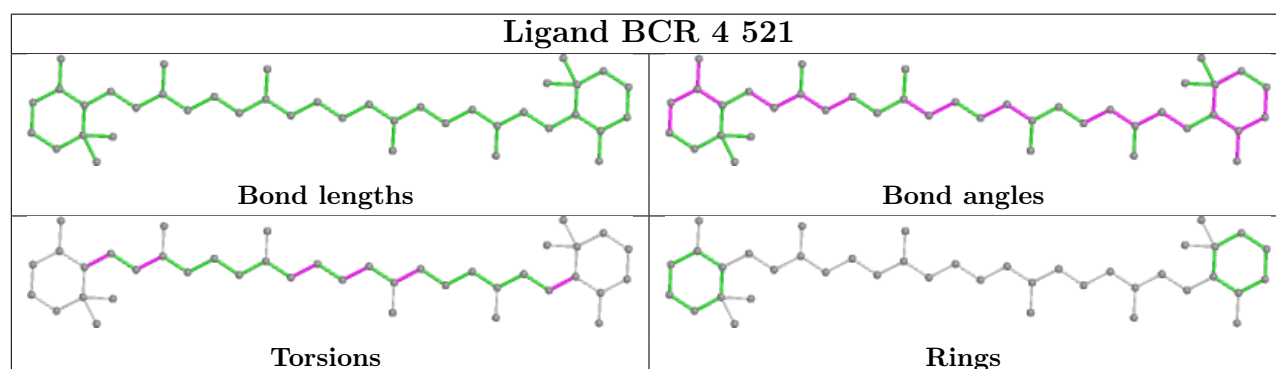
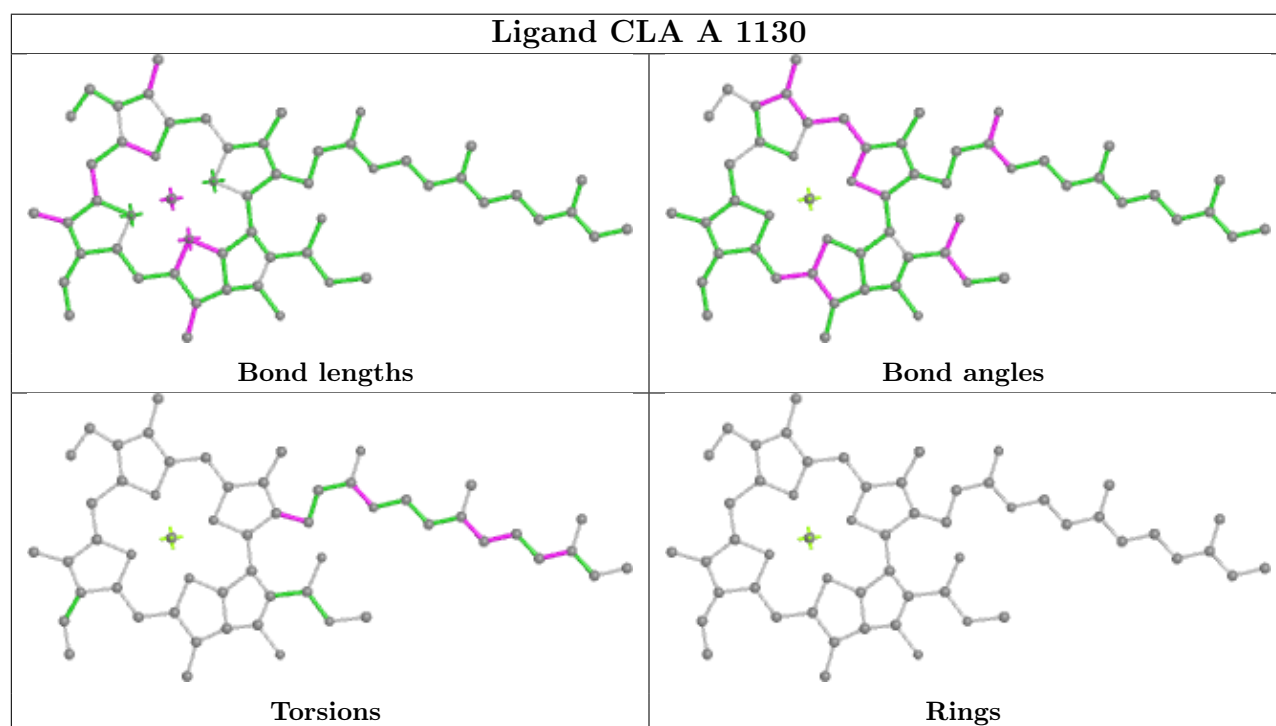
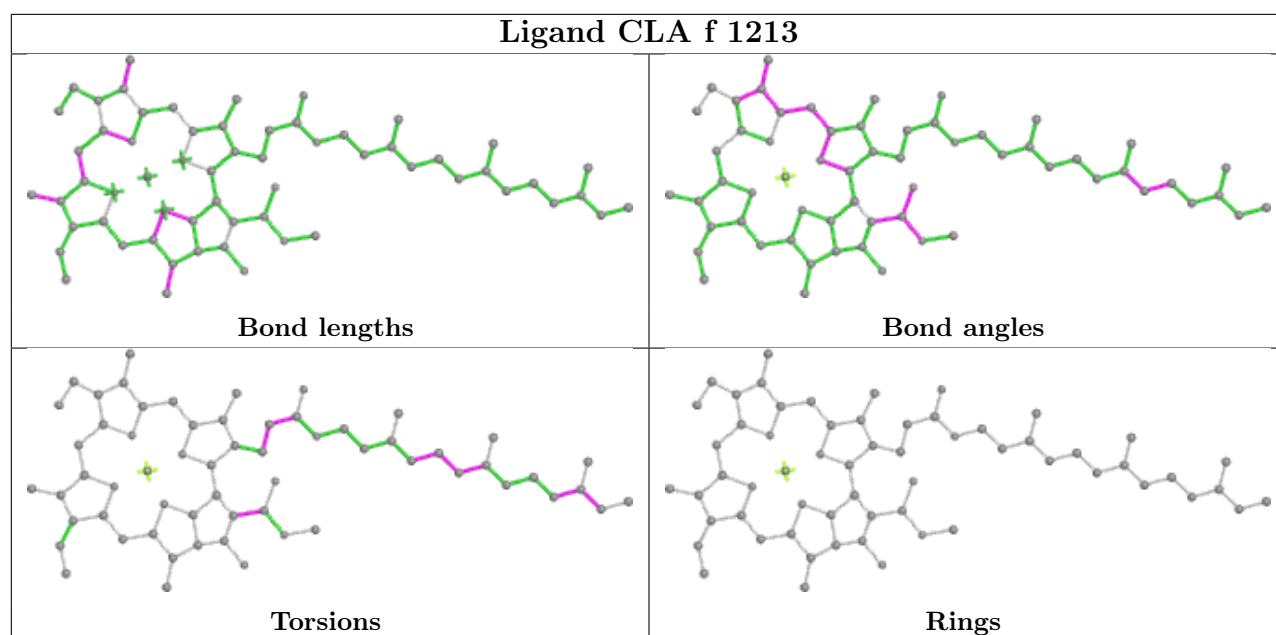


Torsions

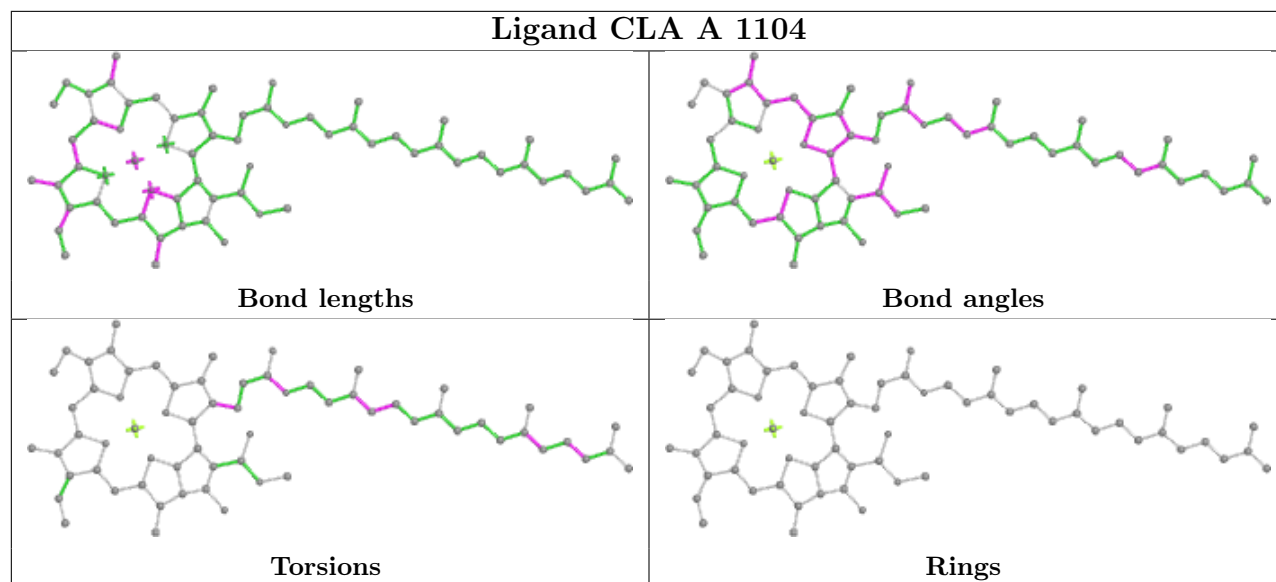


Rings

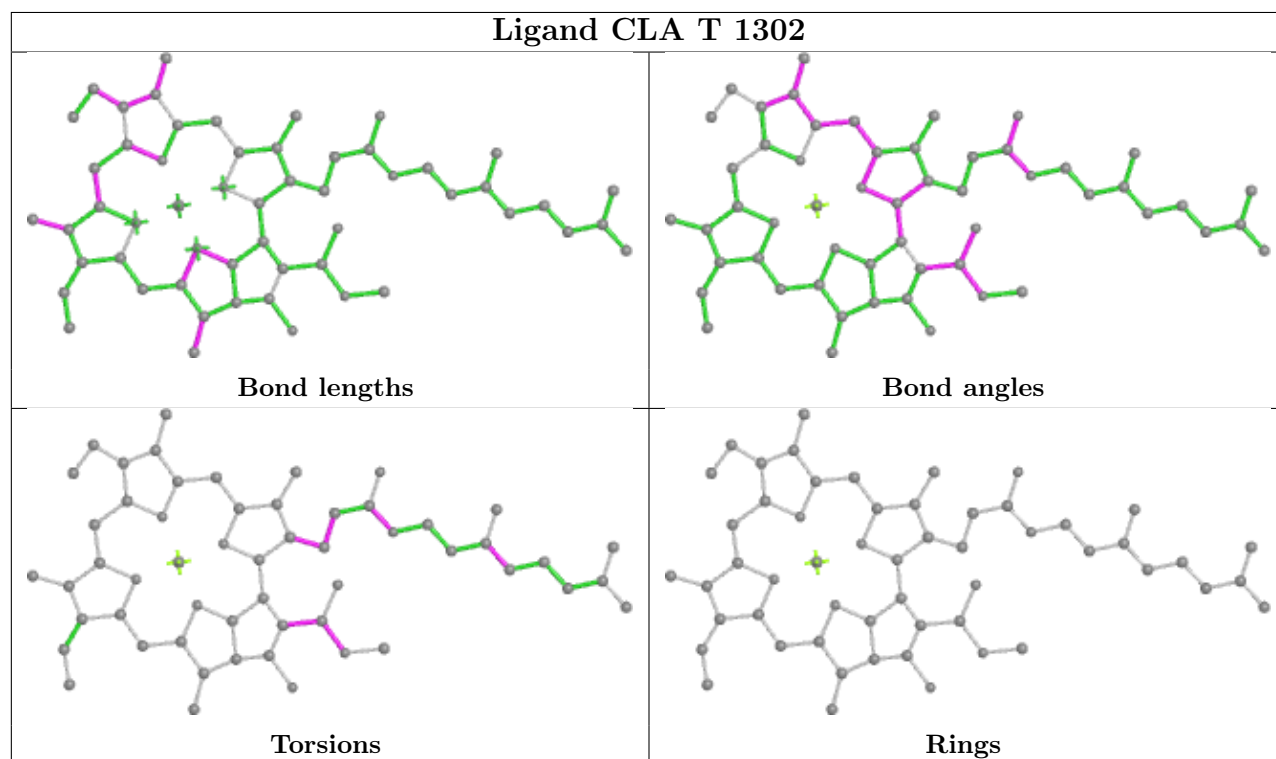




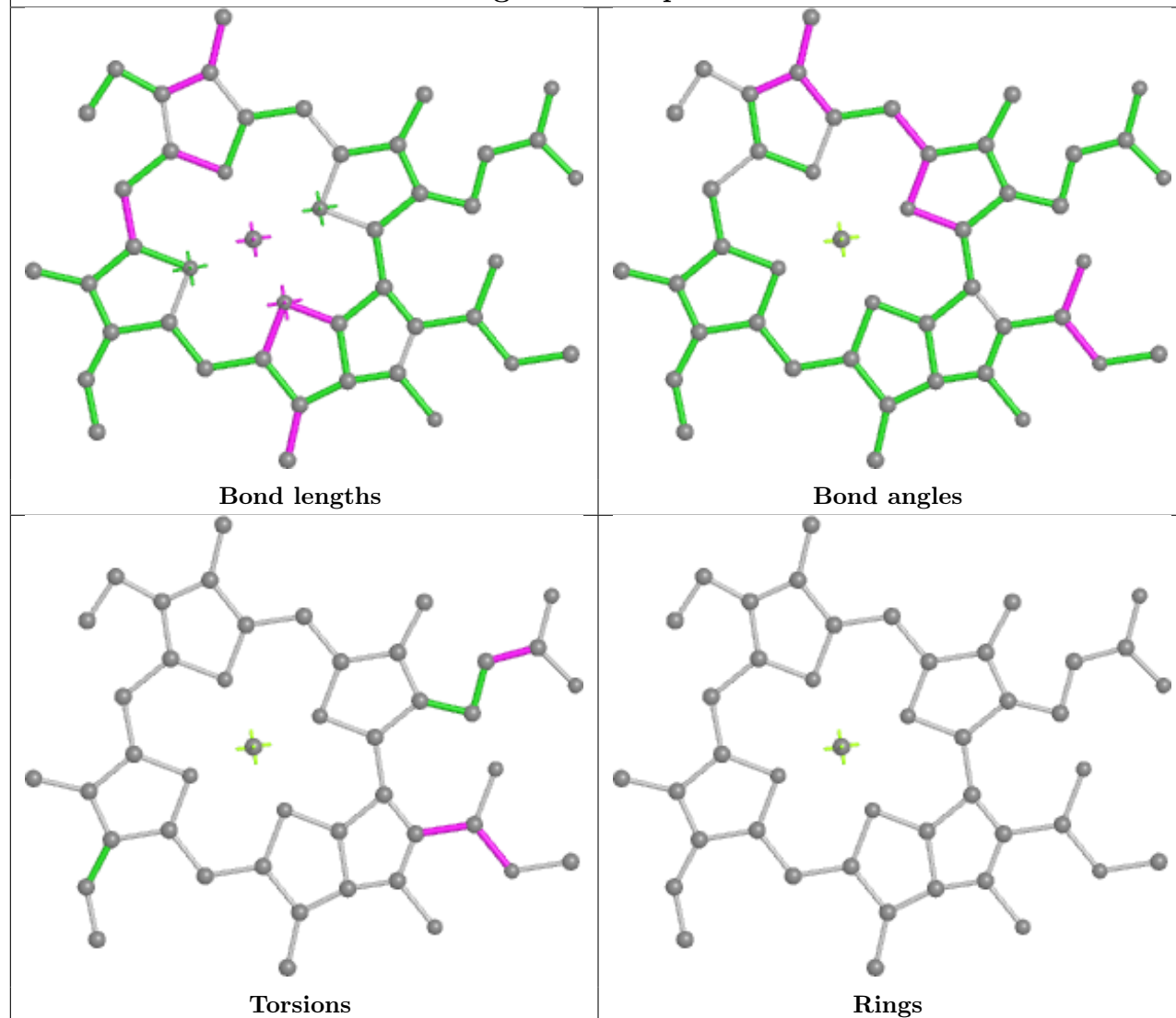
Ligand CLA A 1104



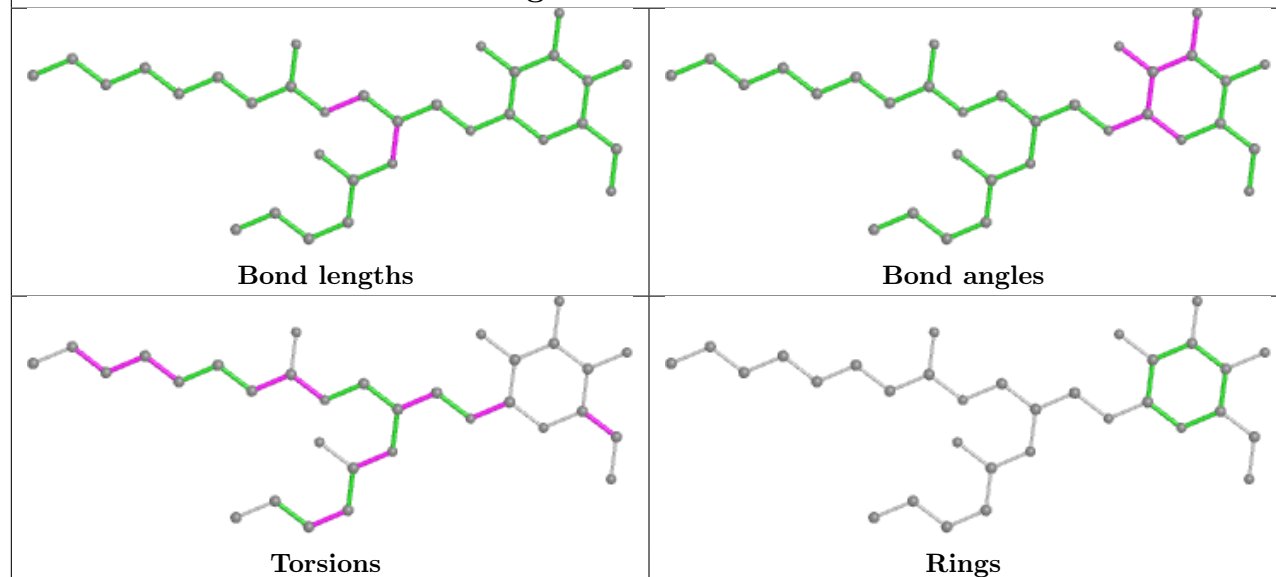
Ligand CLA T 1302



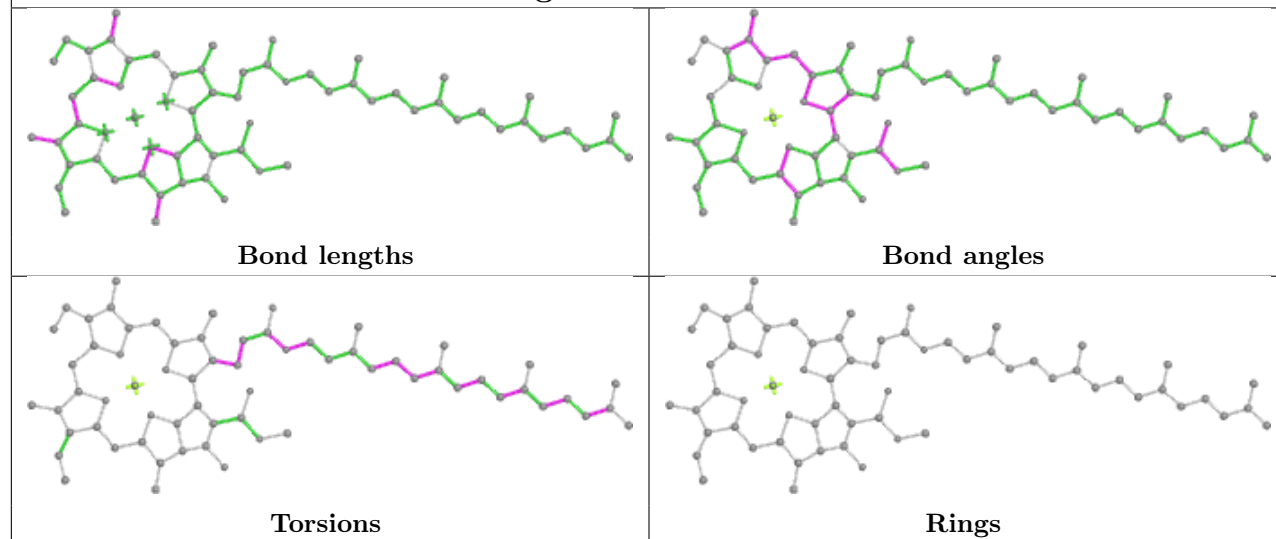
Ligand CLA q 512



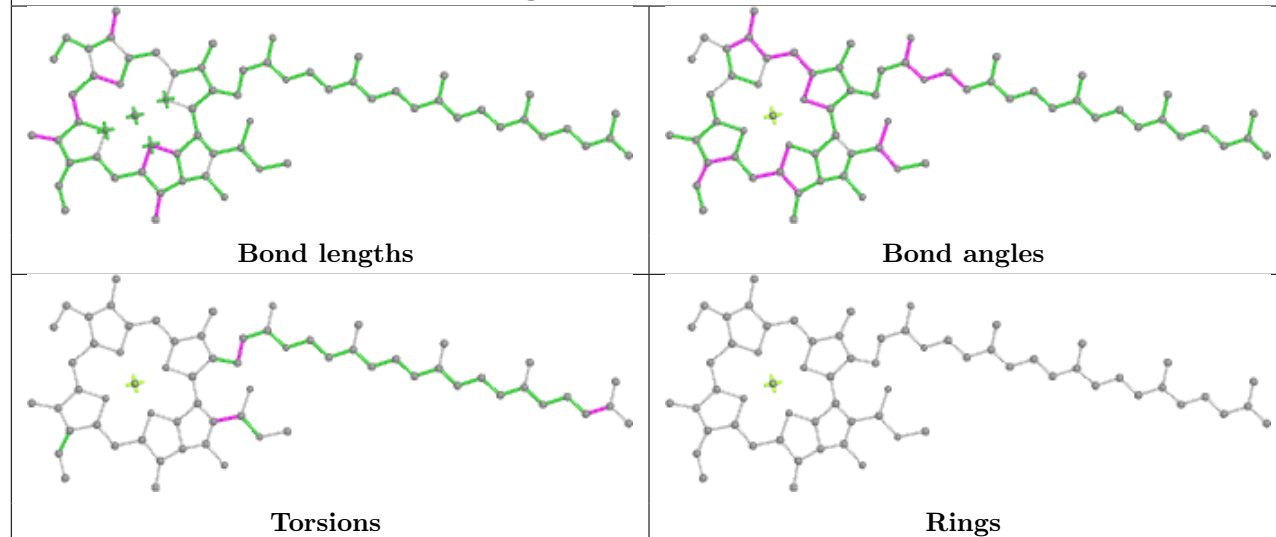
Ligand LMG 1 5104



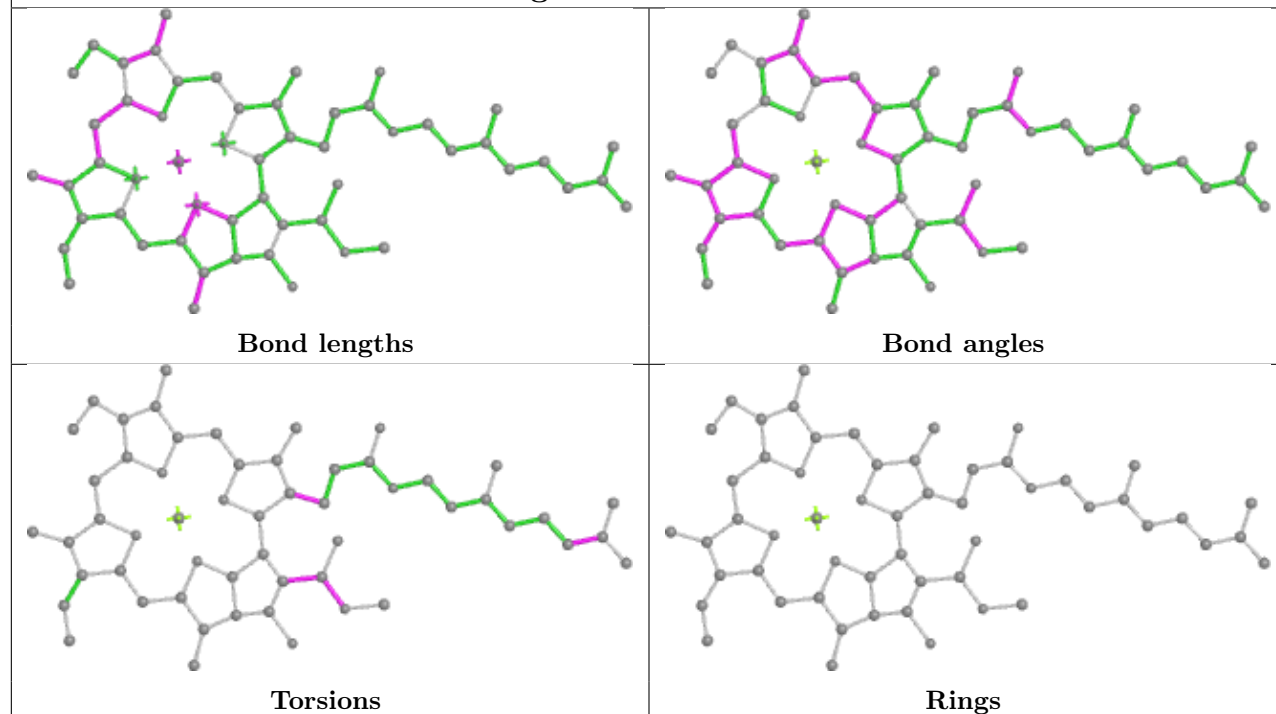
Ligand CLA d 505



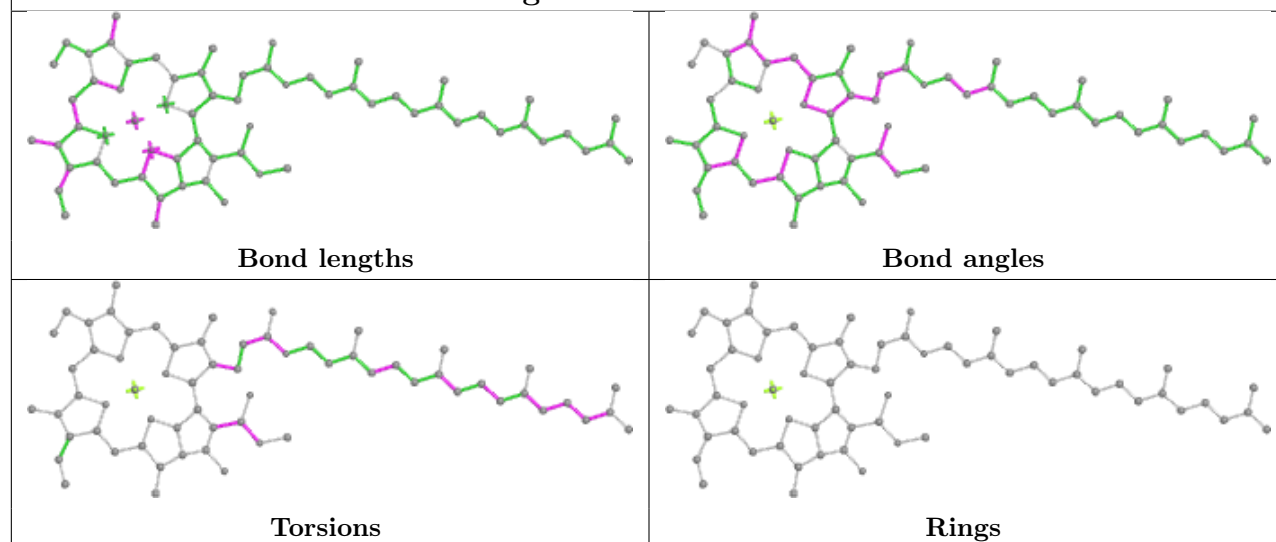
Ligand CLA H 1238



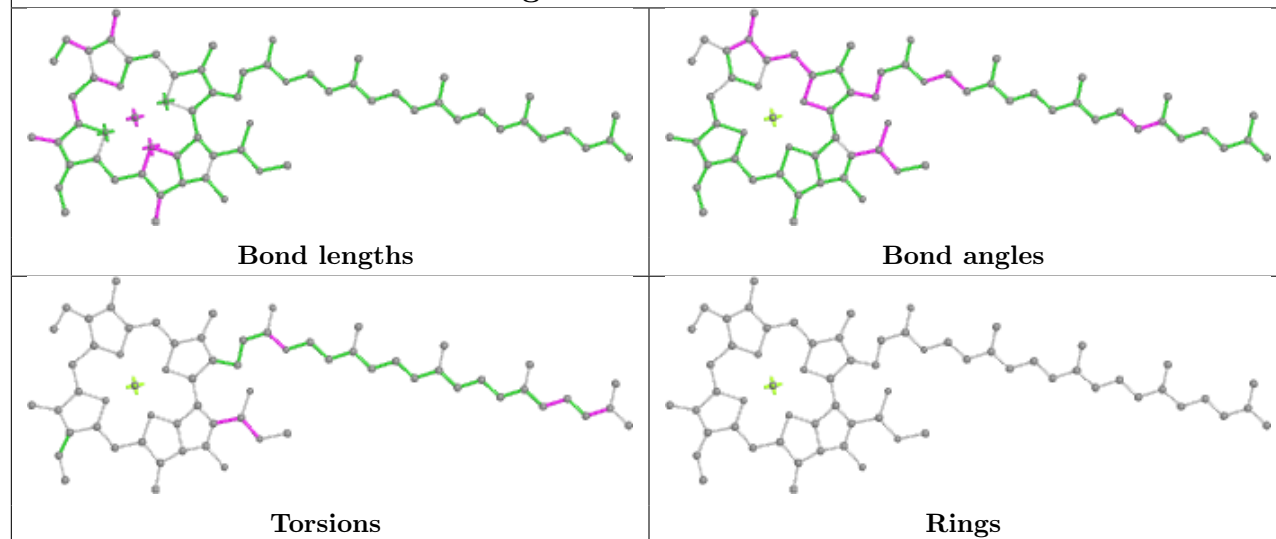
Ligand CLA f 1226



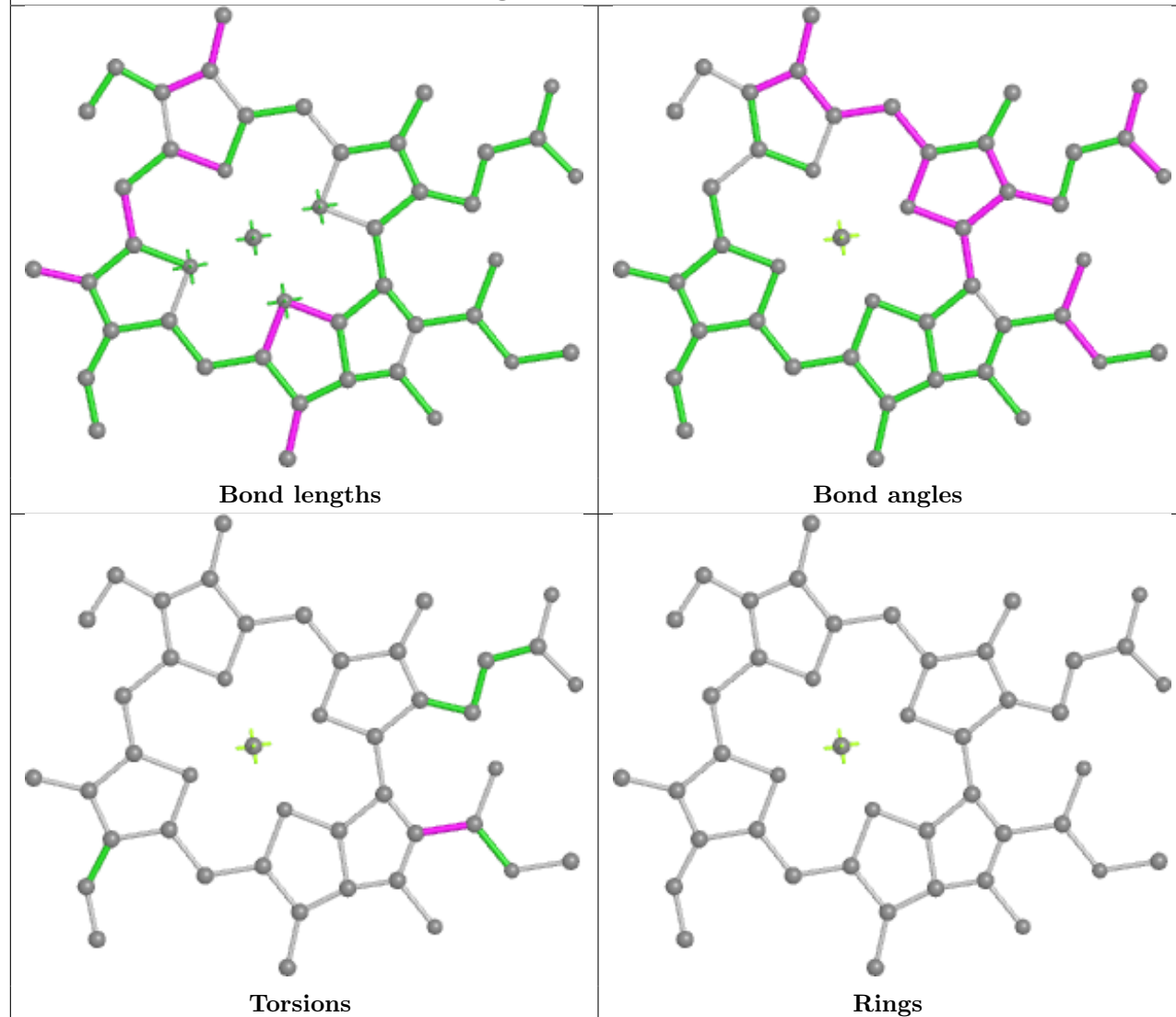
Ligand CLA A 1103



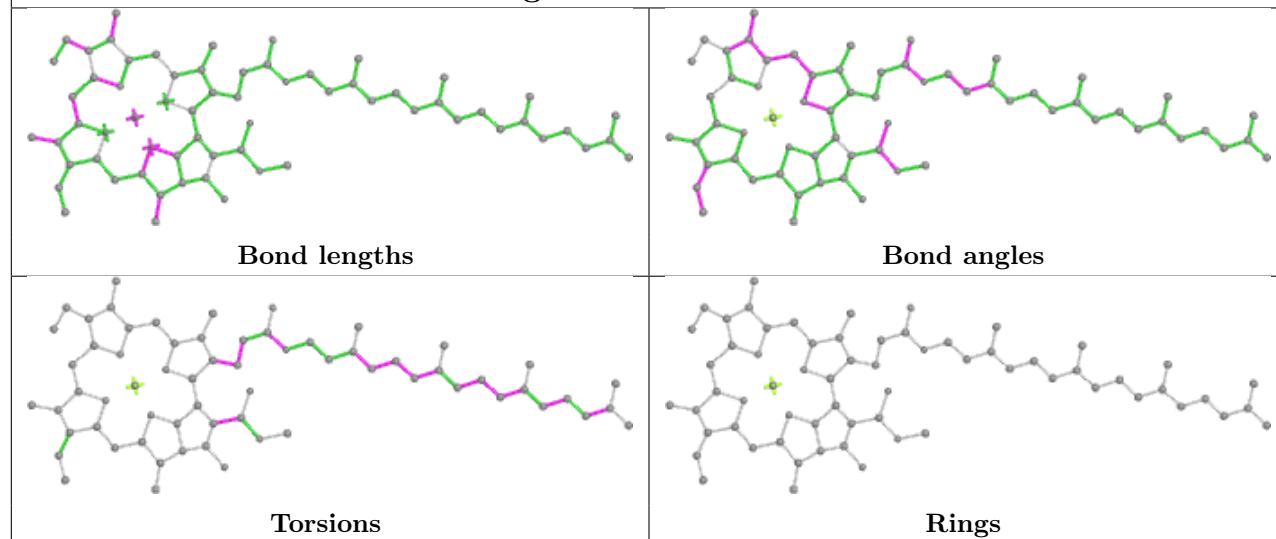
Ligand CLA H 1021



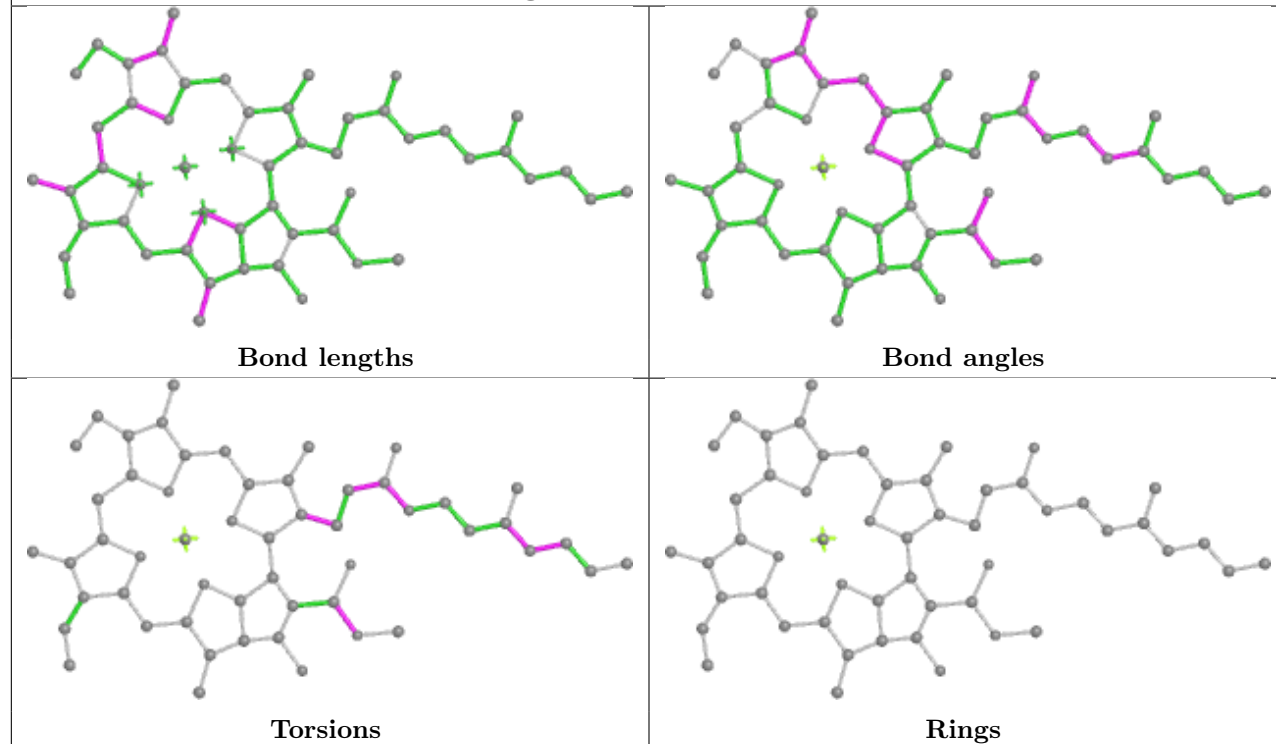
Ligand CLA a 502

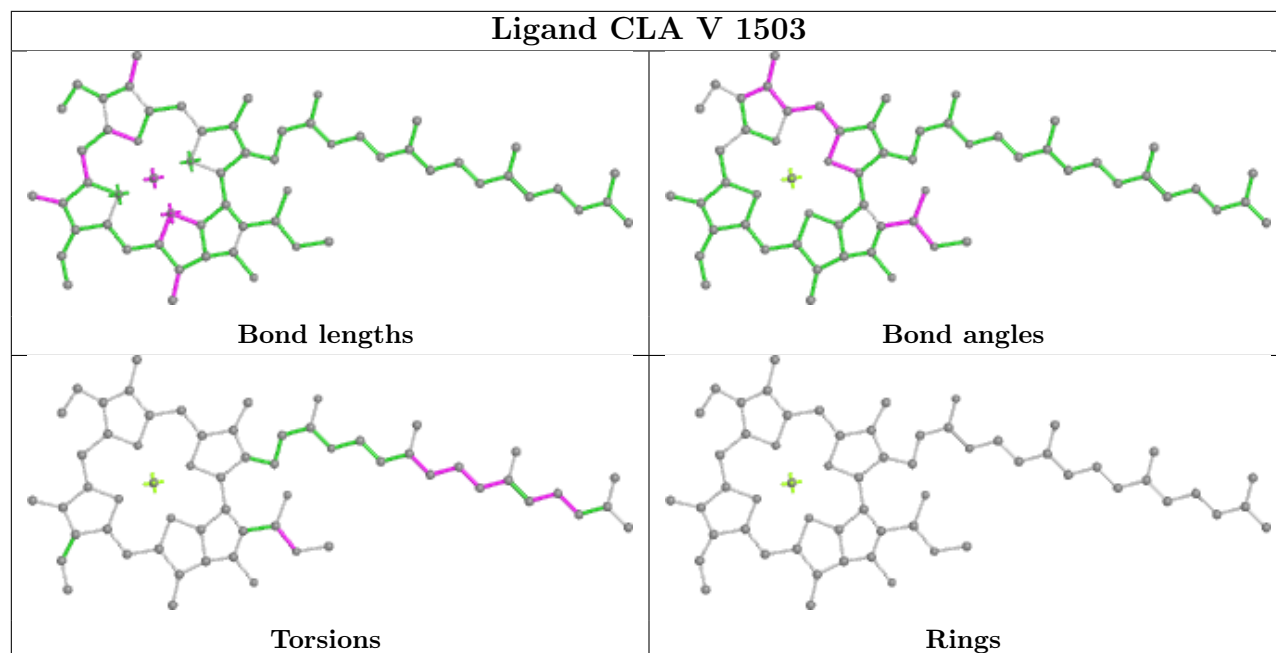
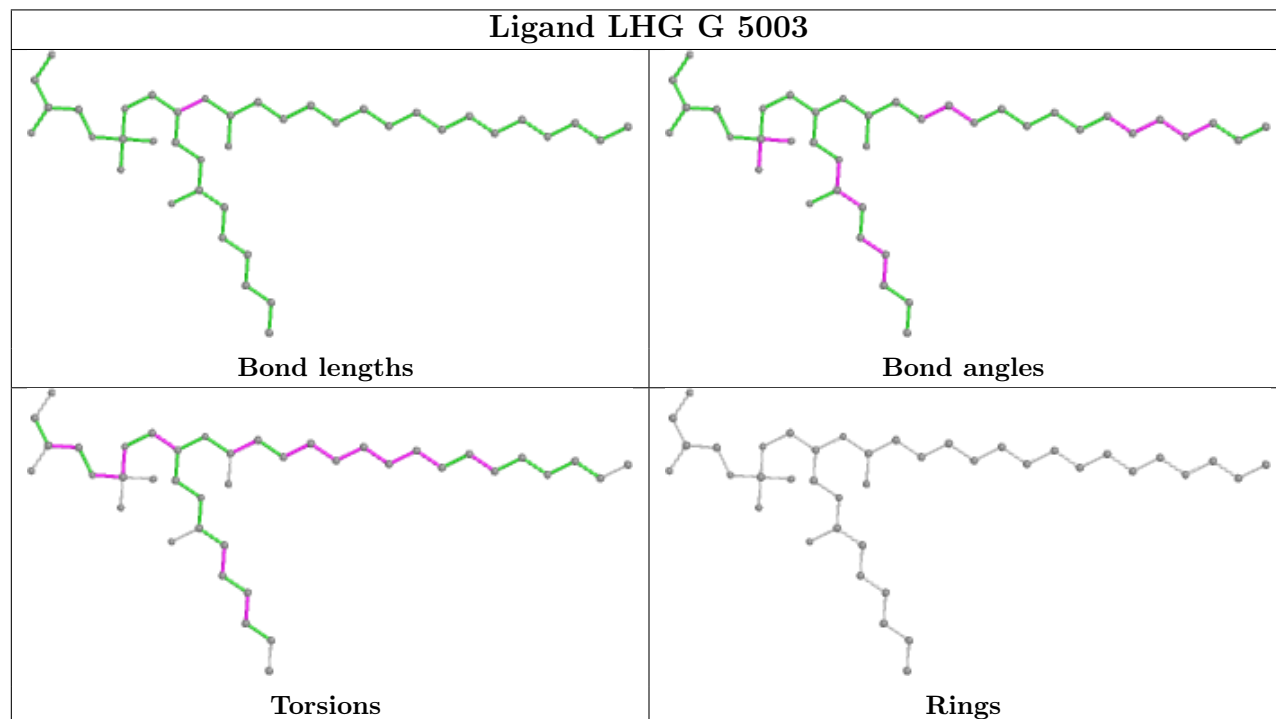


Ligand CLA B 1210

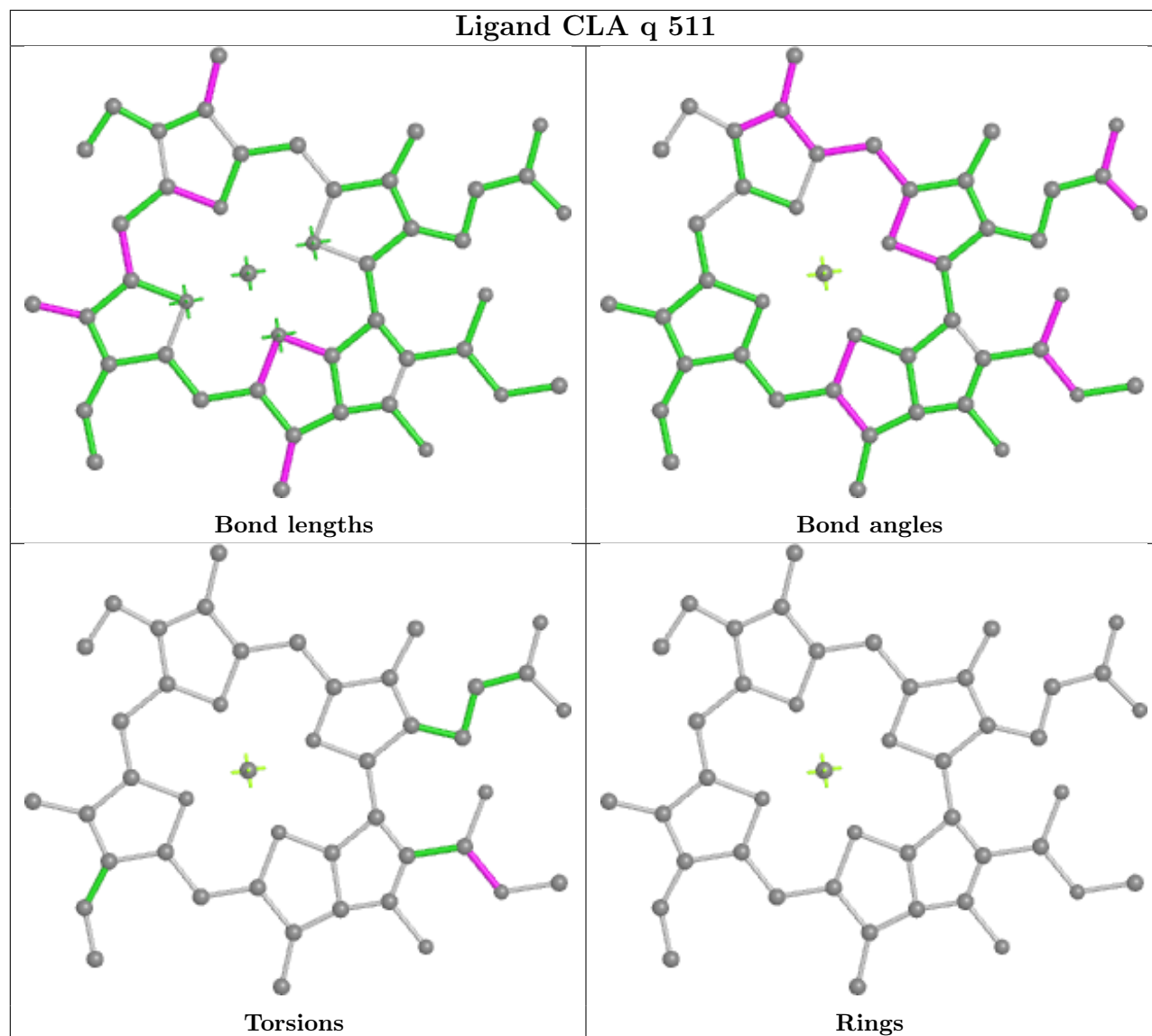


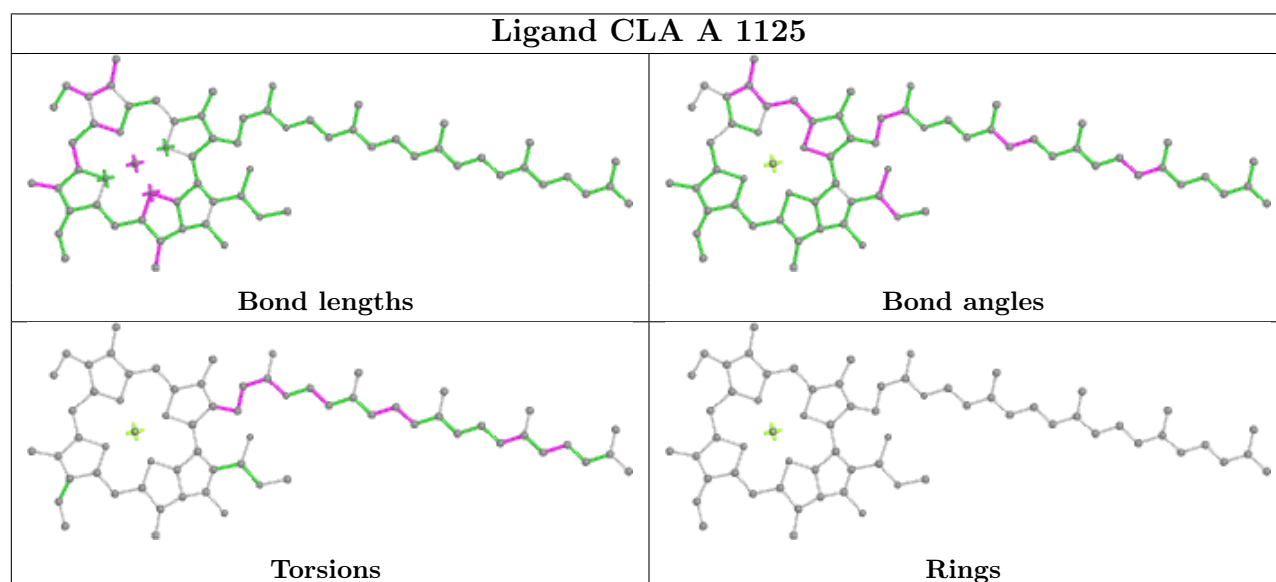
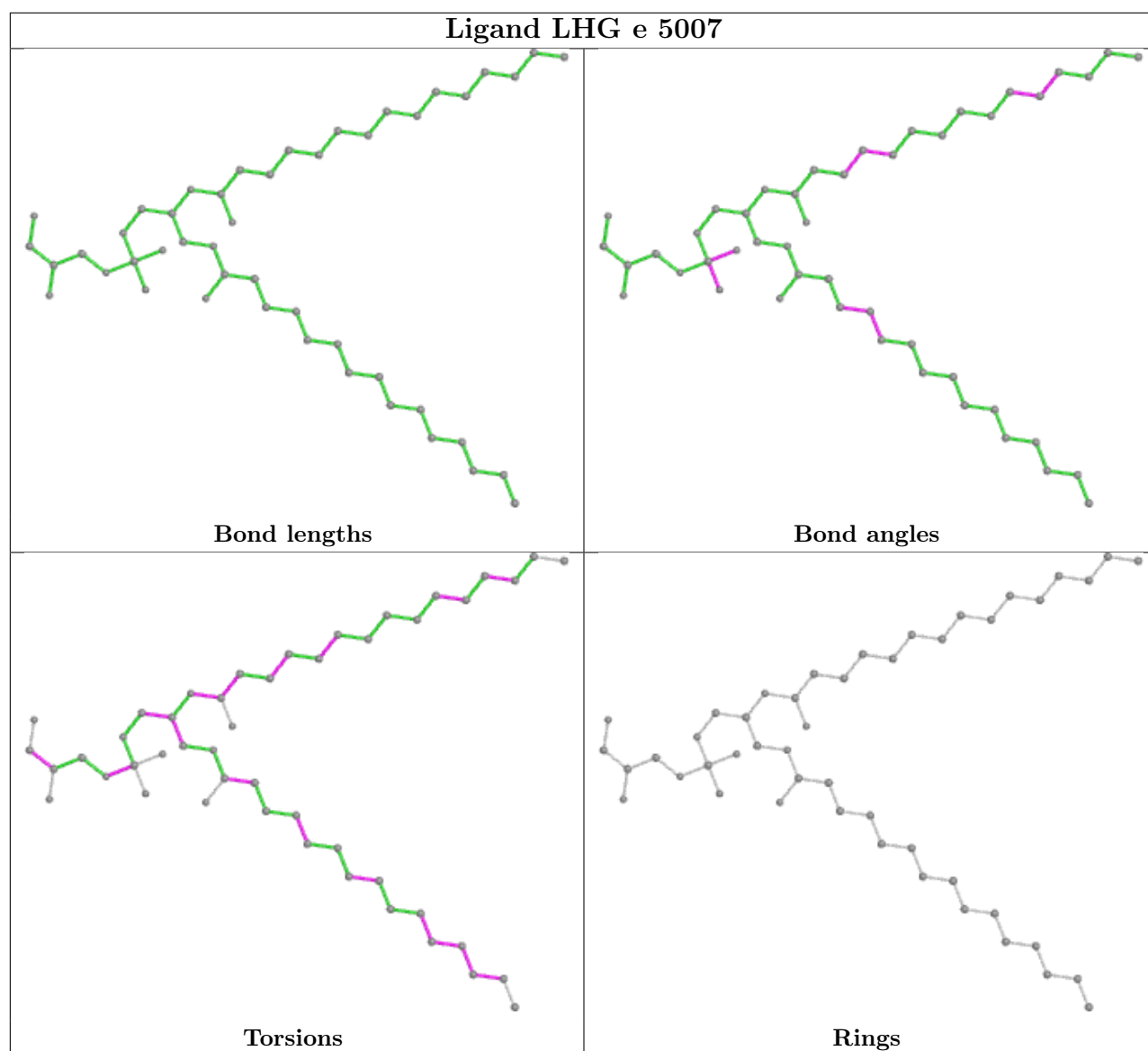
Ligand CLA G 1110



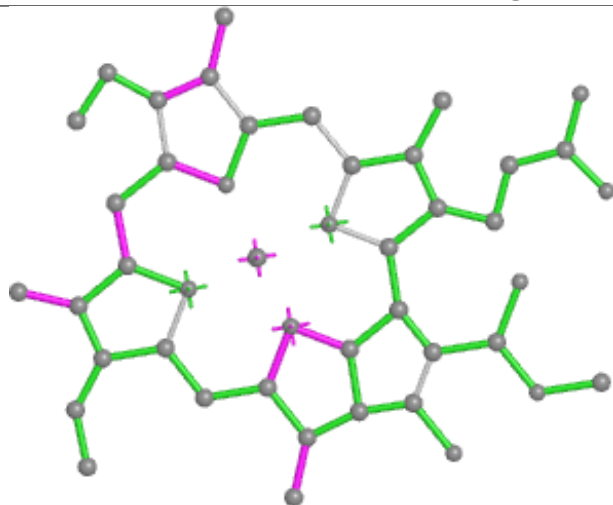
Ligand CLA V 1503**Ligand LHG G 5003**

Ligand CLA q 511

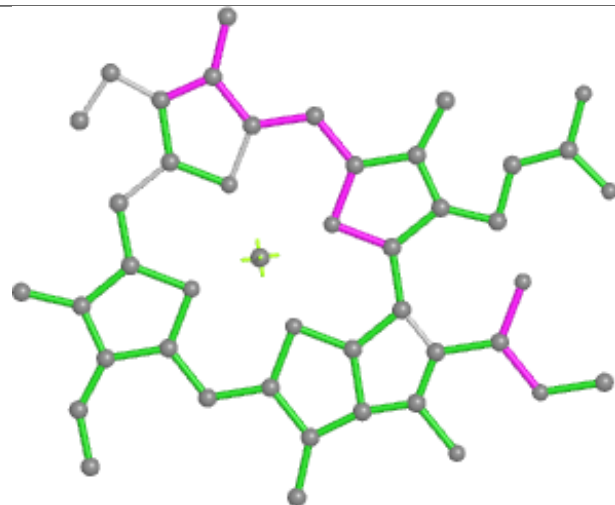




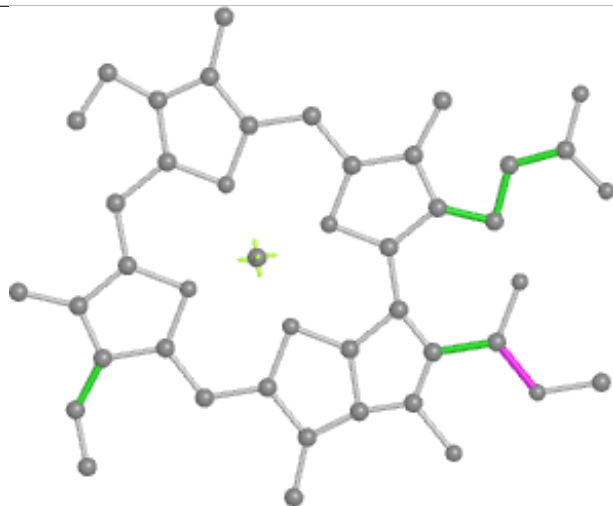
Ligand CLA F 1301



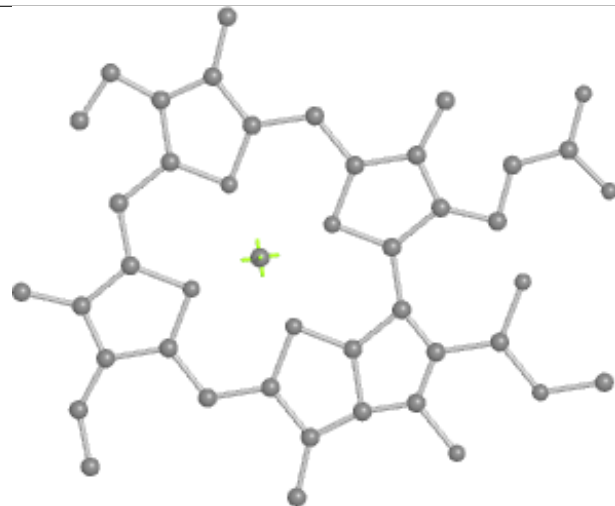
Bond lengths



Bond angles

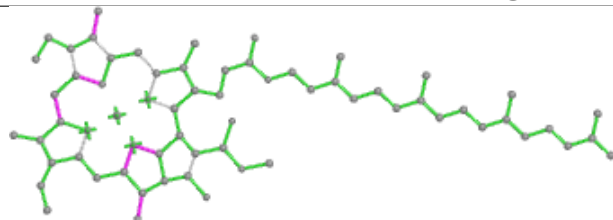


Torsions

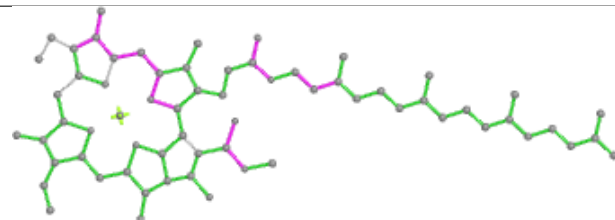


Rings

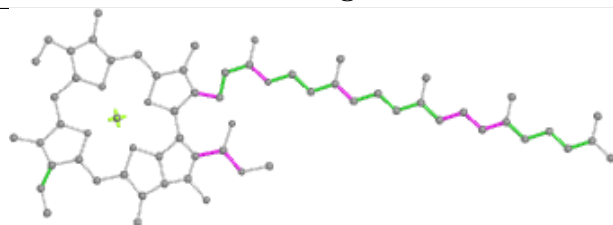
Ligand CLA H 1240



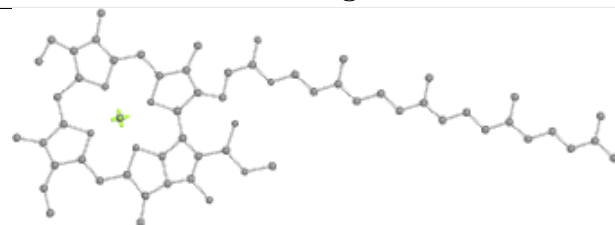
Bond lengths



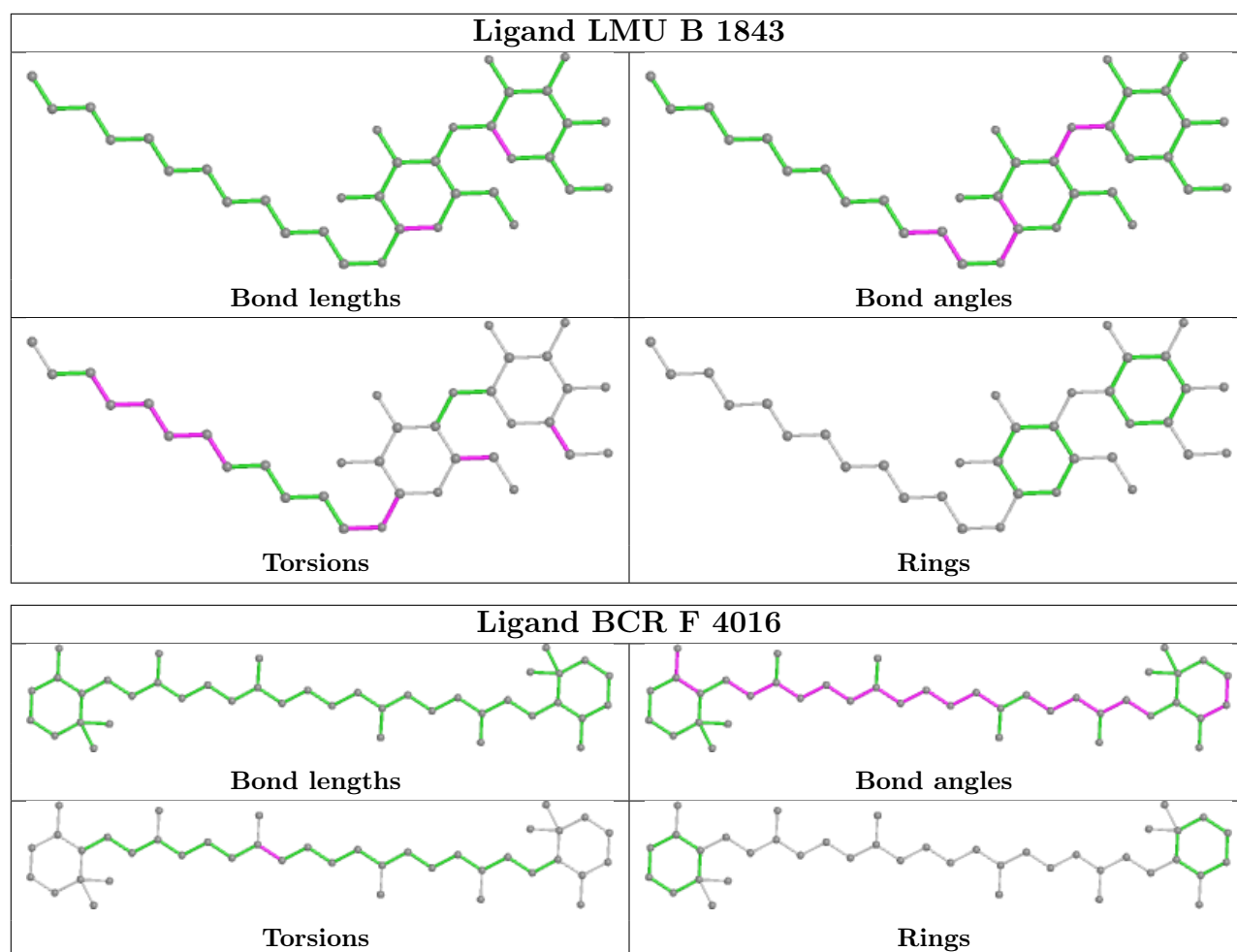
Bond angles



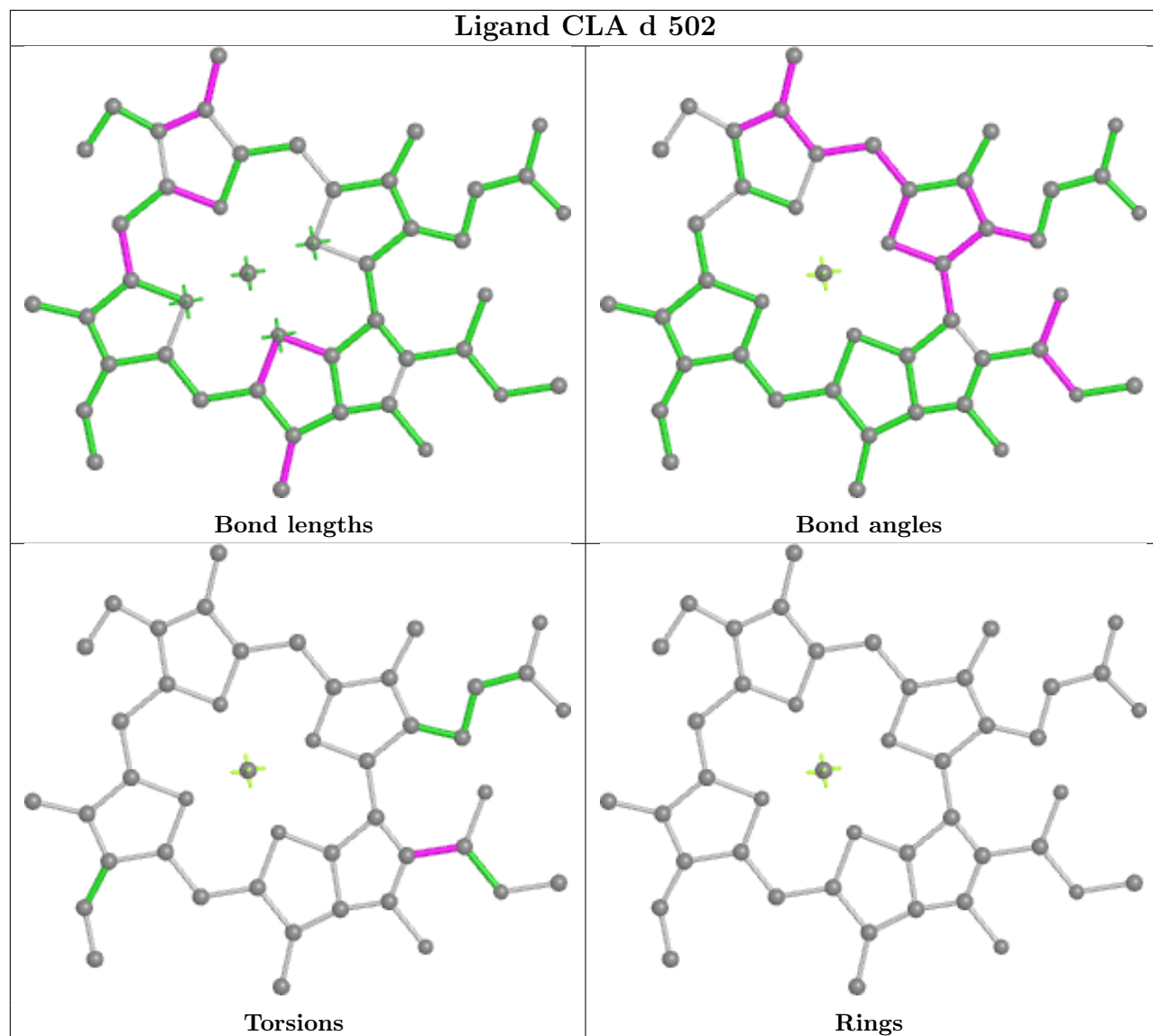
Torsions



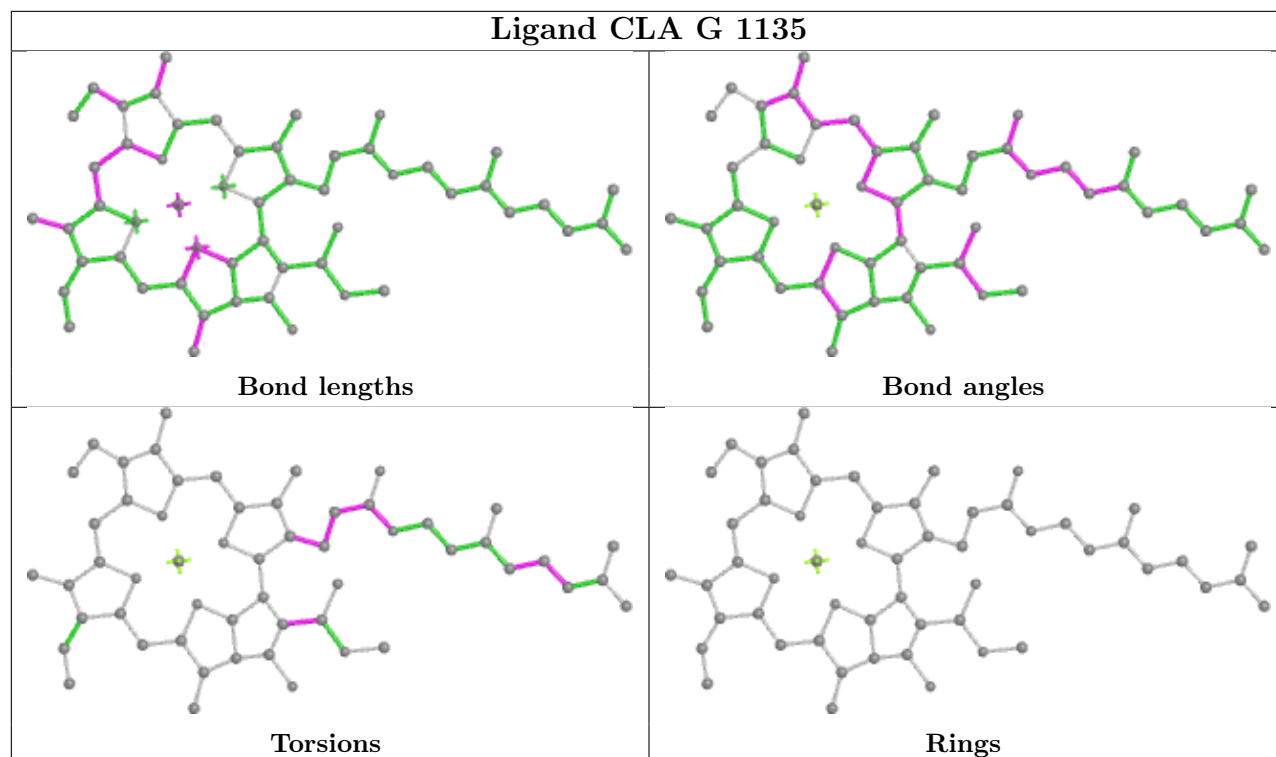
Rings



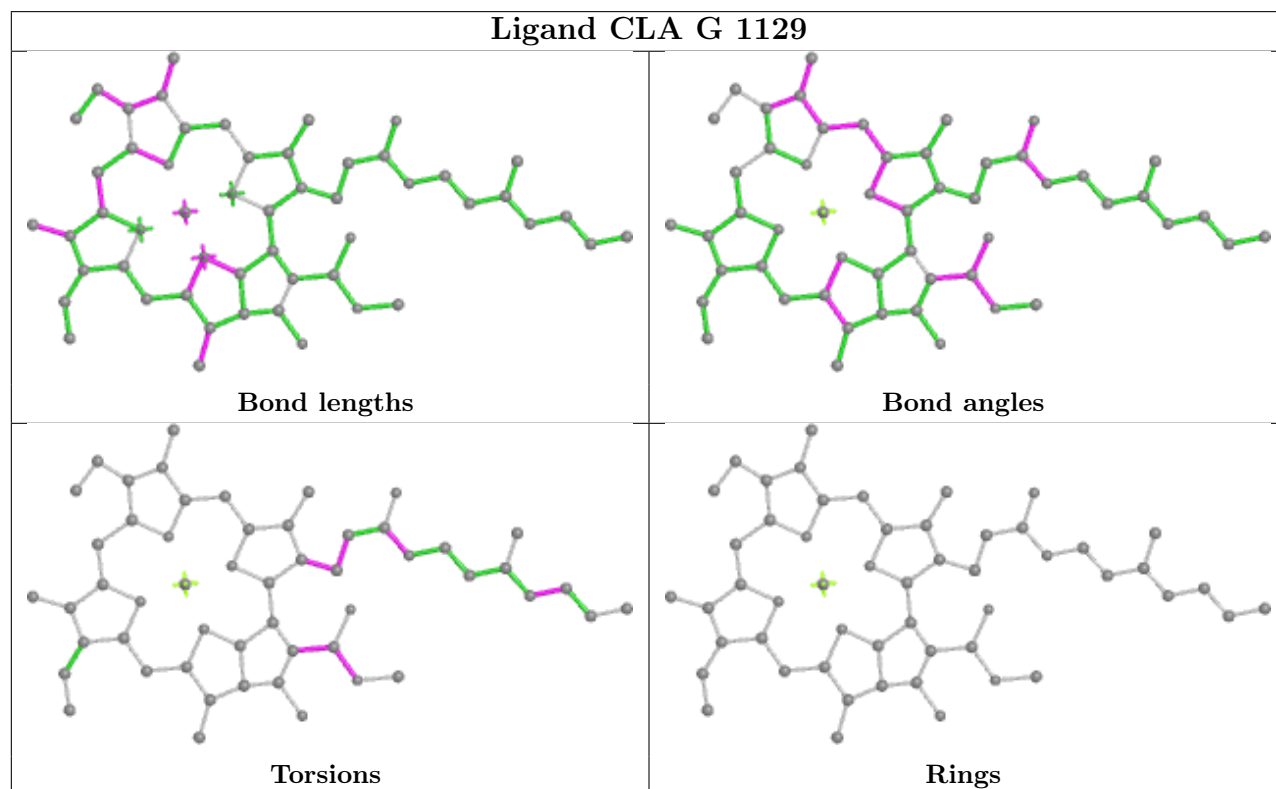
Ligand CLA d 502



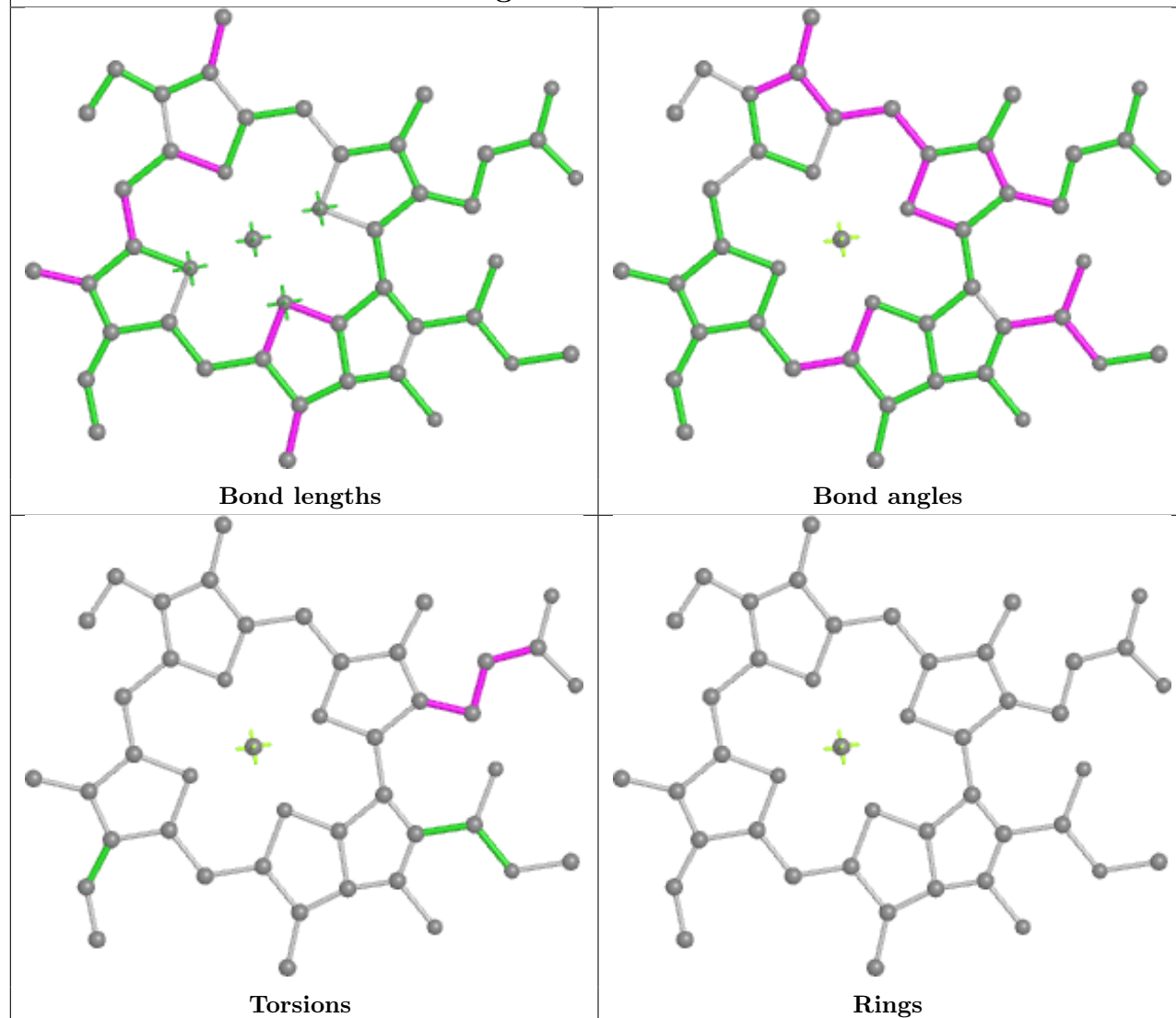
Ligand CLA G 1135



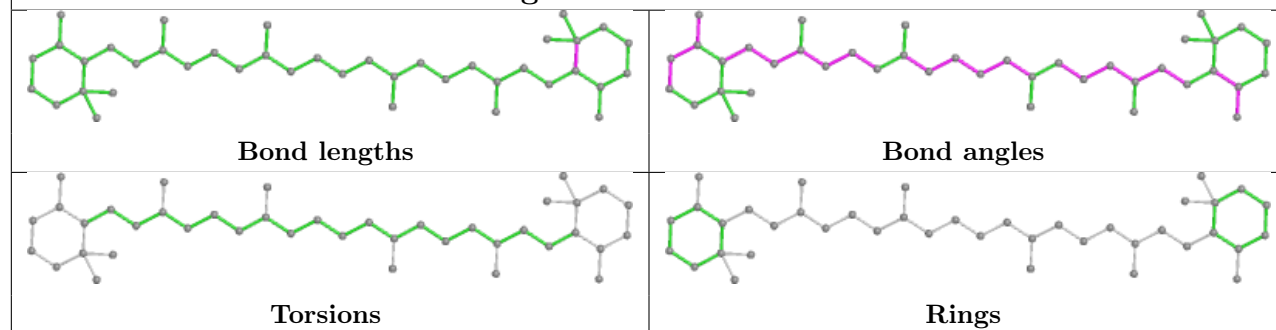
Ligand CLA G 1129



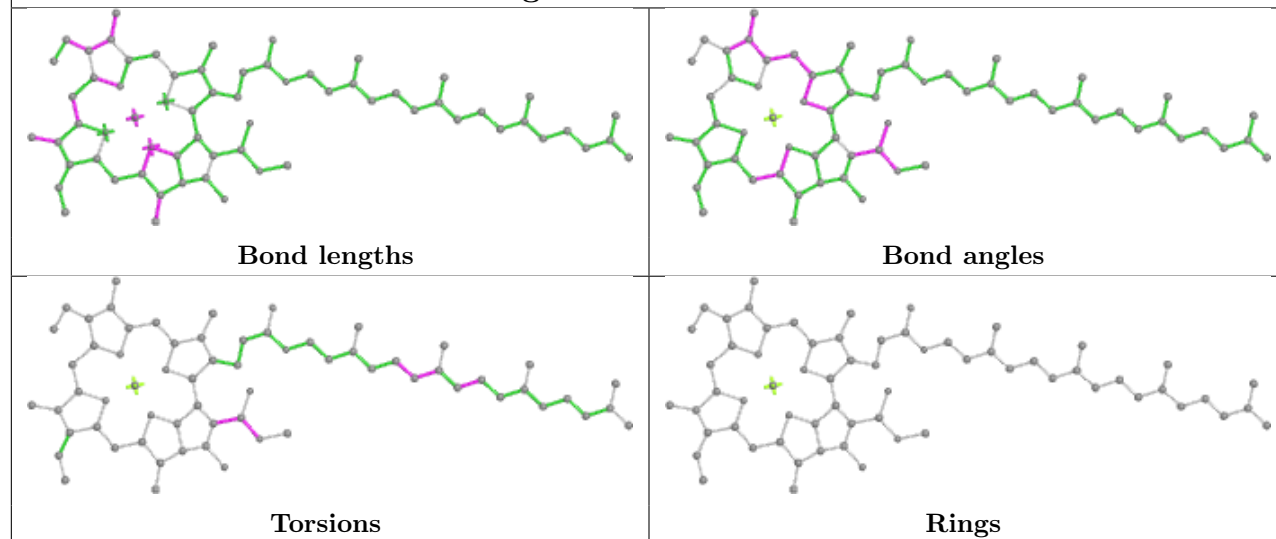
Ligand CLA s 501



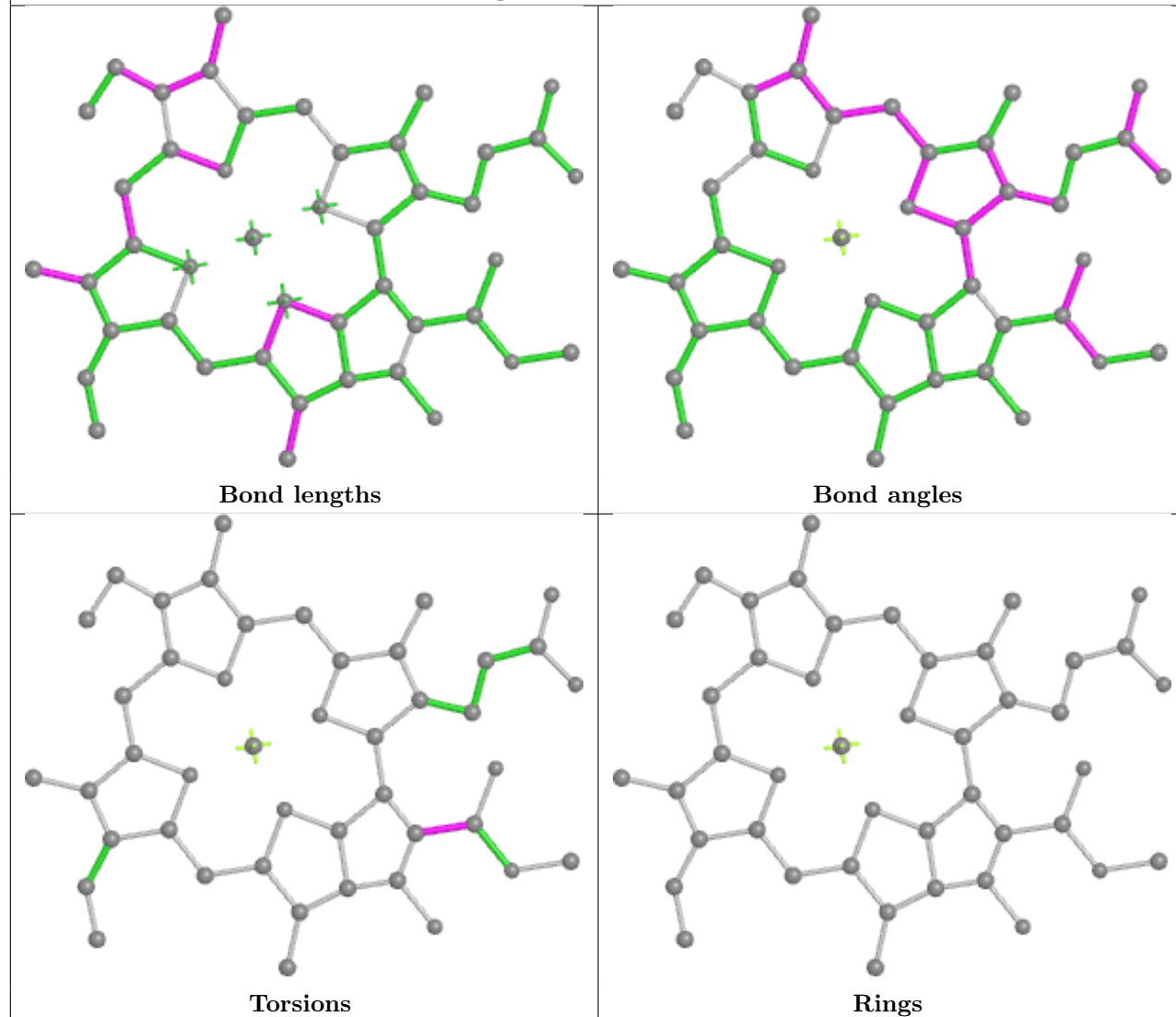
Ligand BCR A 4003

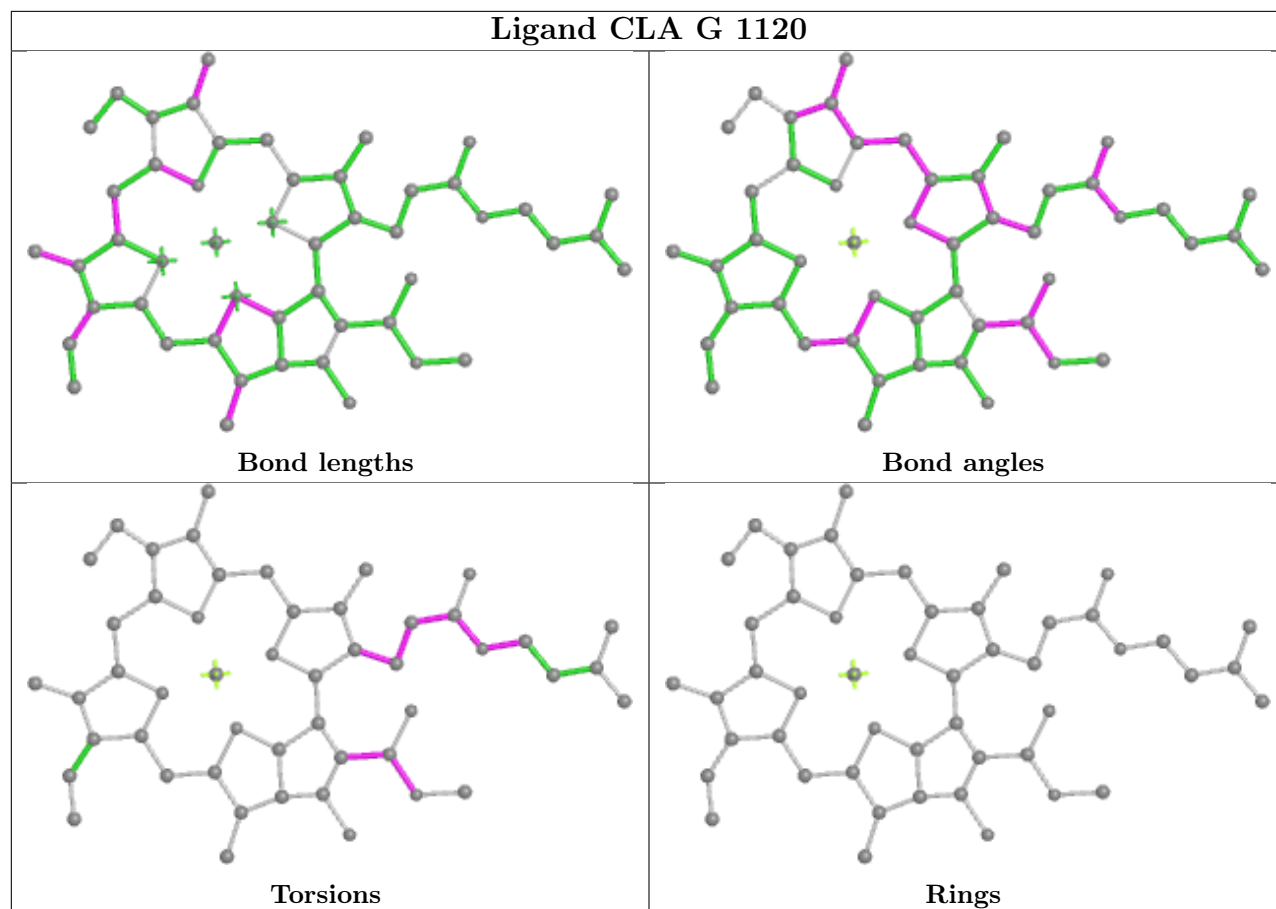


Ligand CLA H 1235

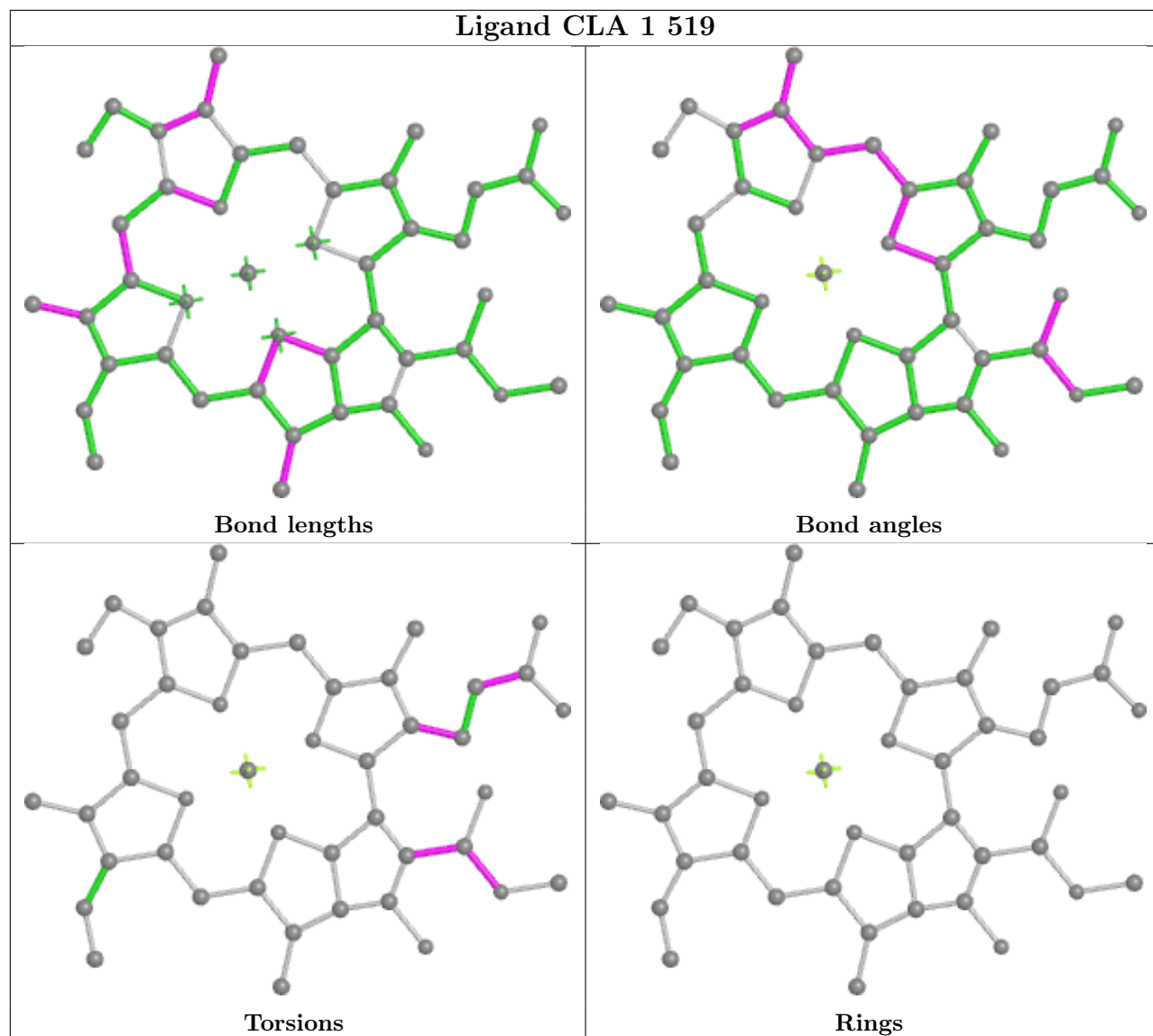


Ligand CLA Z 502

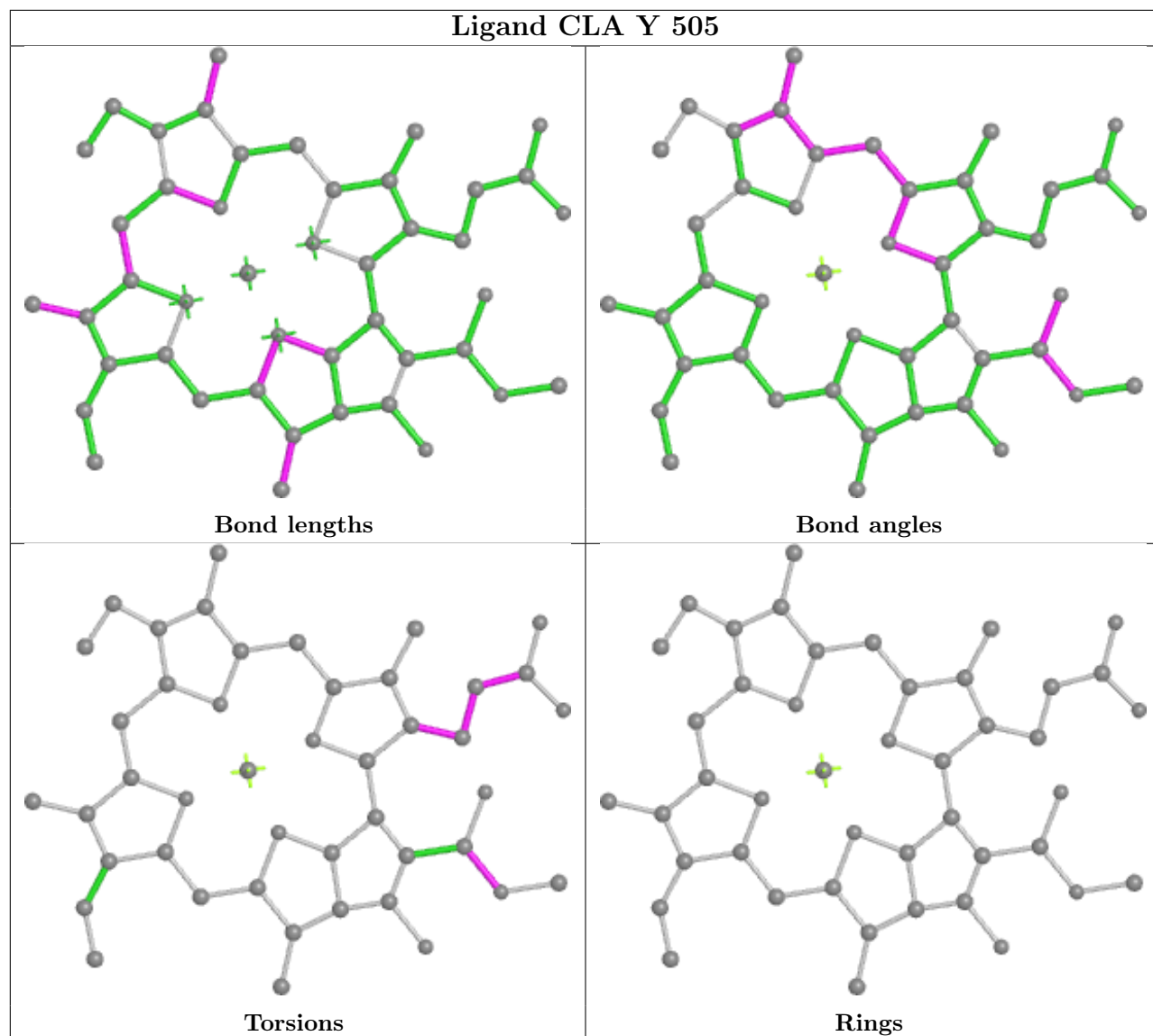




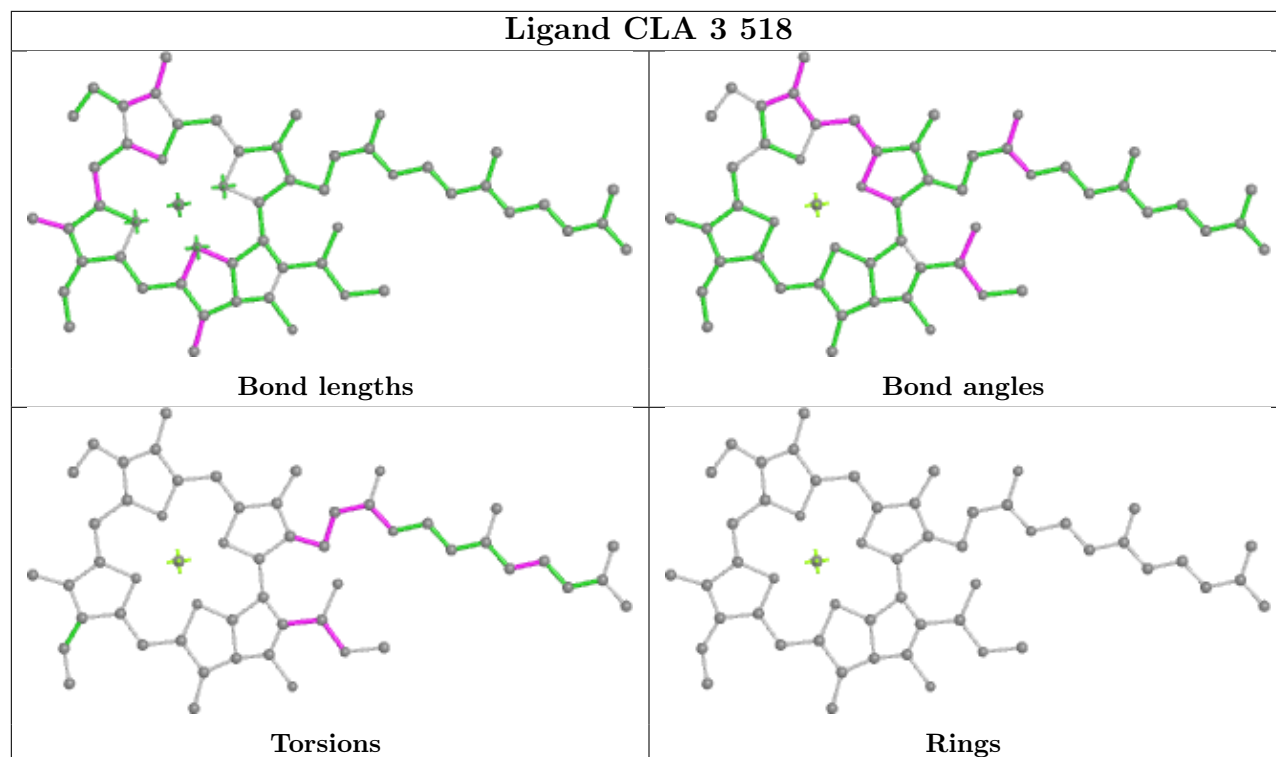
Ligand CLA 1 519



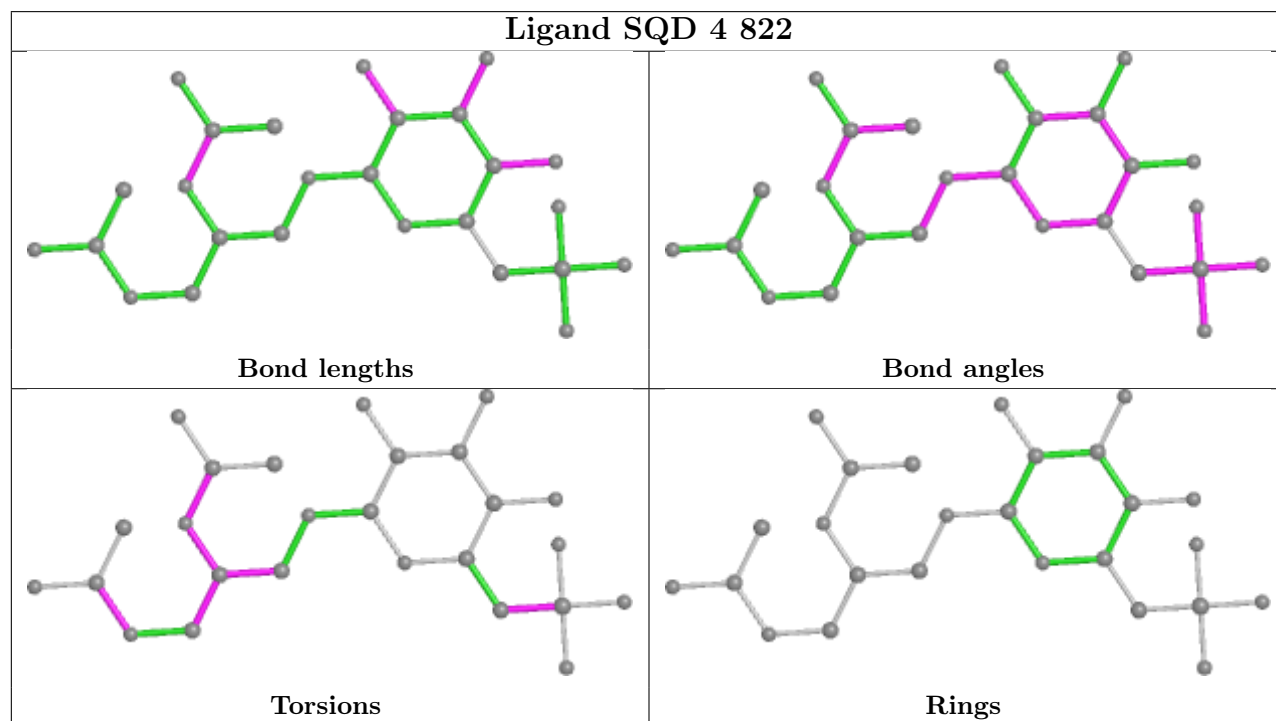
Ligand CLA Y 505

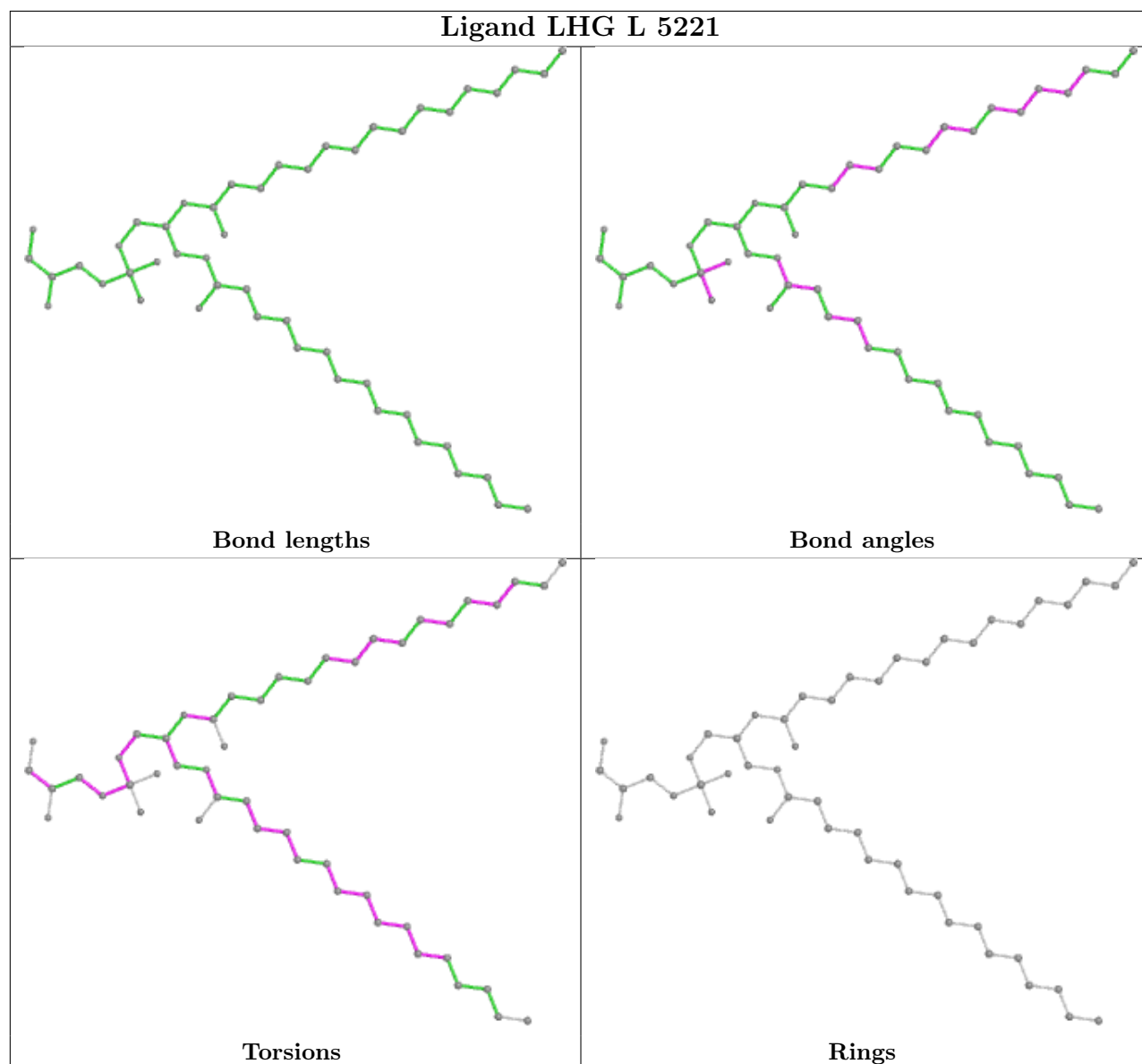
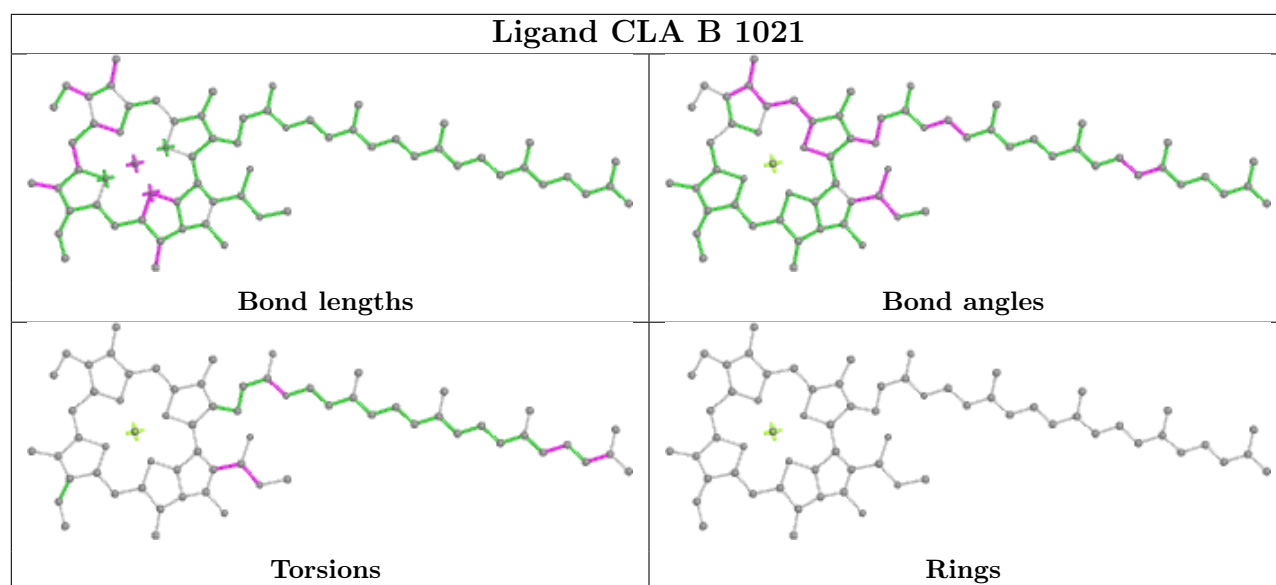


Ligand CLA 3 518

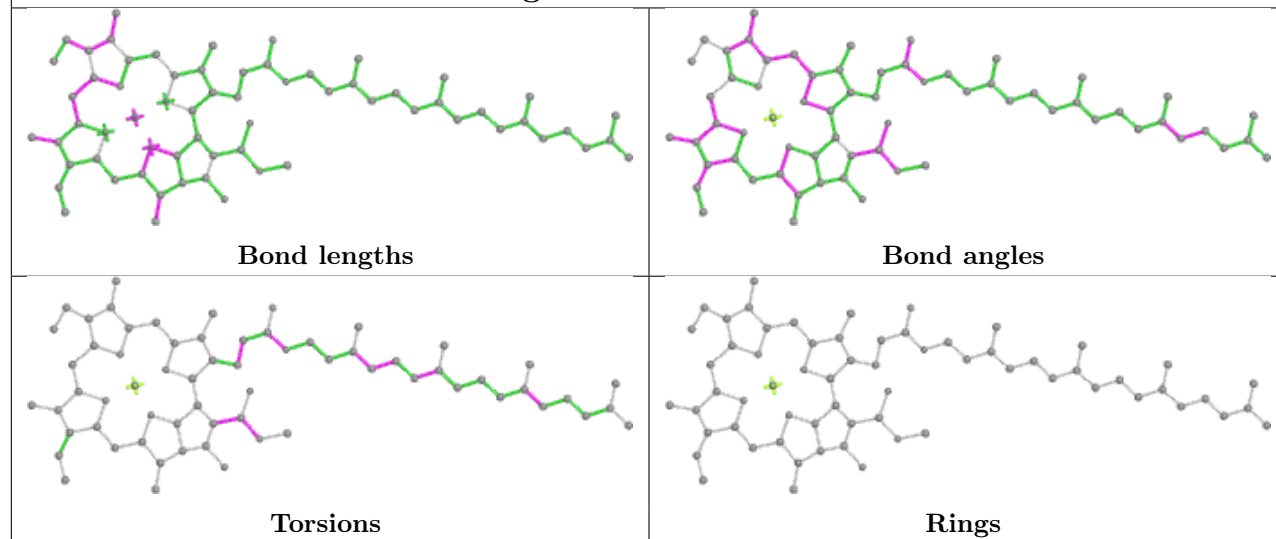


Ligand SQD 4 822

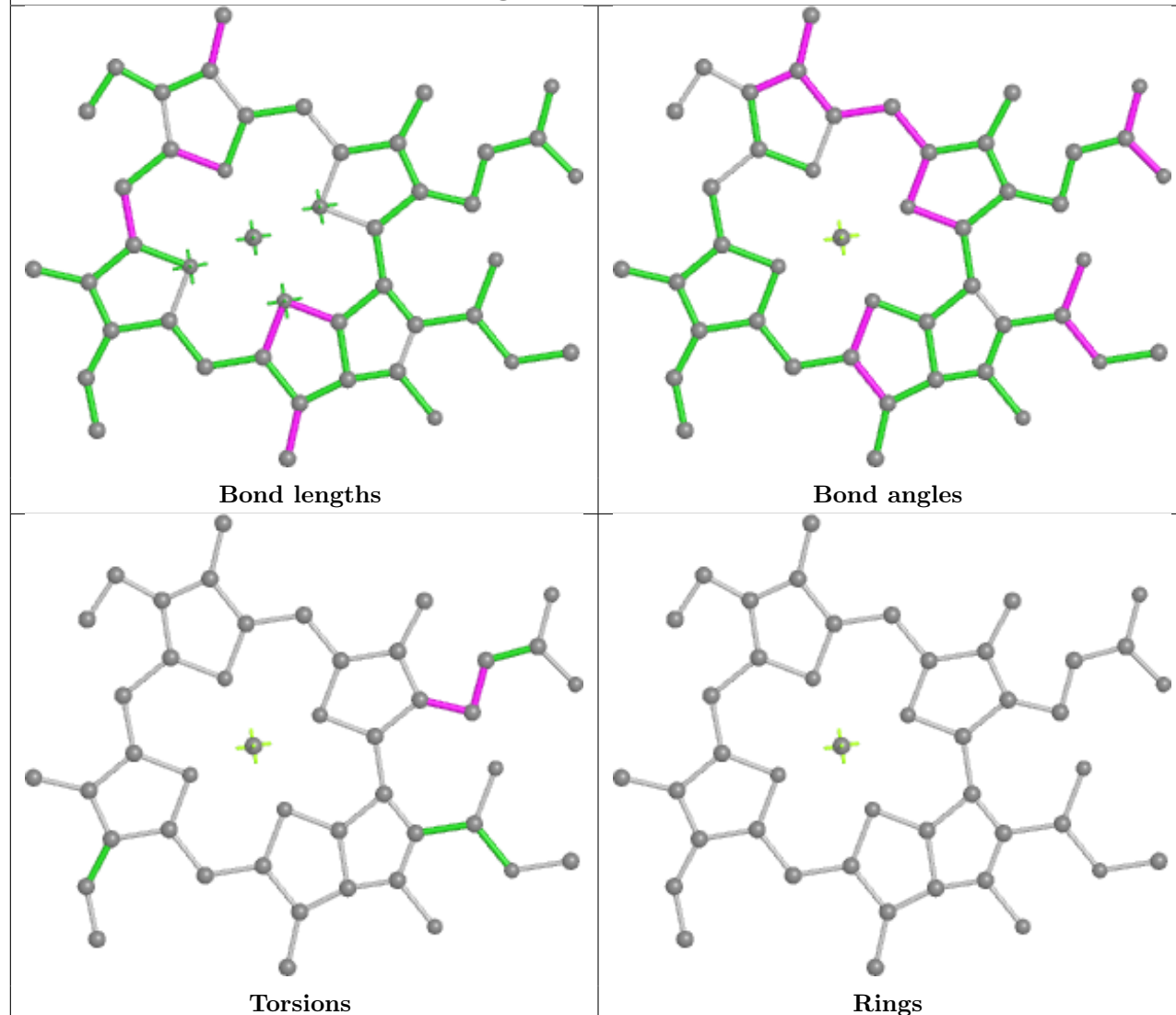


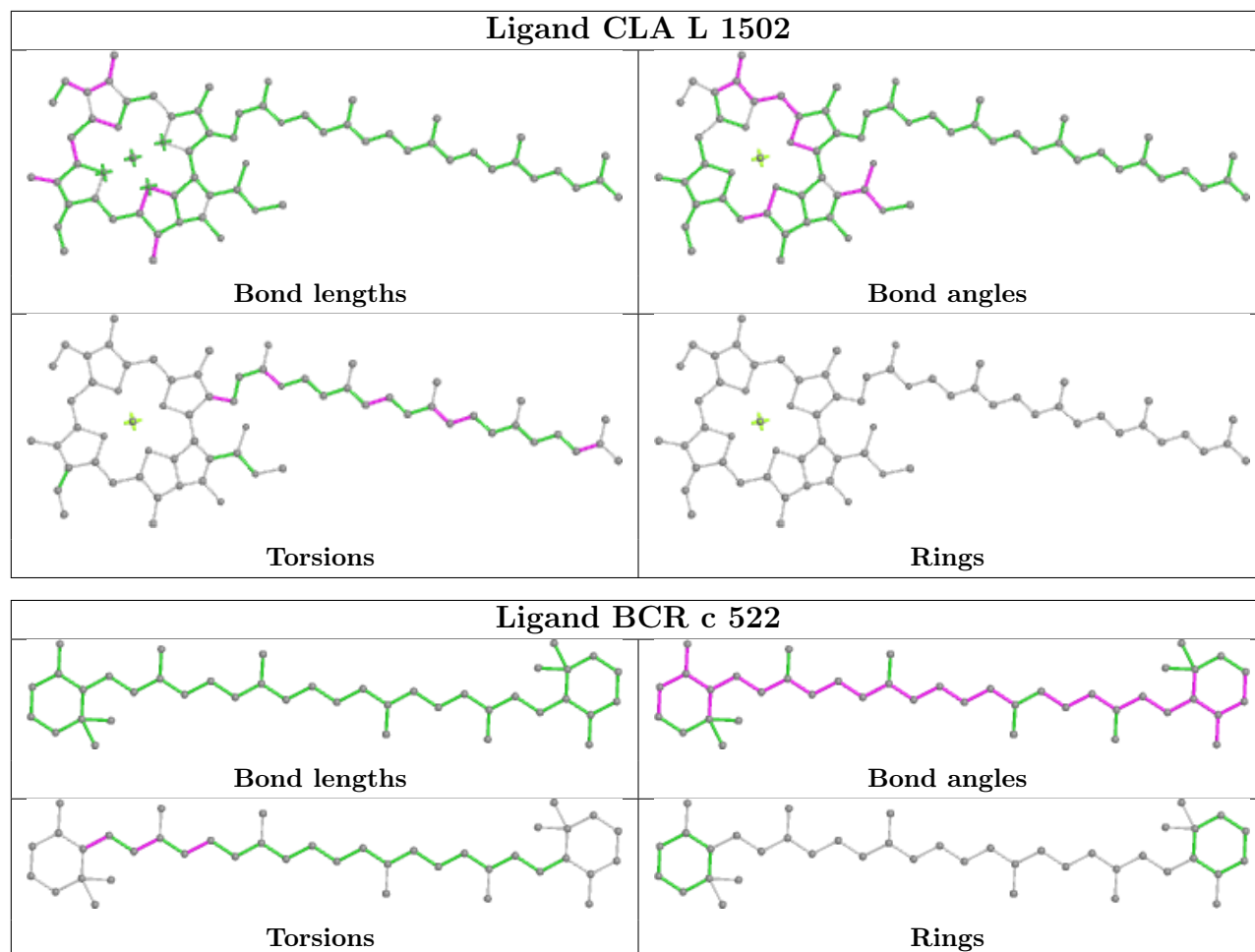


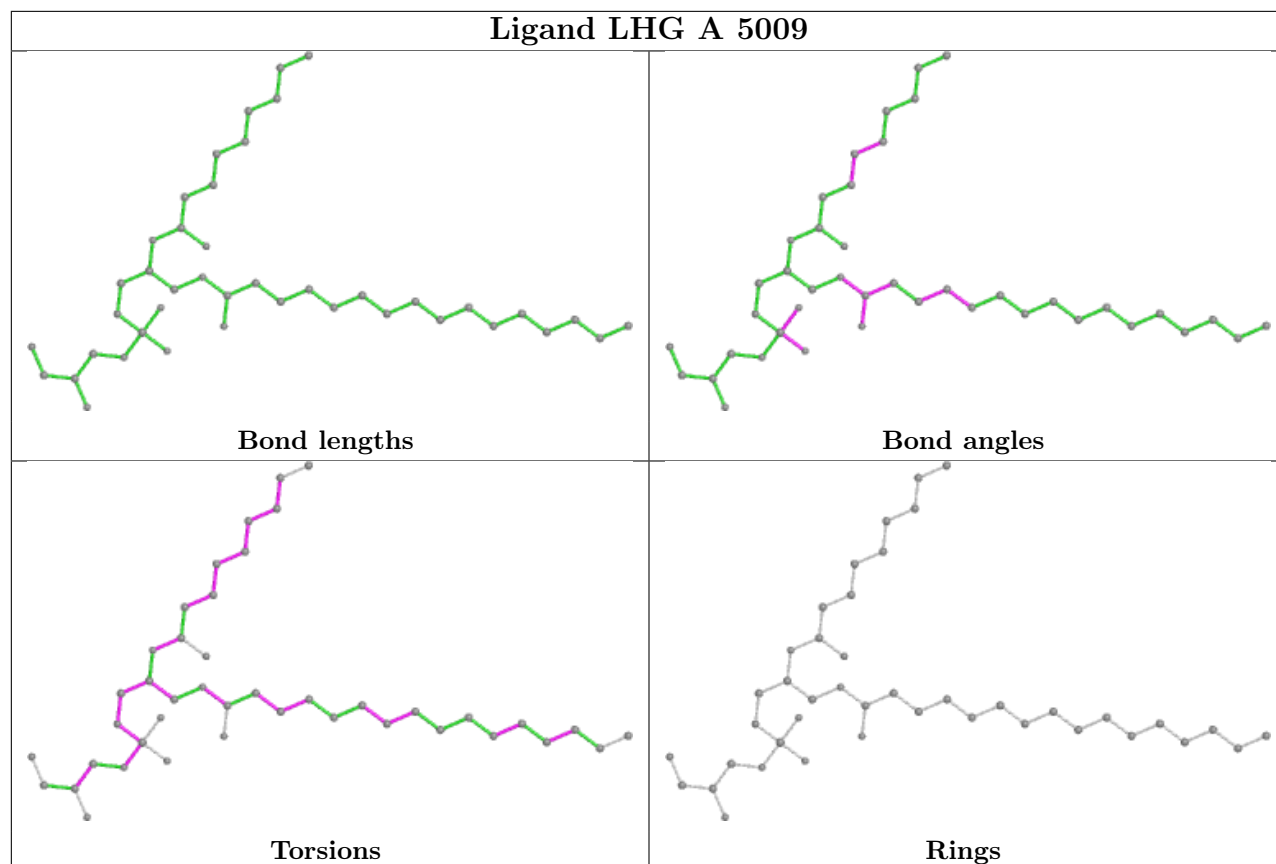
Ligand CLA A 1119

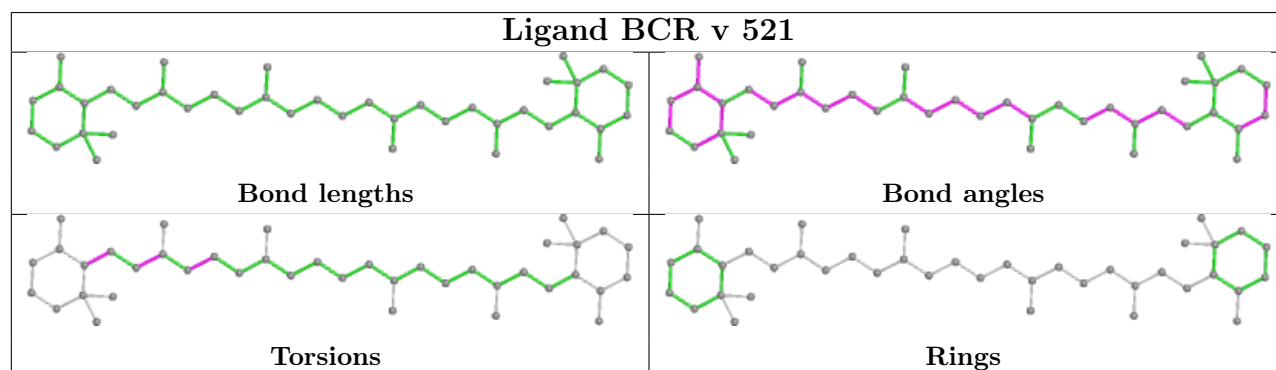
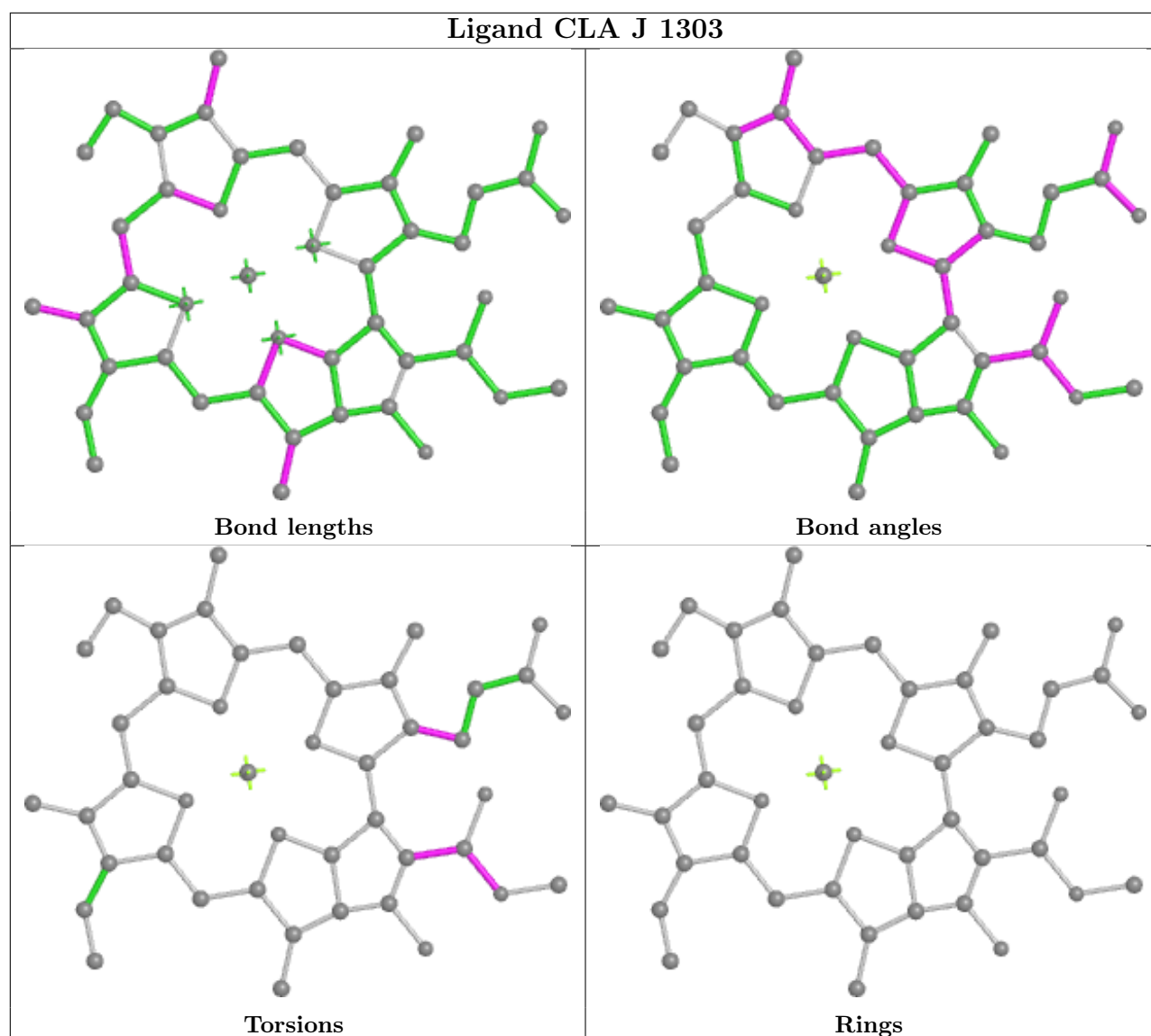


Ligand CLA c 518

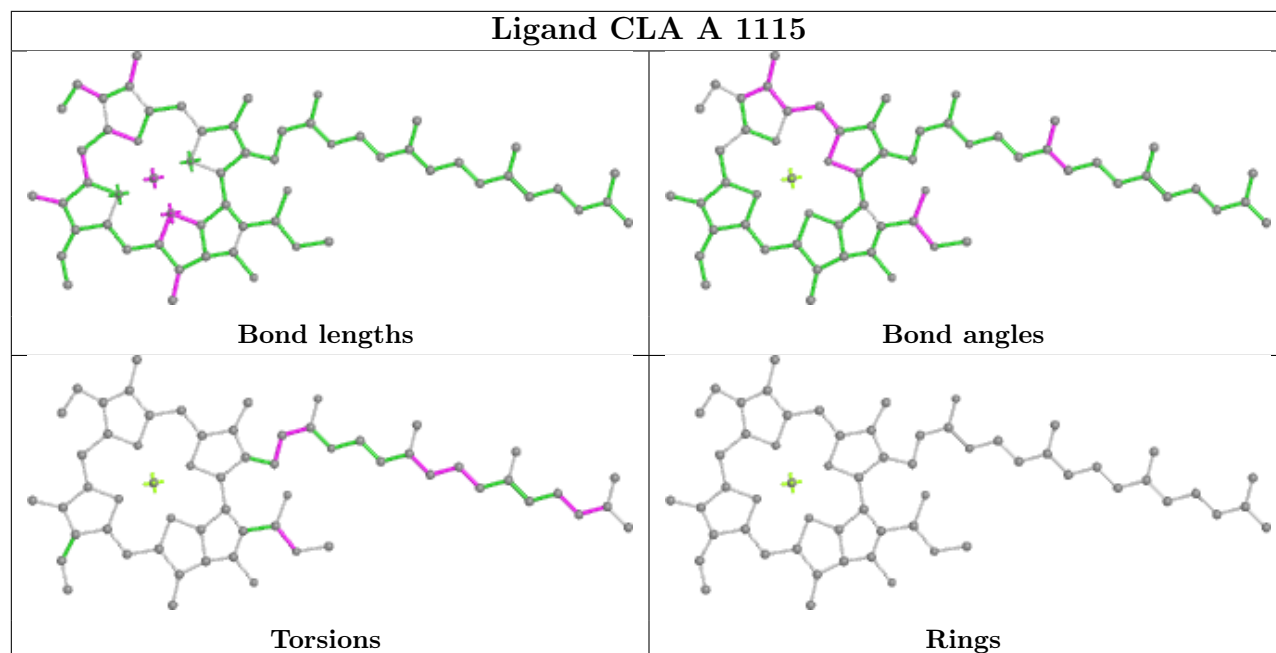




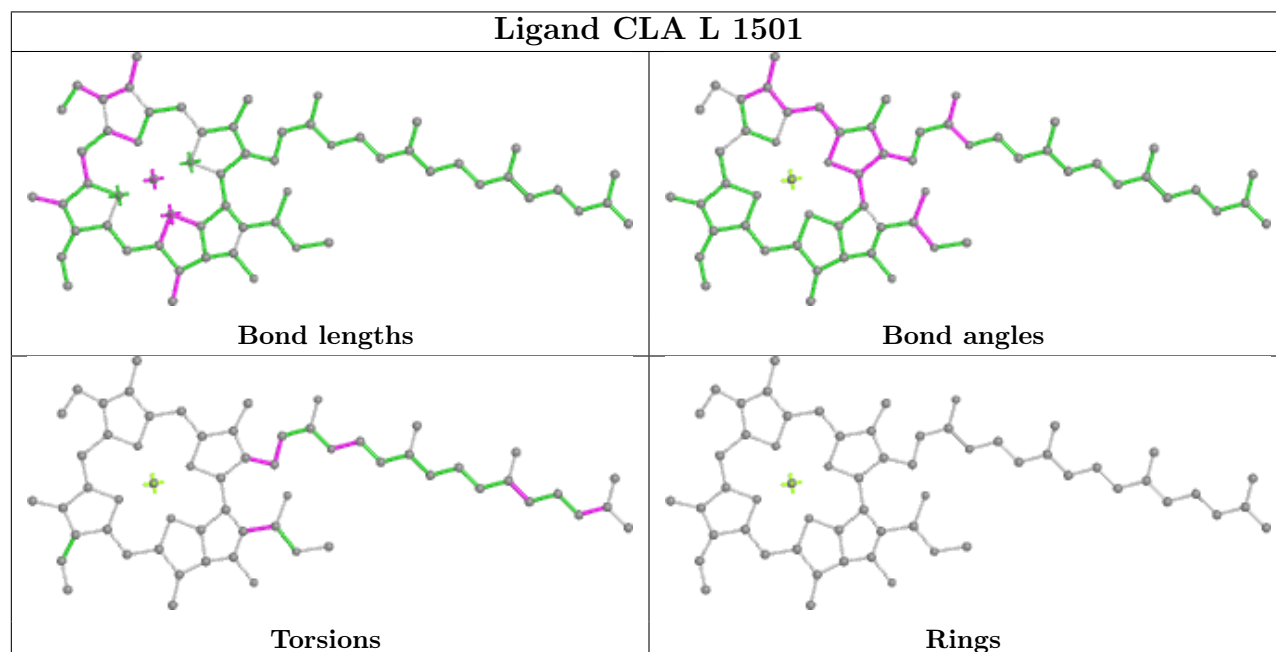




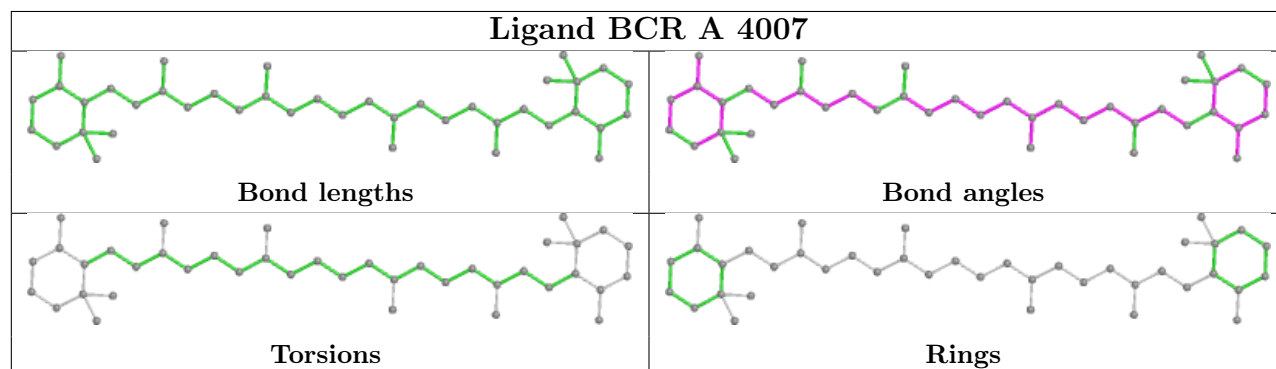
Ligand CLA A 1115



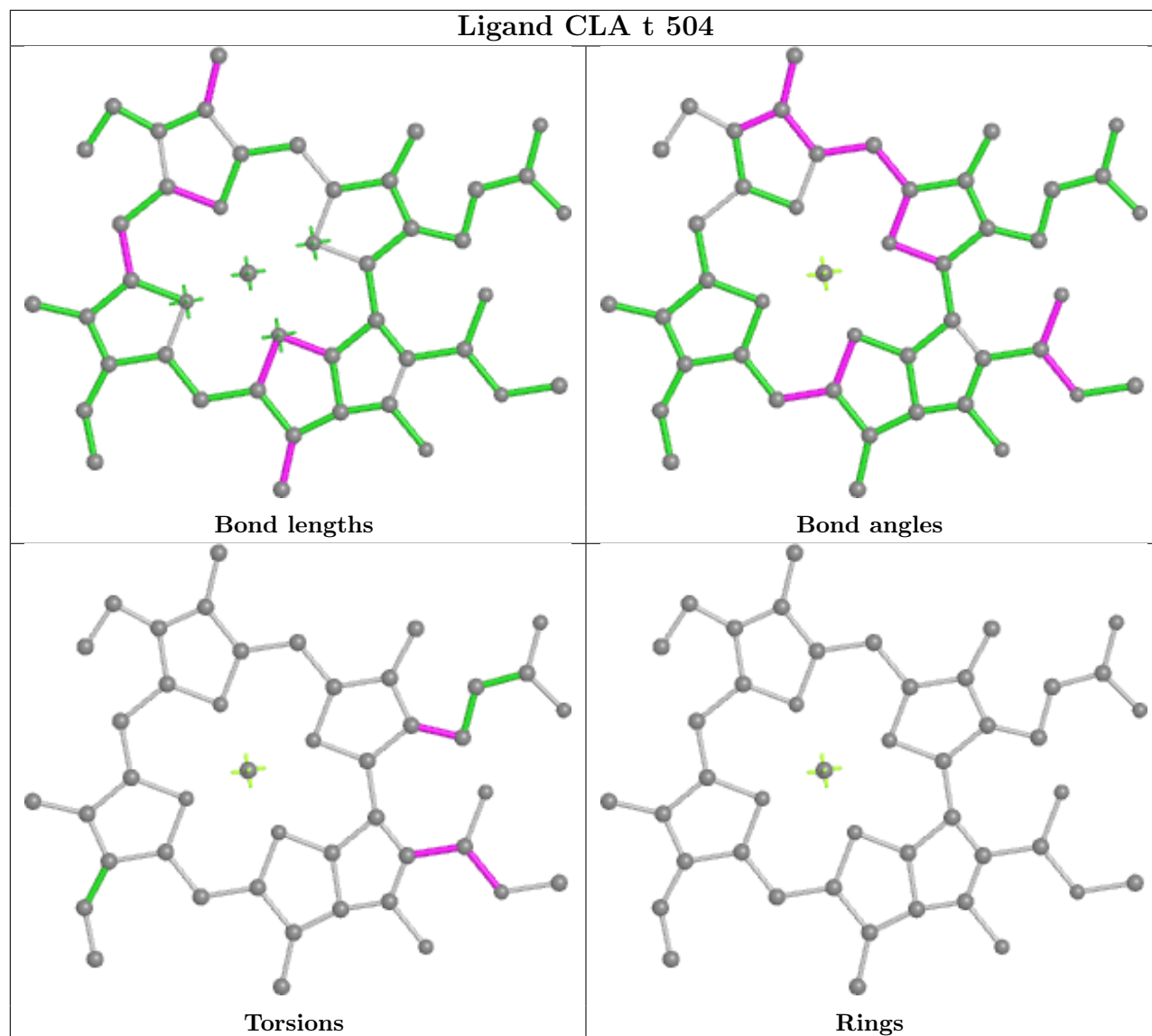
Ligand CLA L 1501



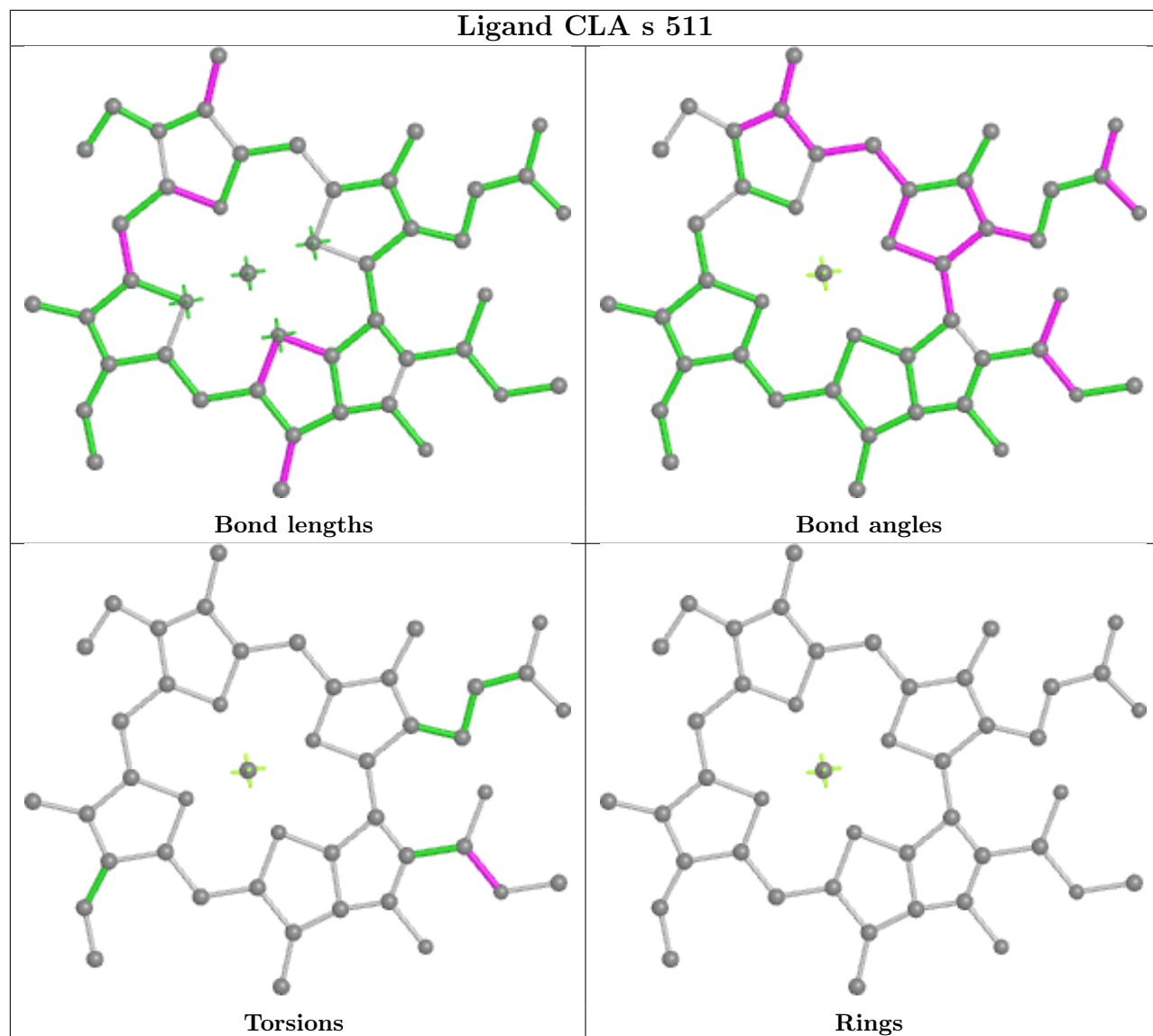
Ligand BCR A 4007



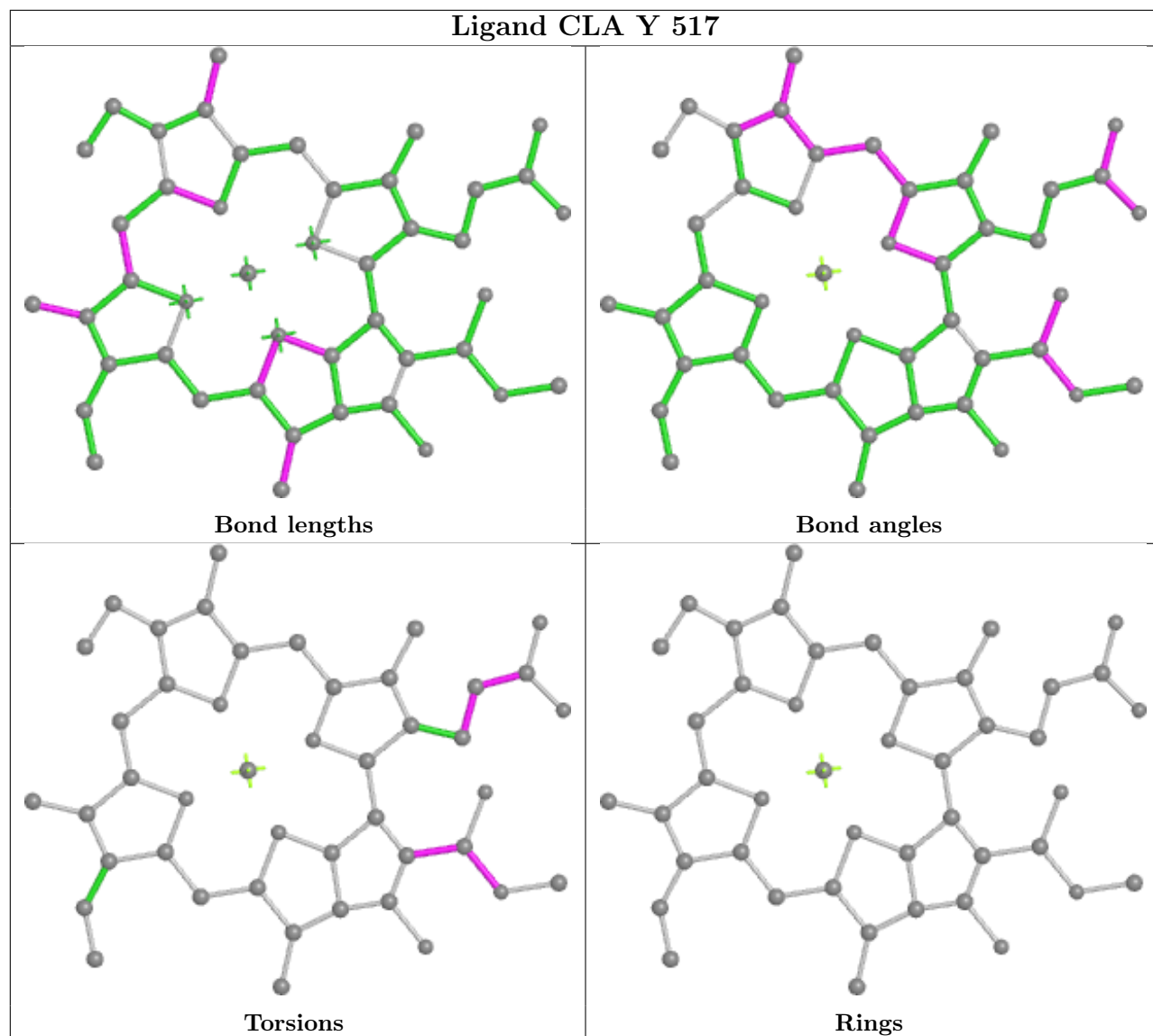
Ligand CLA t 504



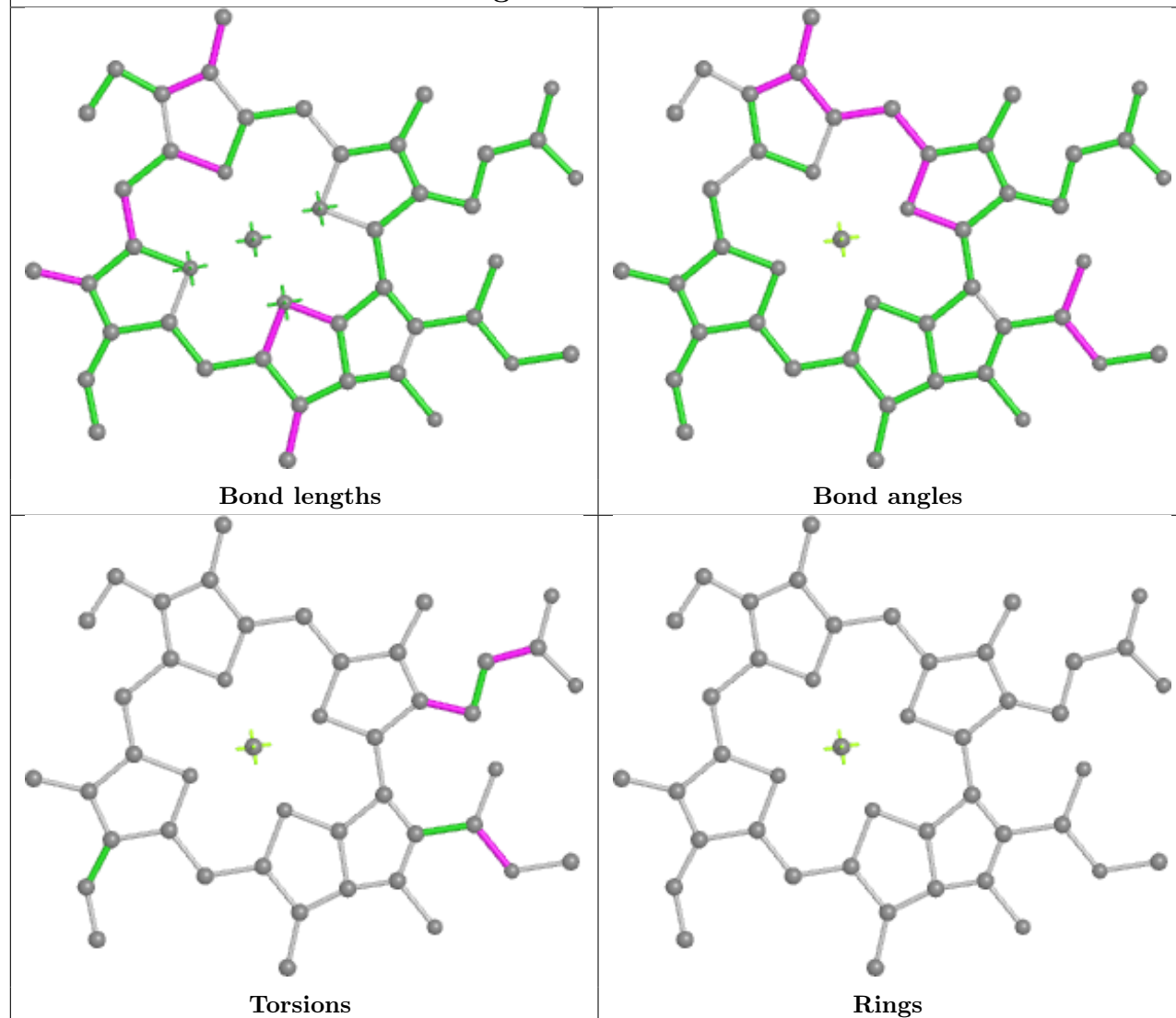
Ligand CLA s 511



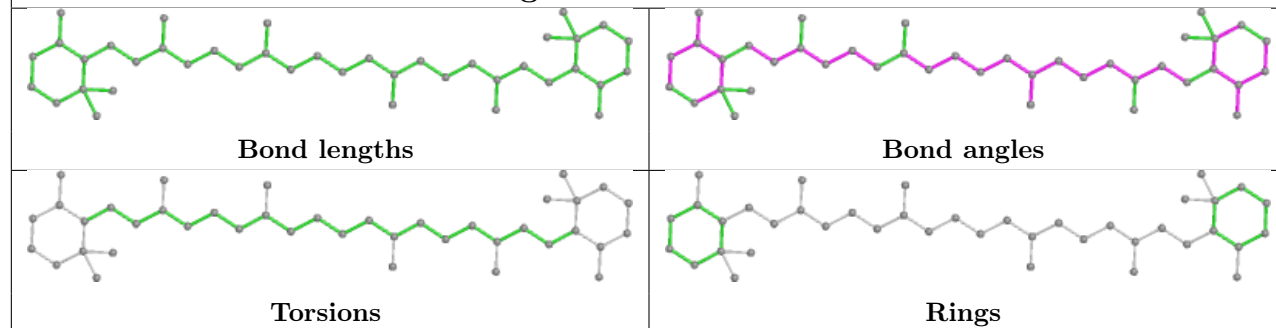
Ligand CLA Y 517

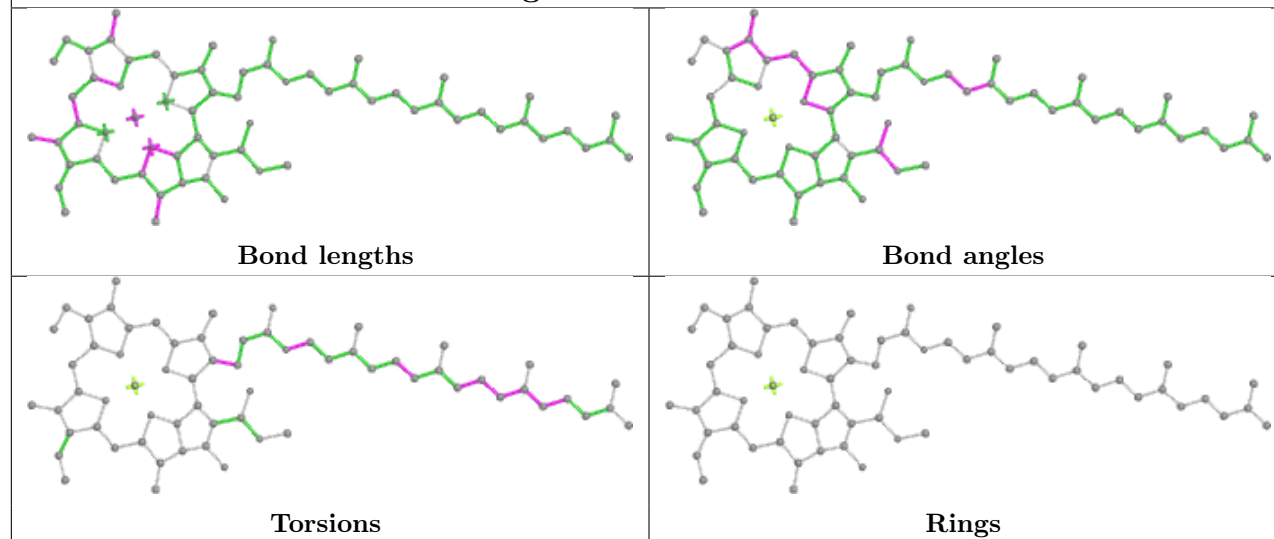
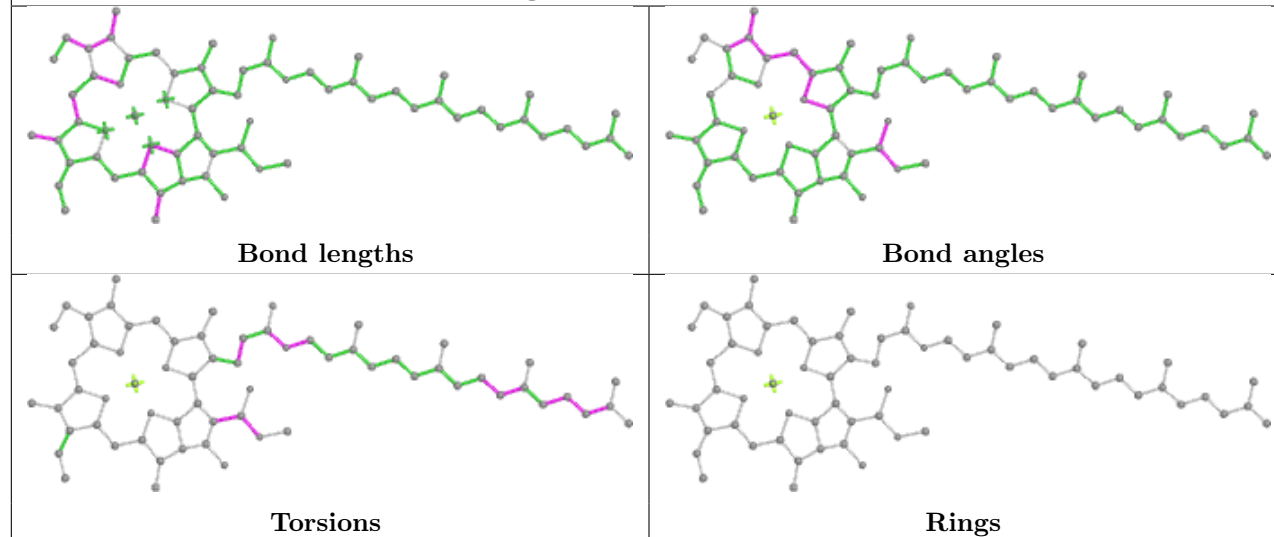


Ligand CLA u 513

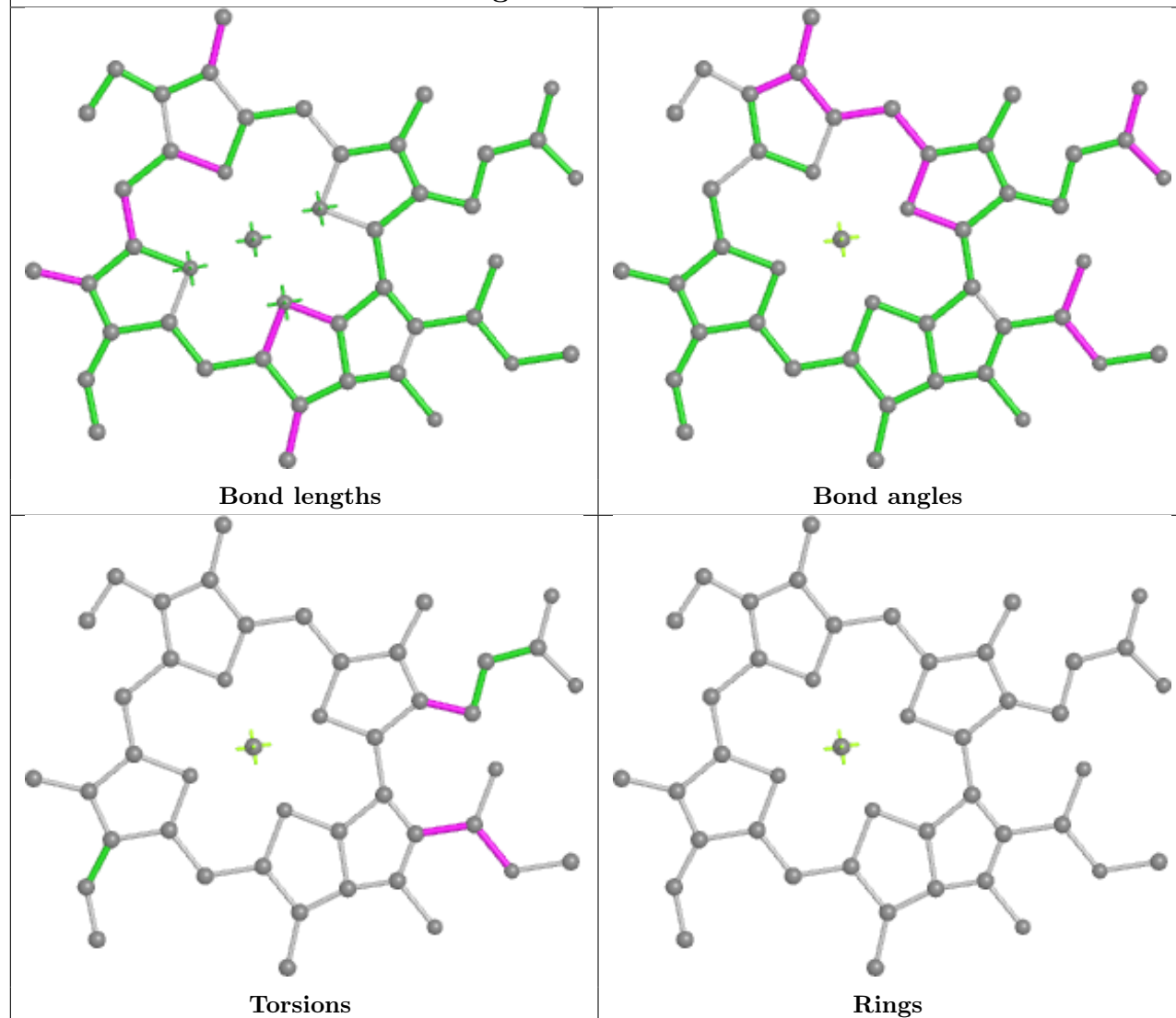


Ligand BCR G 4007

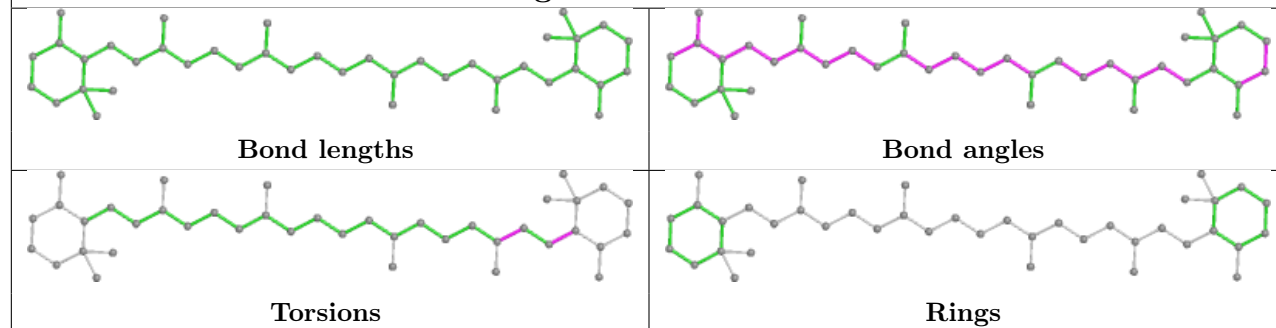


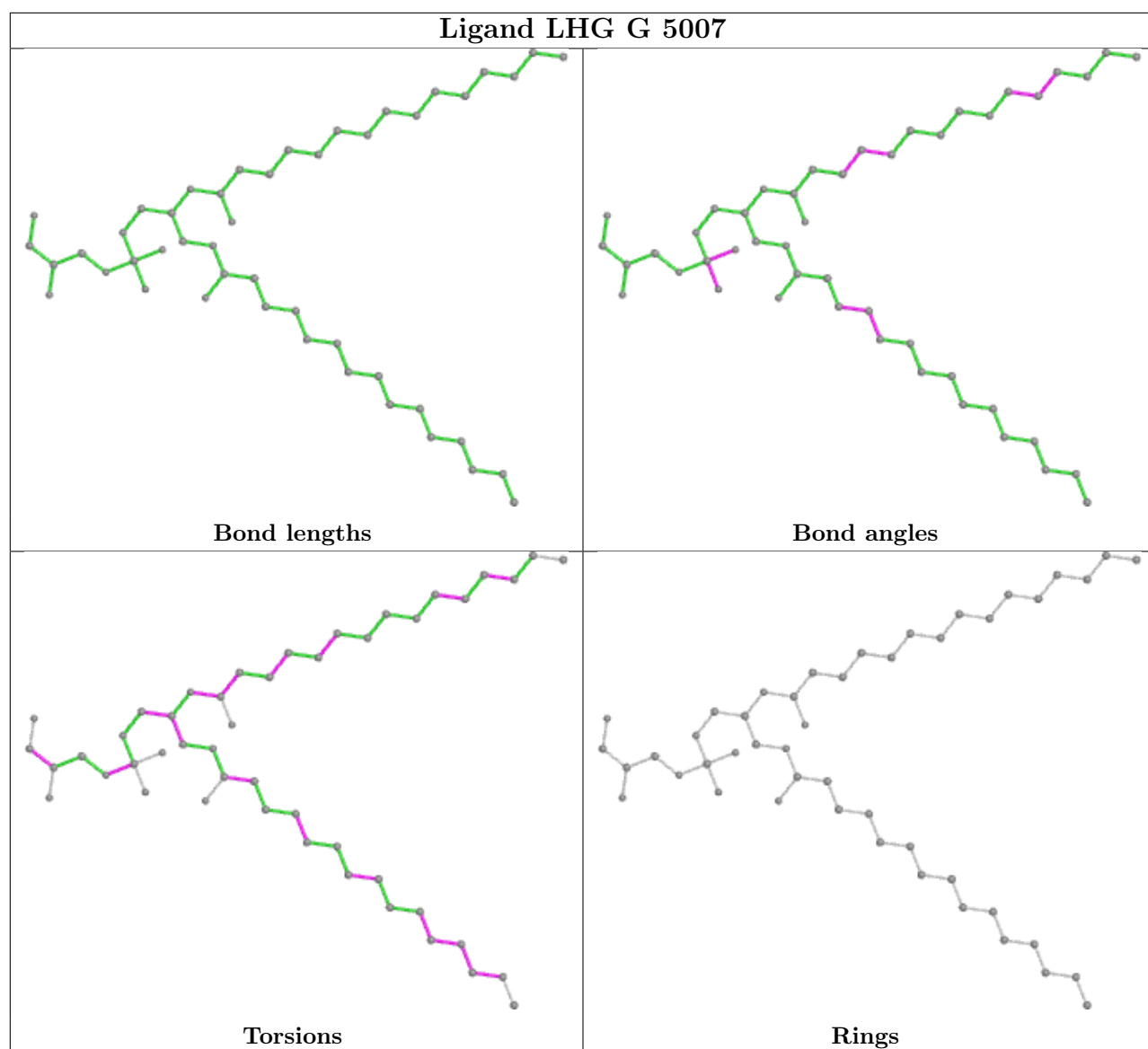
Ligand CLA H 1223**Ligand CLA B 1207**

Ligand CLA Z 511

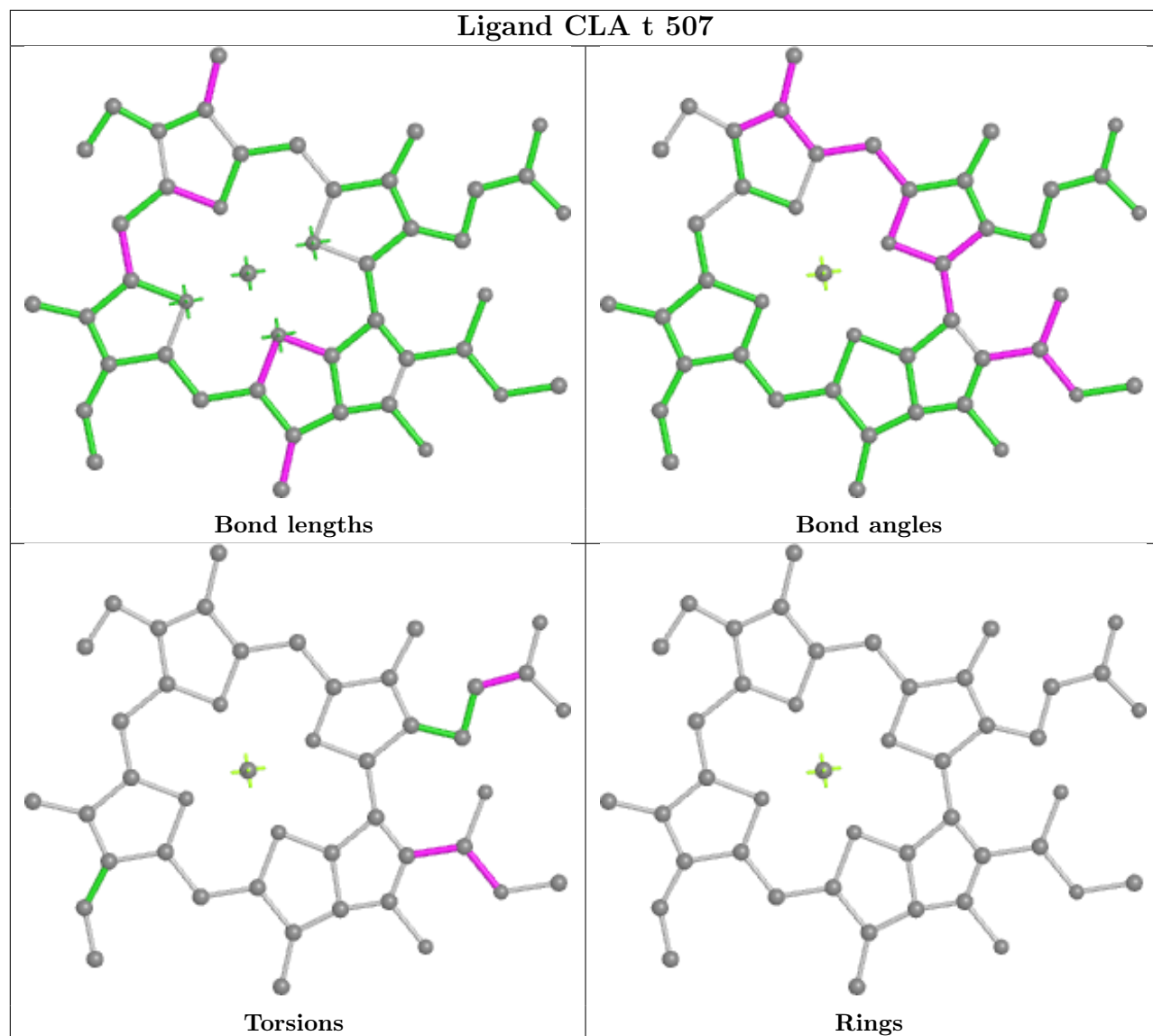


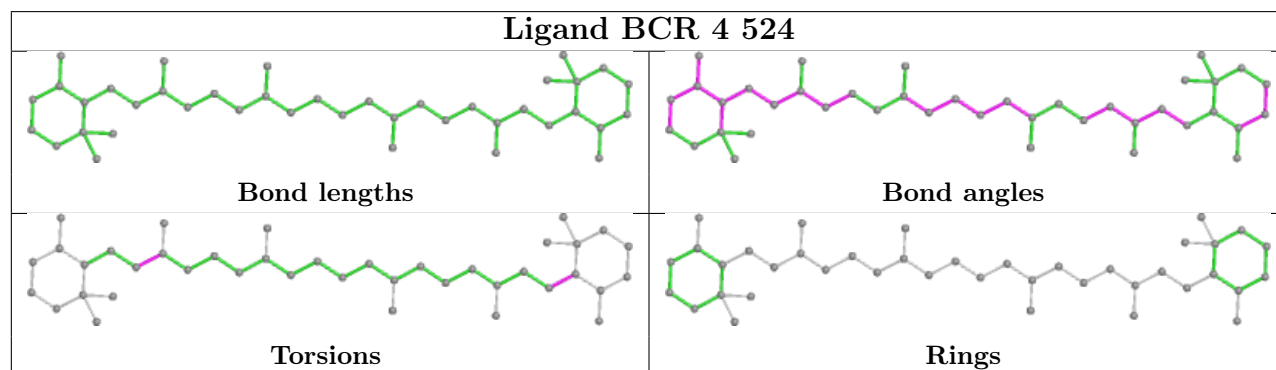
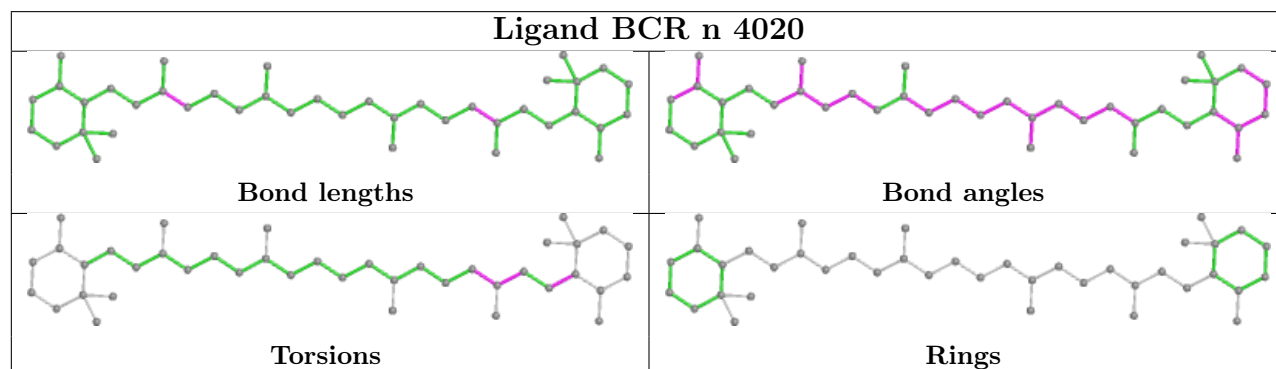
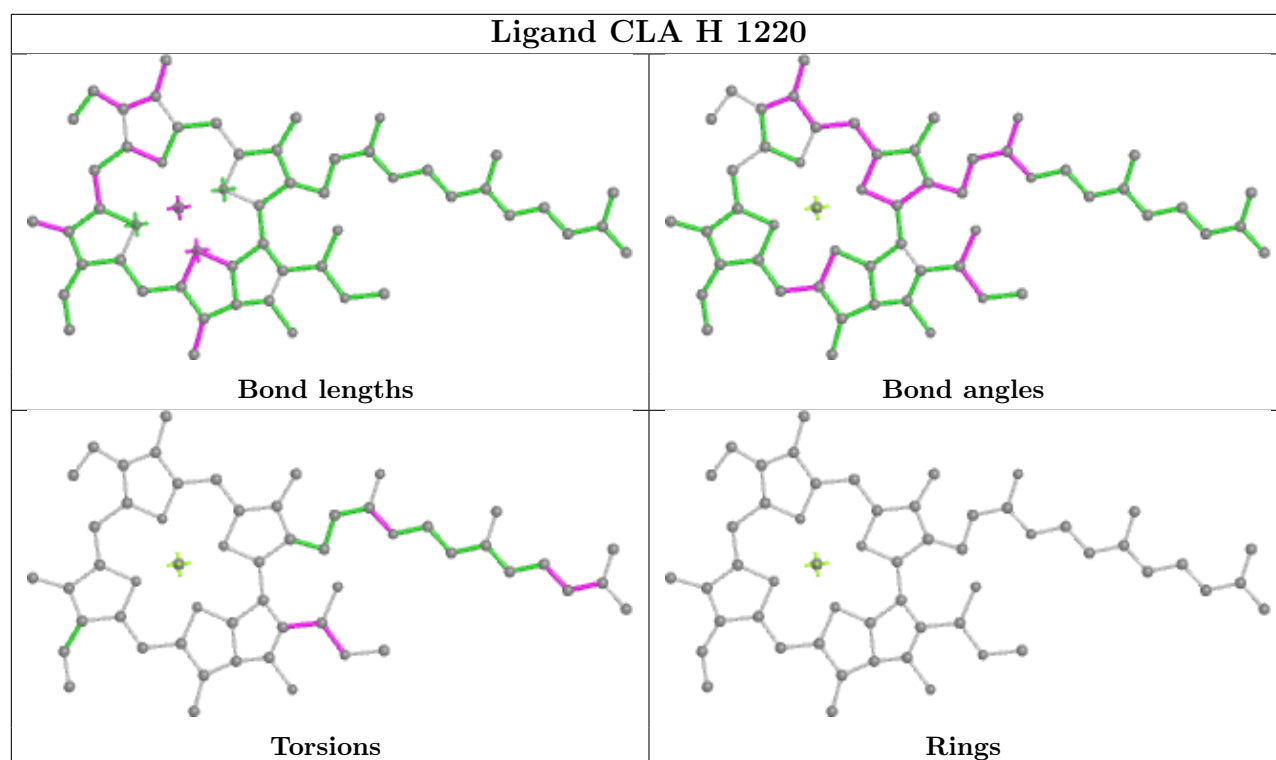
Ligand BCR 6 523



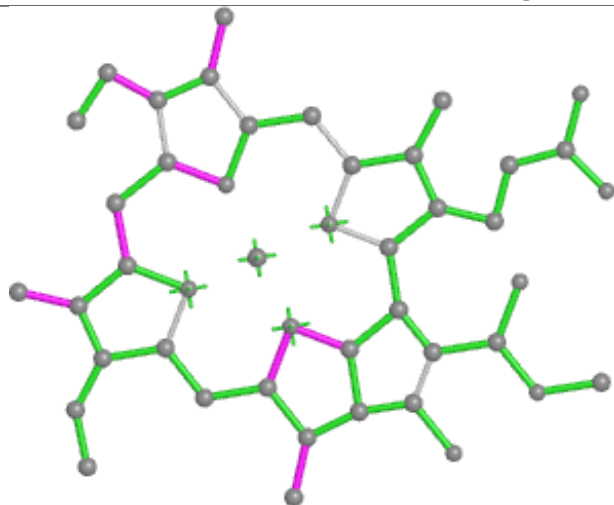


Ligand CLA t 507

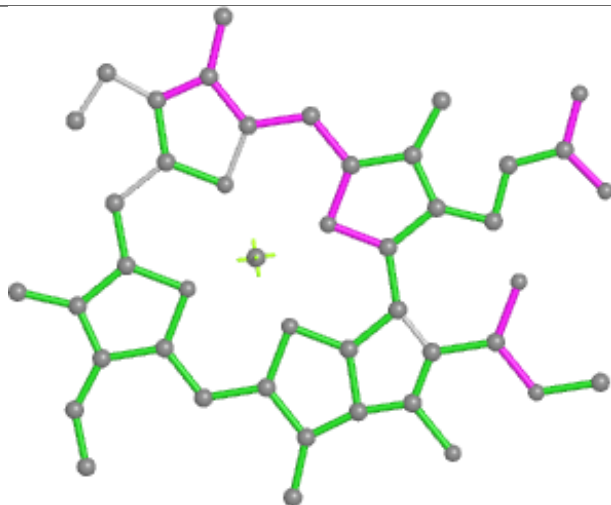




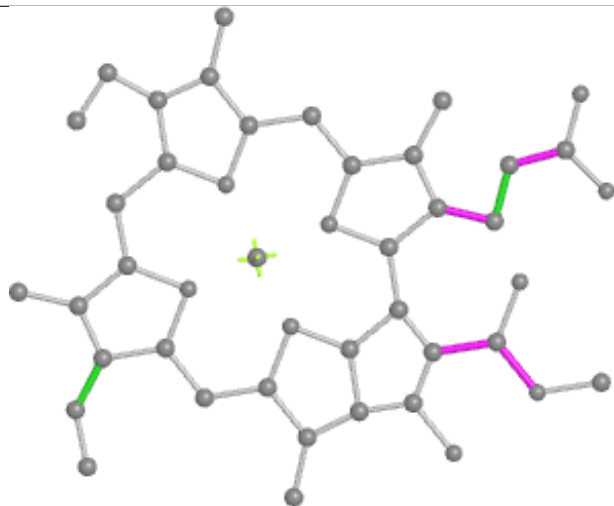
Ligand CLA v 517



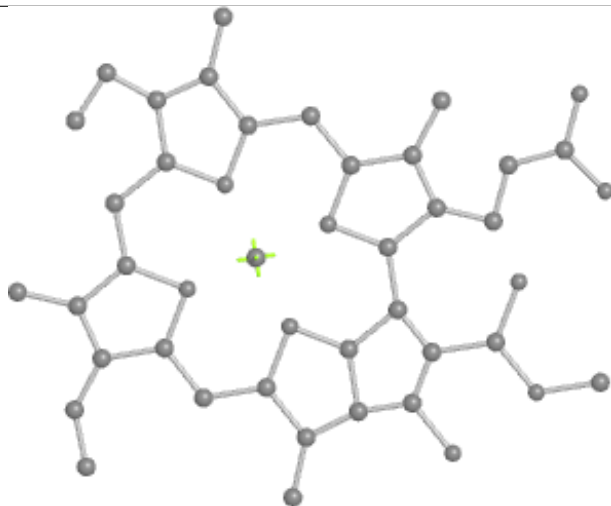
Bond lengths



Bond angles

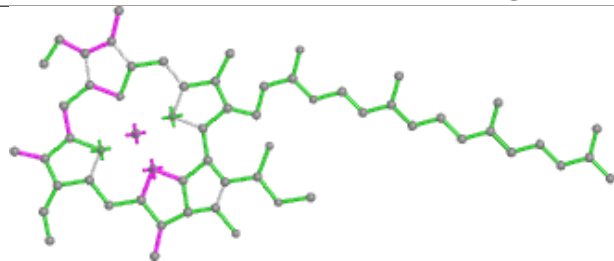


Torsions

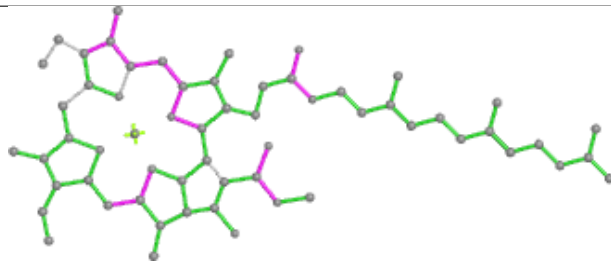


Rings

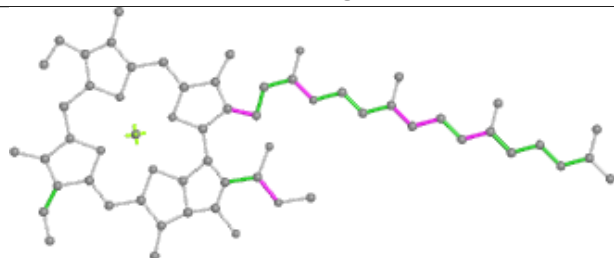
Ligand CLA B 1227



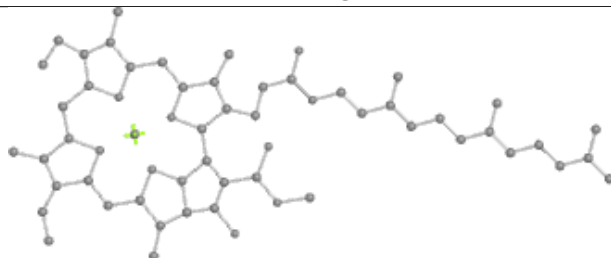
Bond lengths



Bond angles

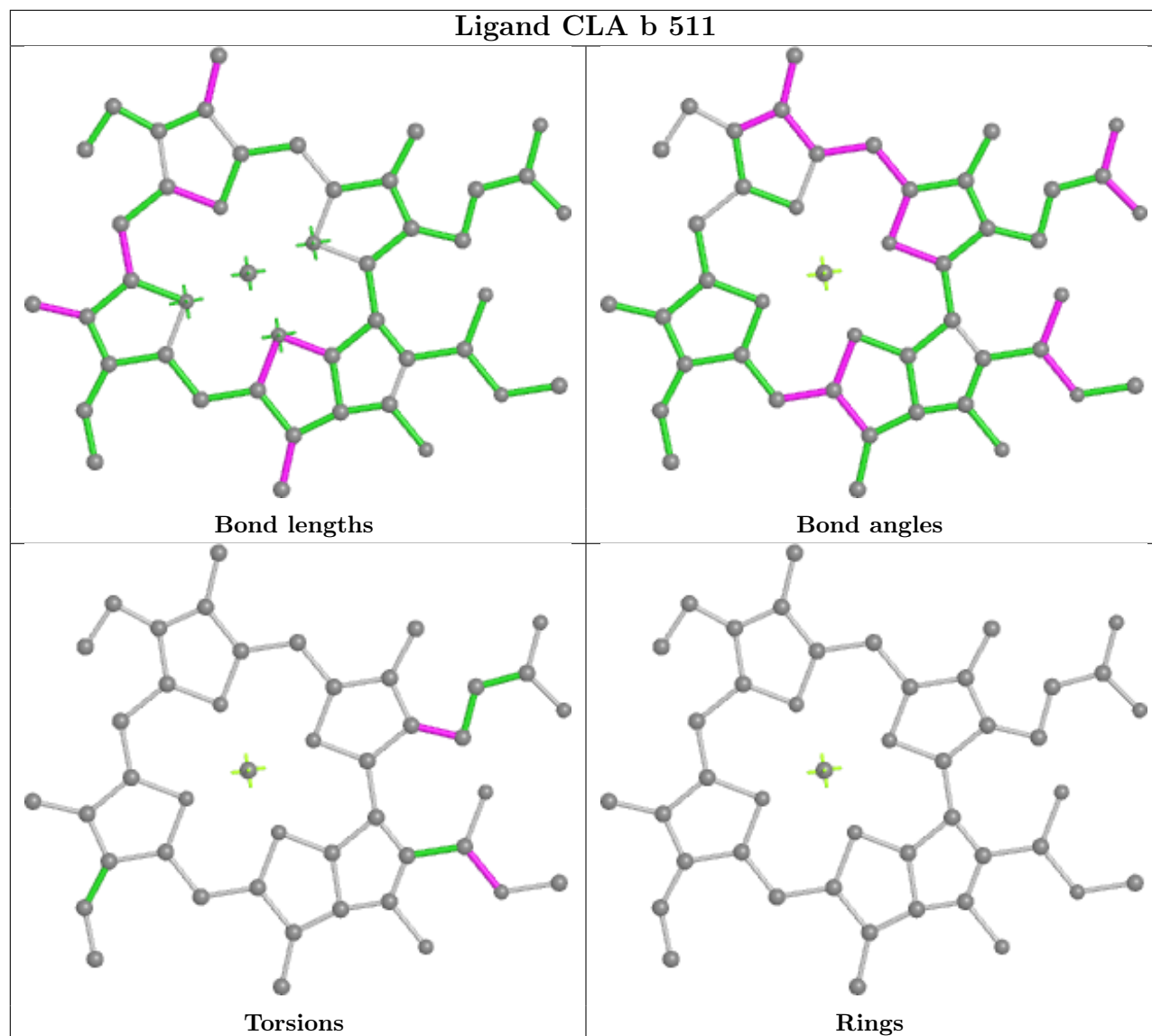


Torsions

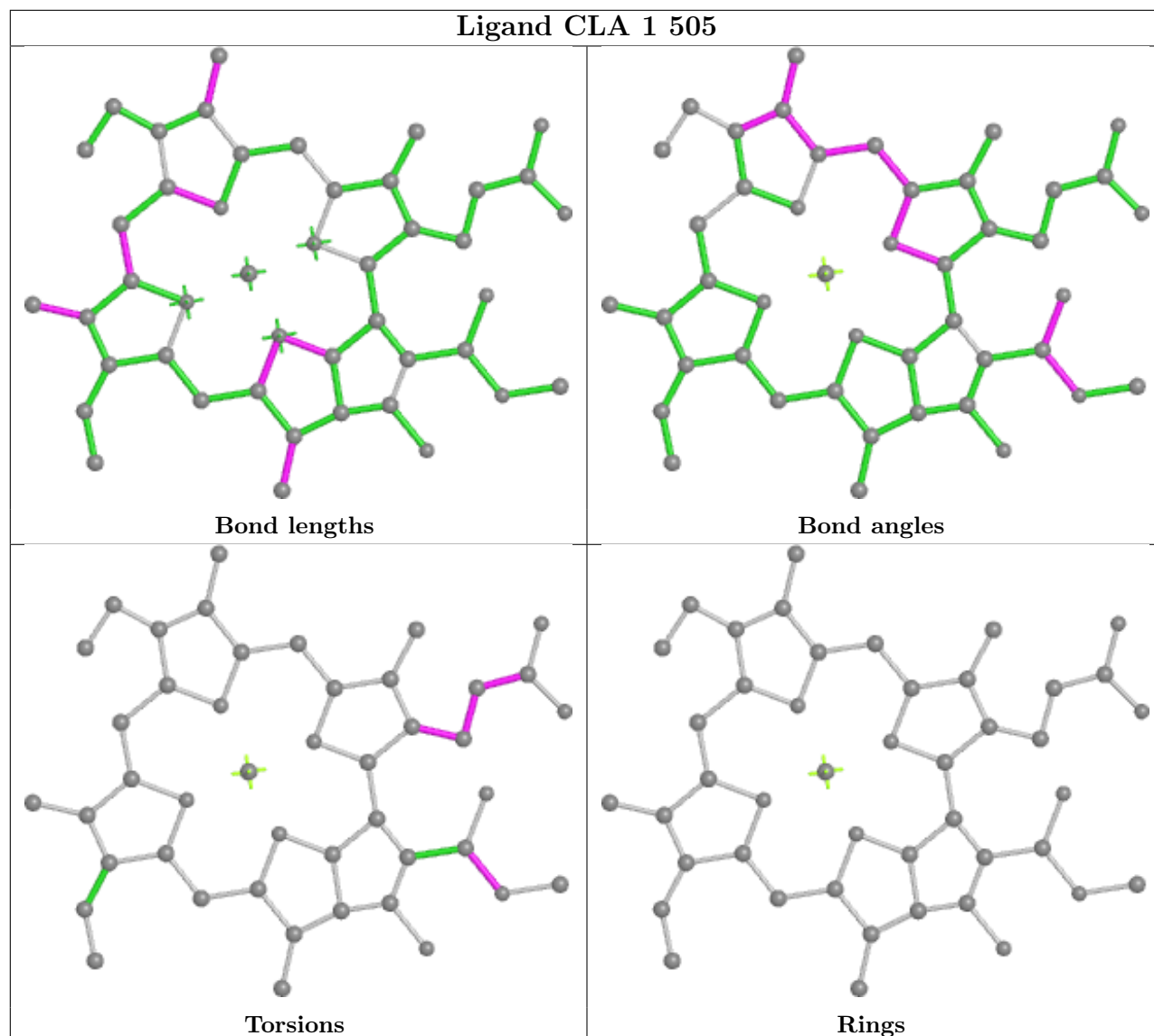


Rings

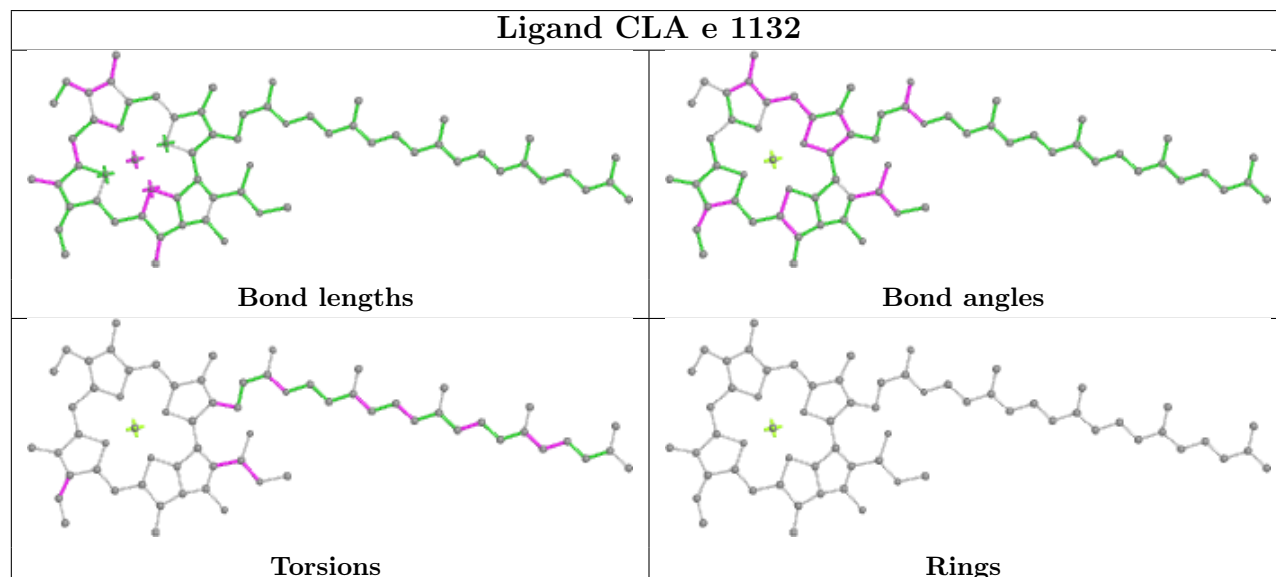
Ligand CLA b 511



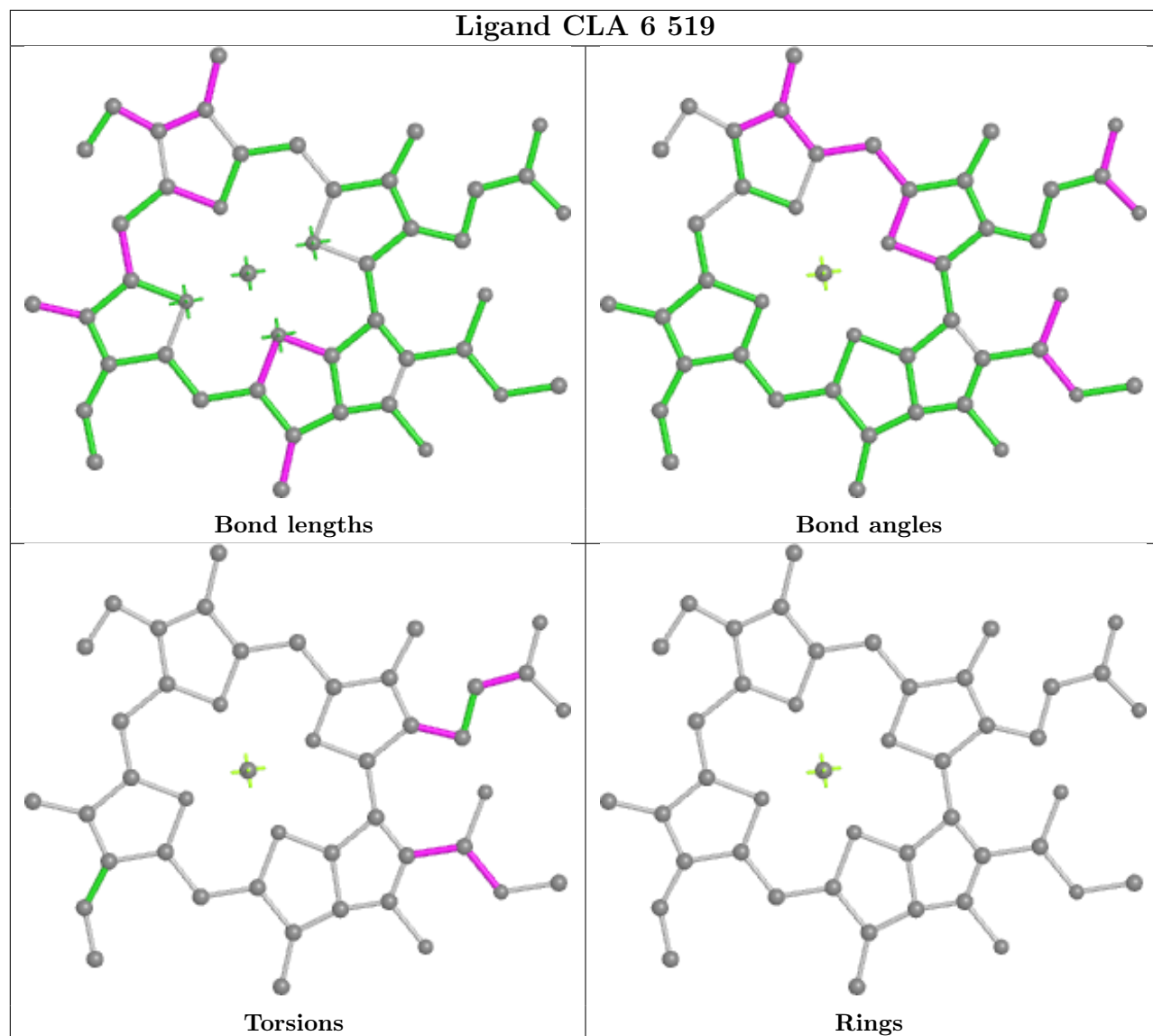
Ligand CLA 1 505



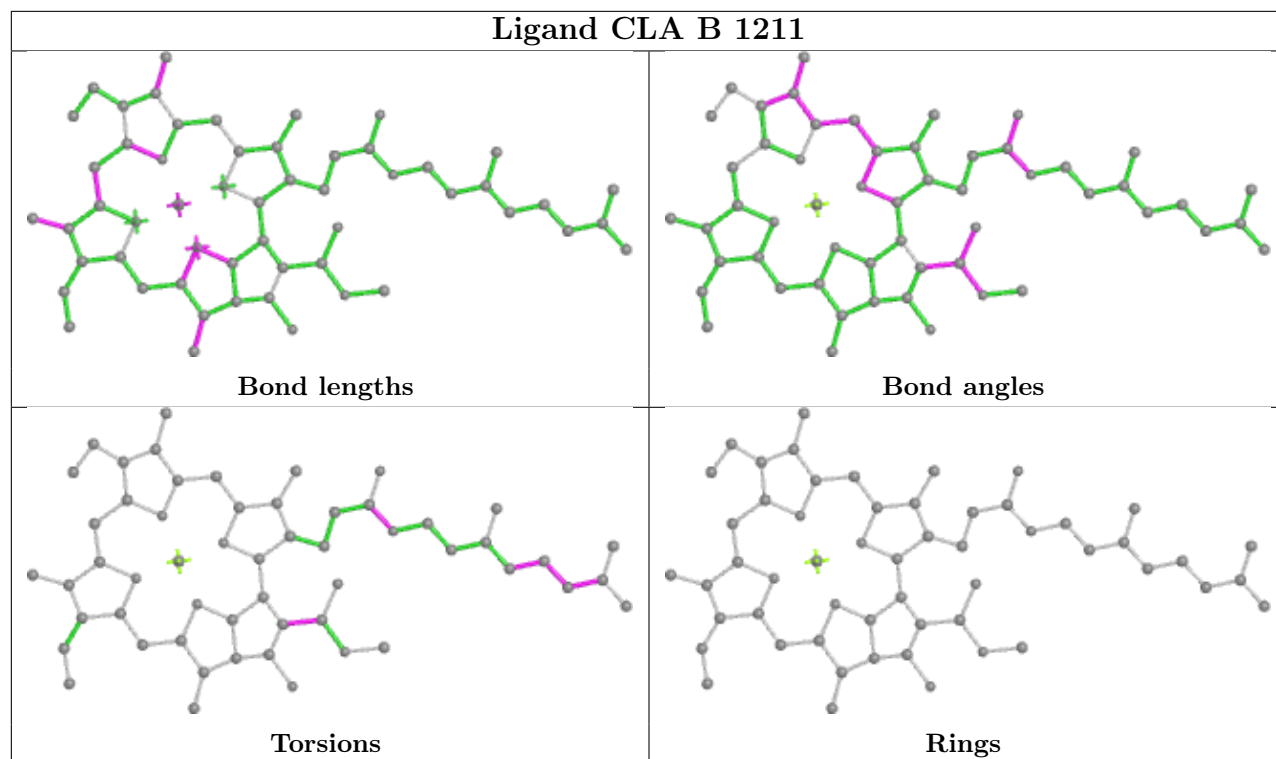
Ligand CLA e 1132



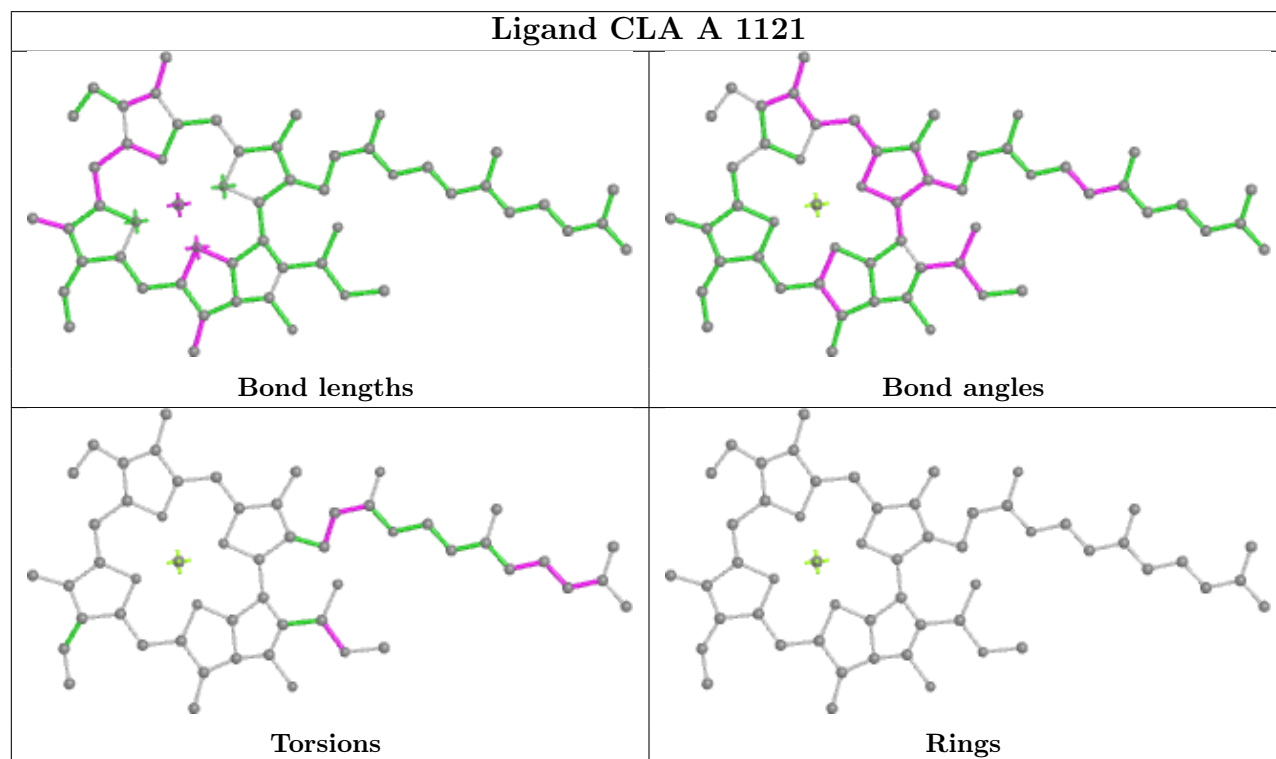
Ligand CLA 6 519



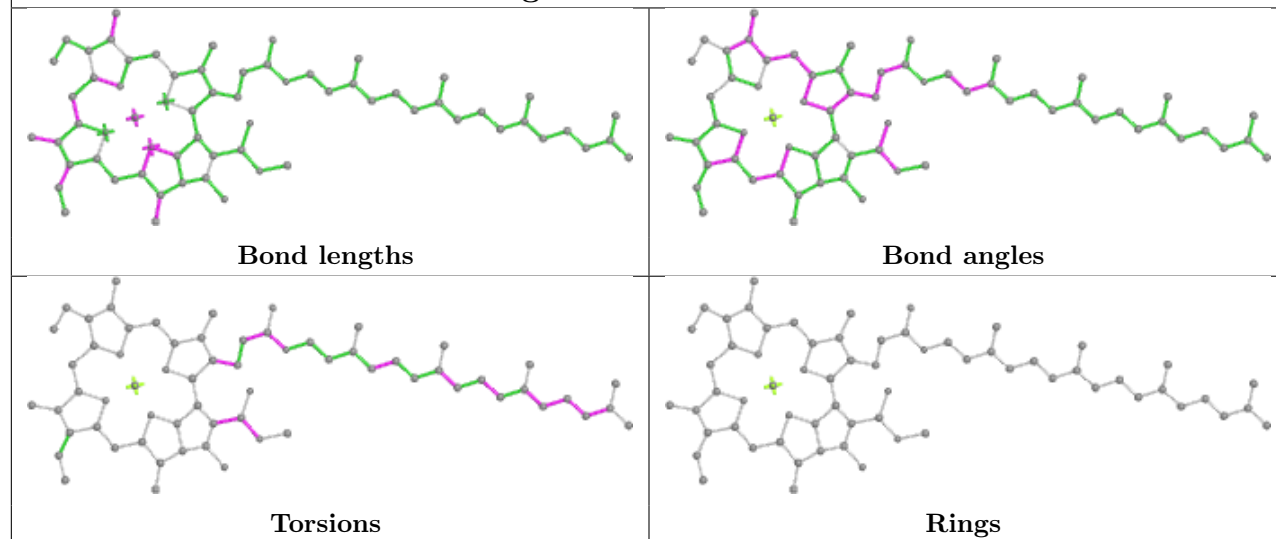
Ligand CLA B 1211



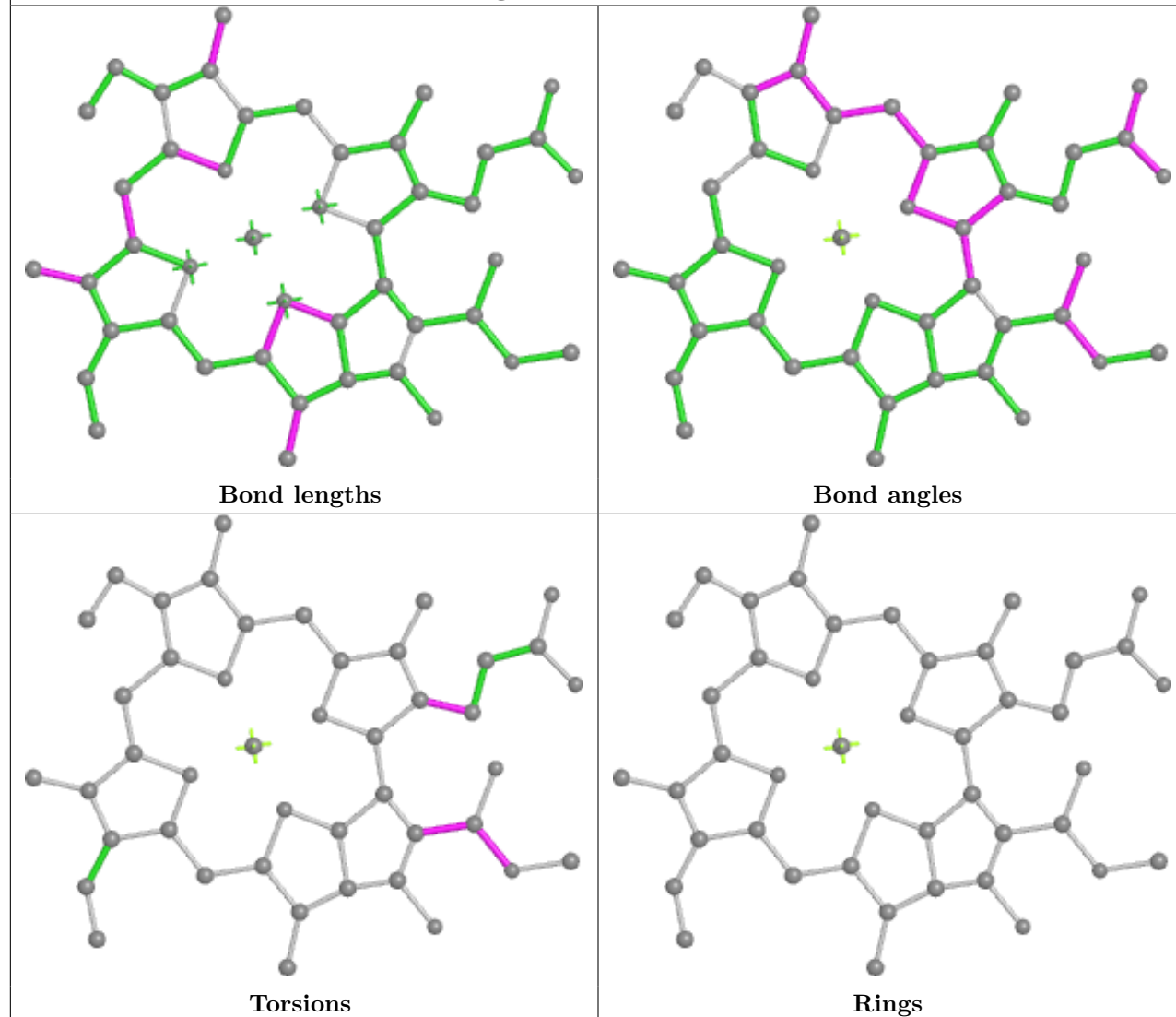
Ligand CLA A 1121



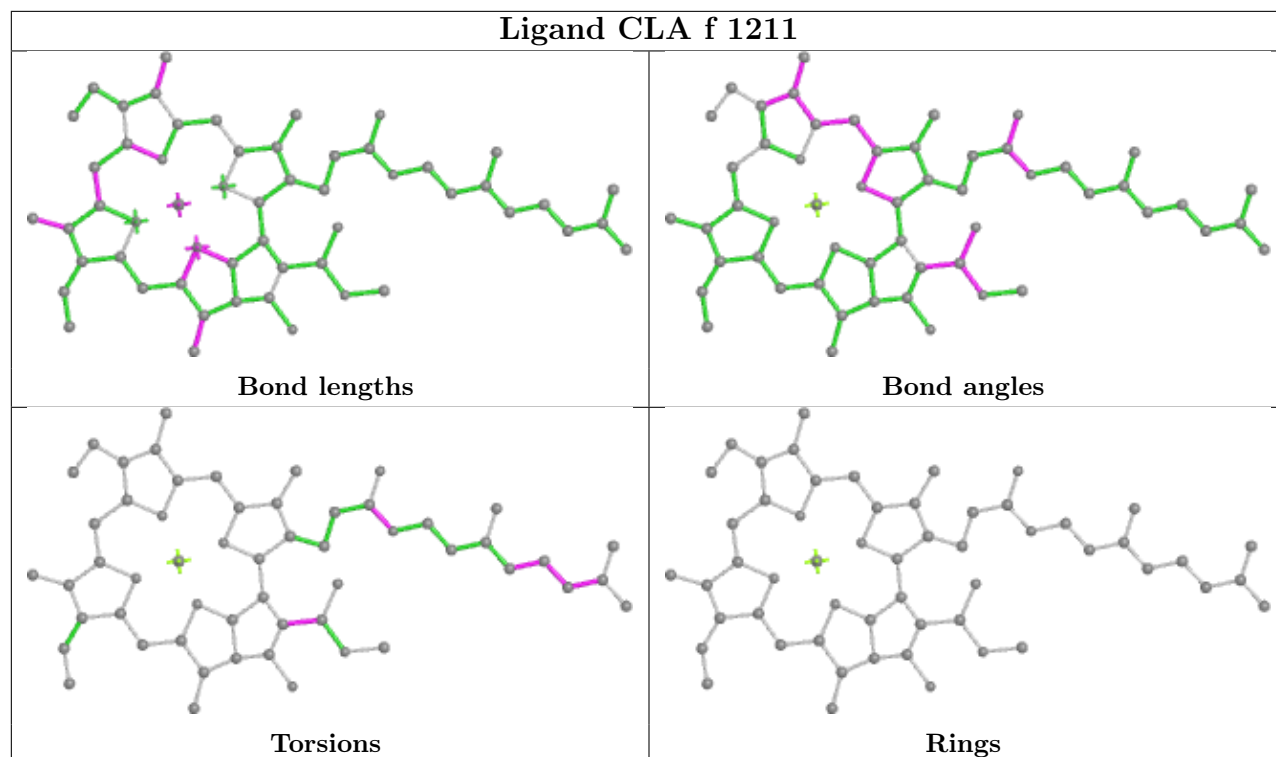
Ligand CLA G 1103



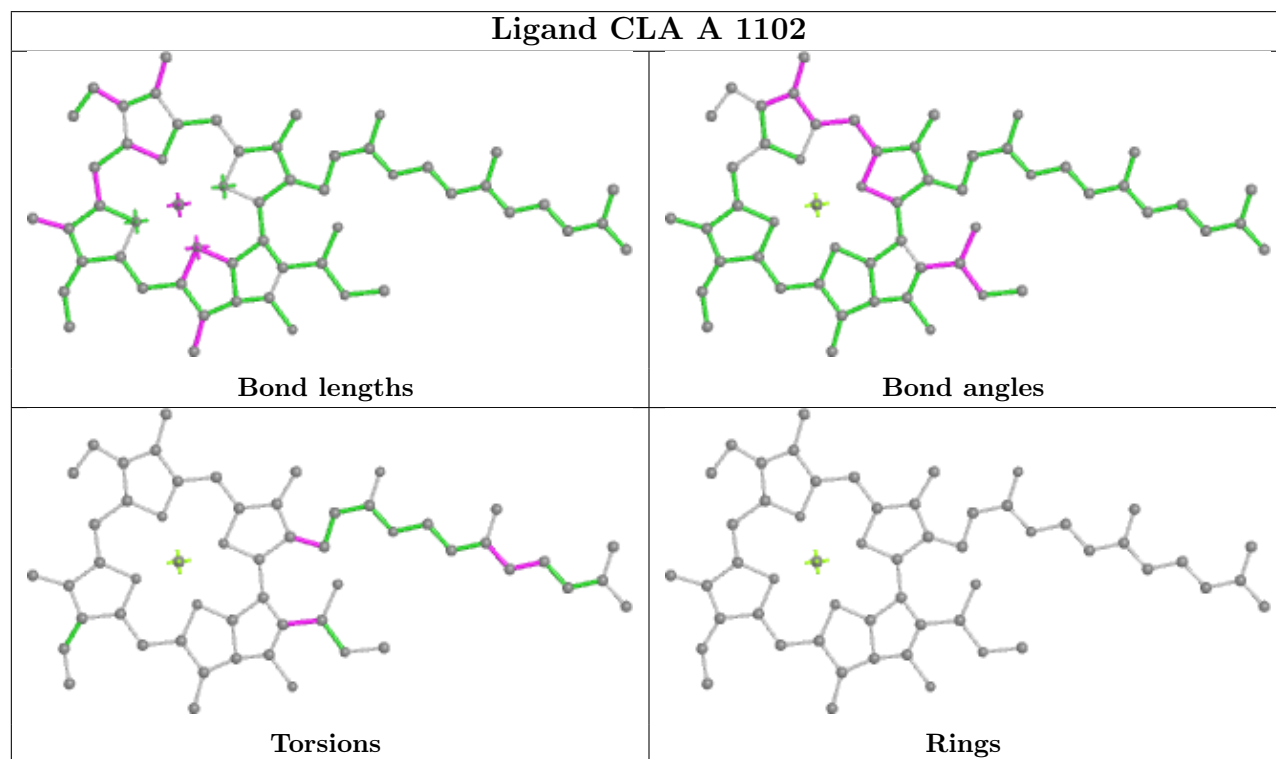
Ligand CLA b 517



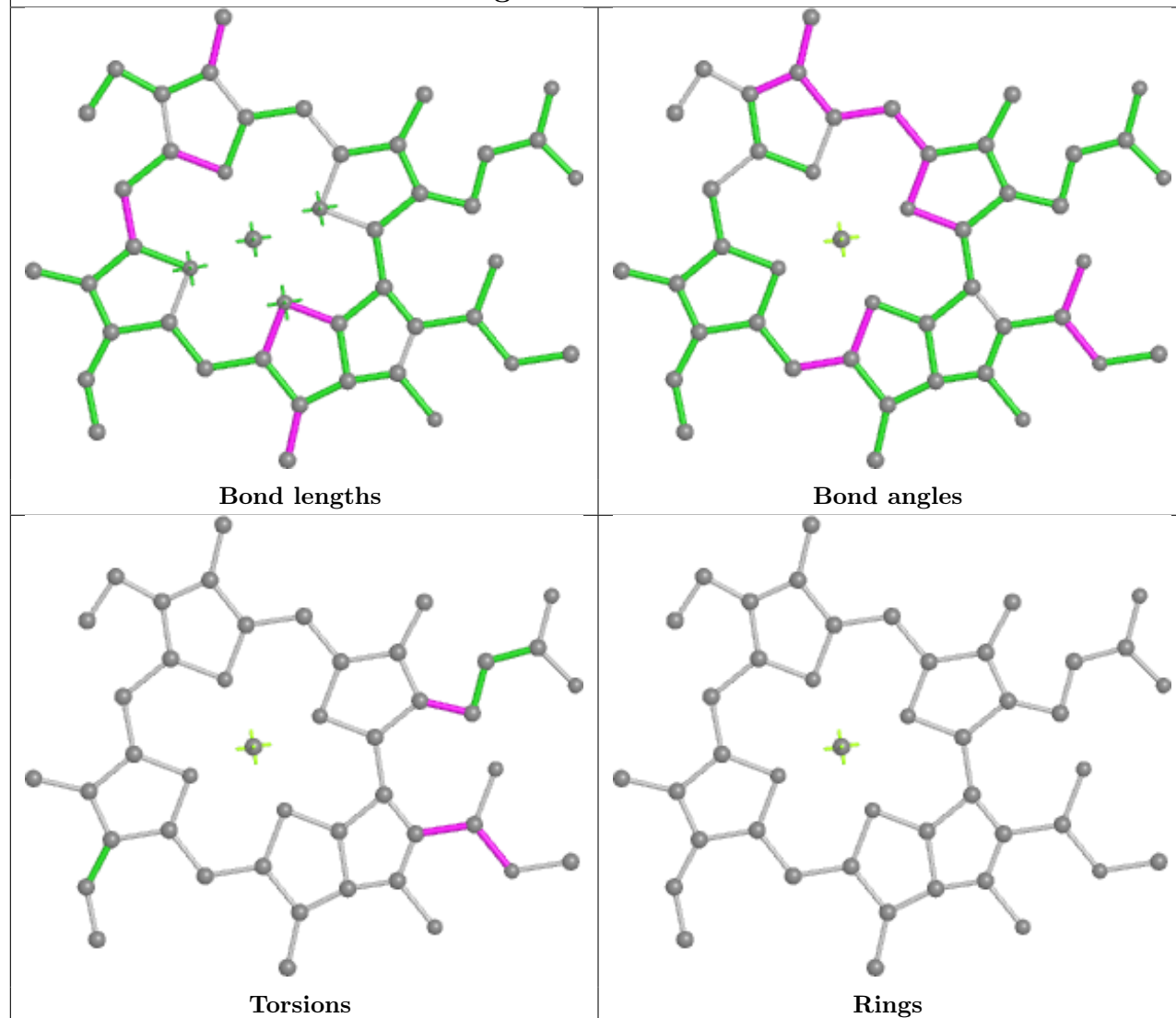
Ligand CLA f 1211



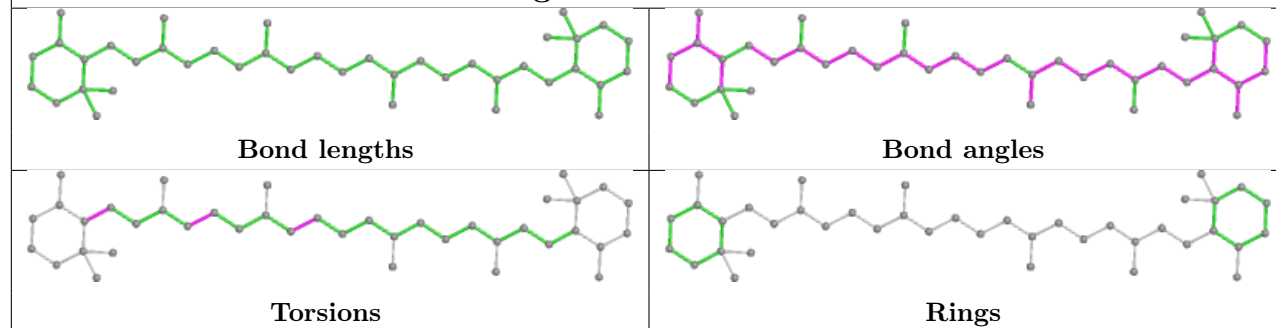
Ligand CLA A 1102

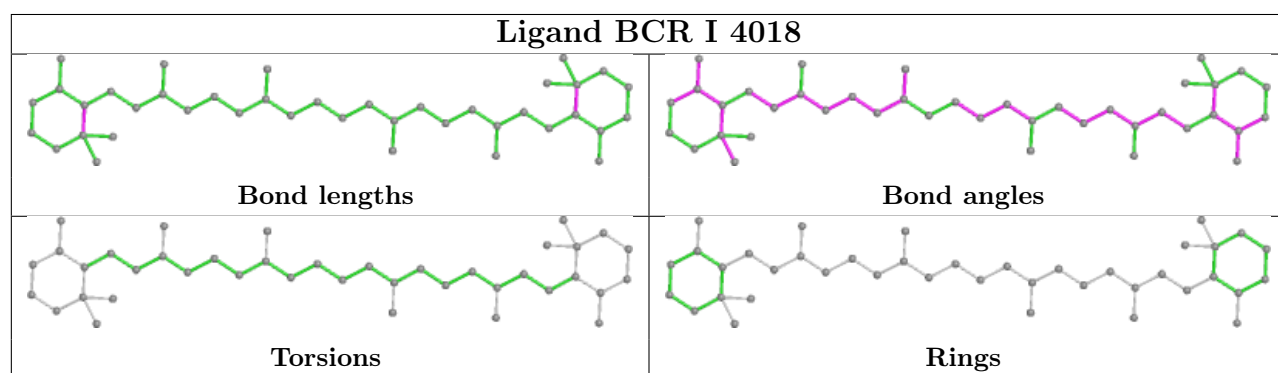
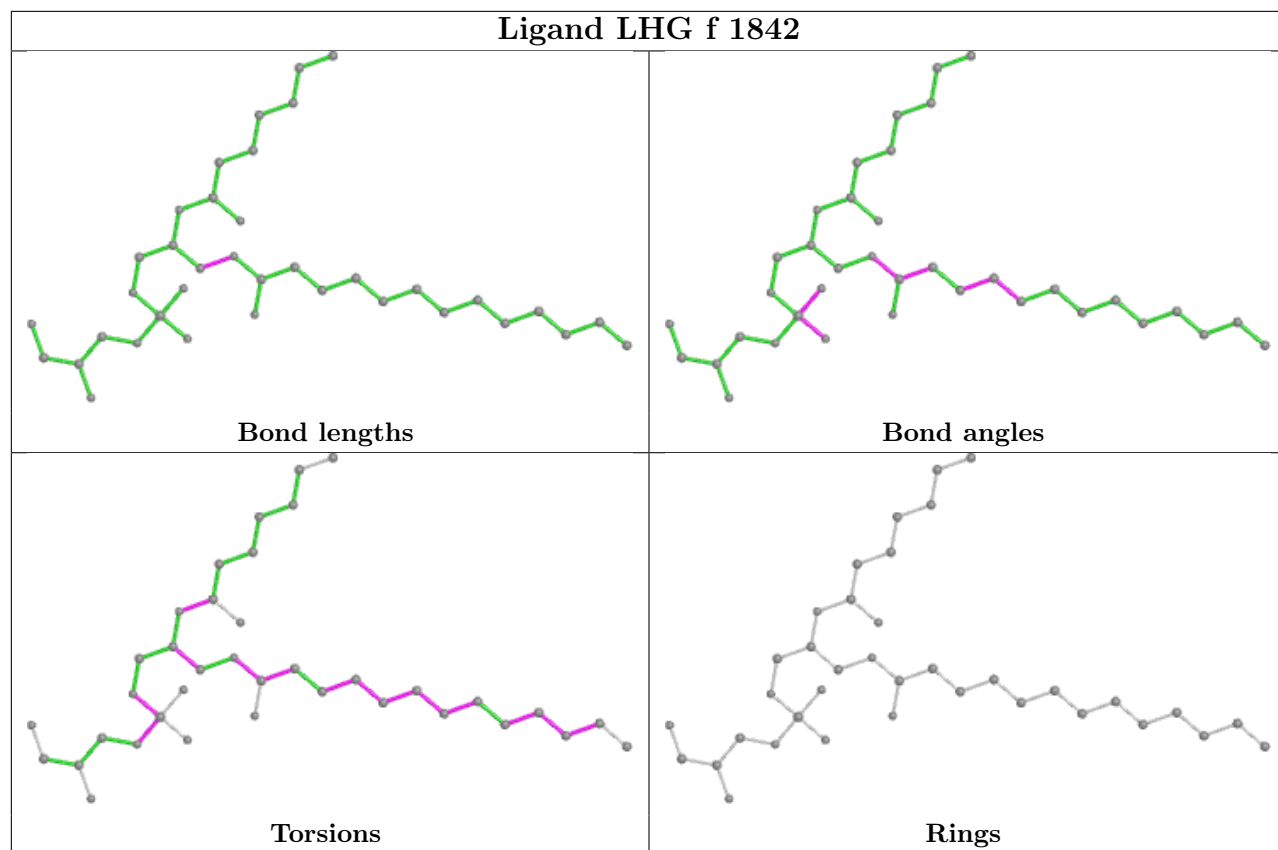


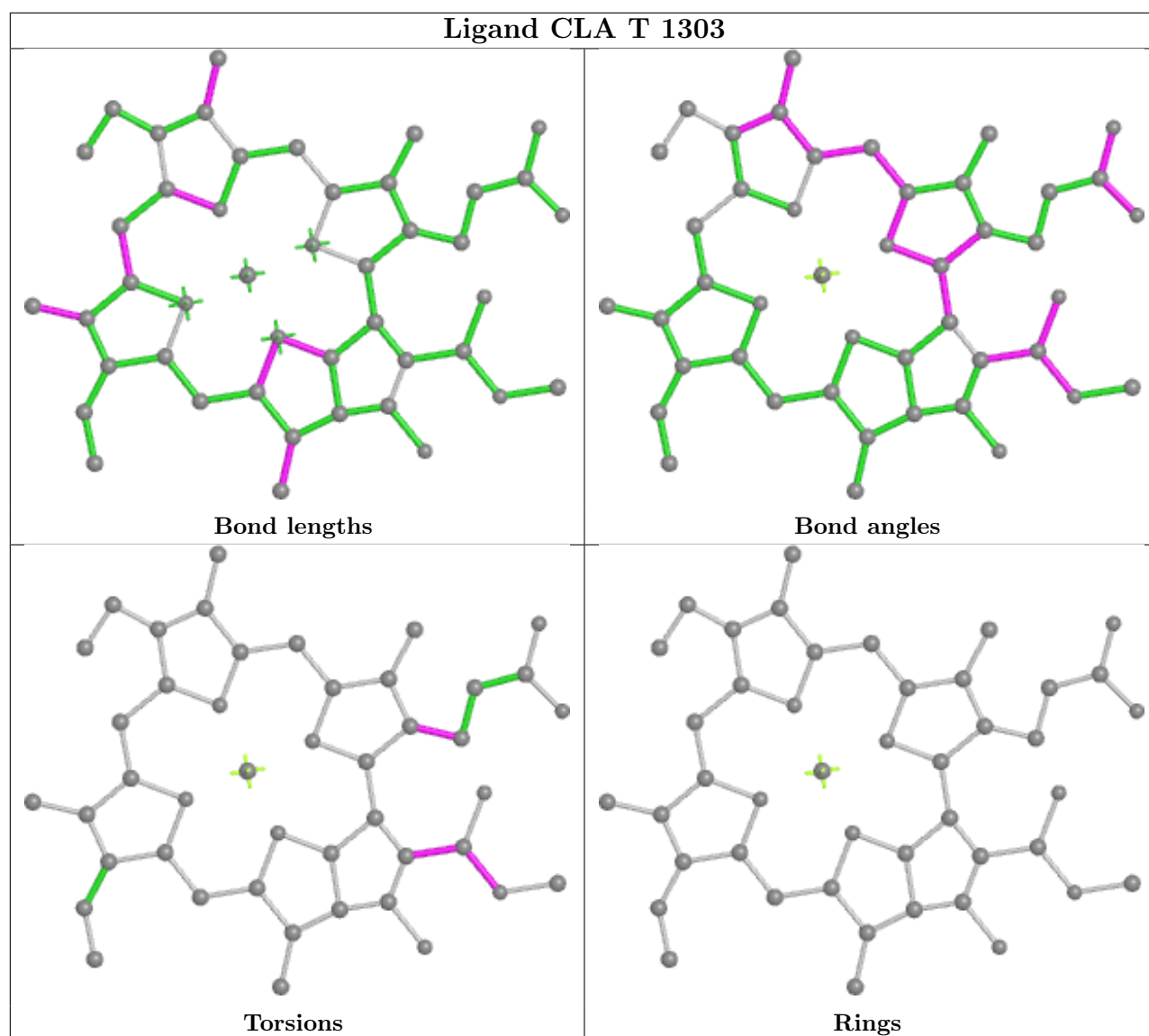
Ligand CLA 4 504



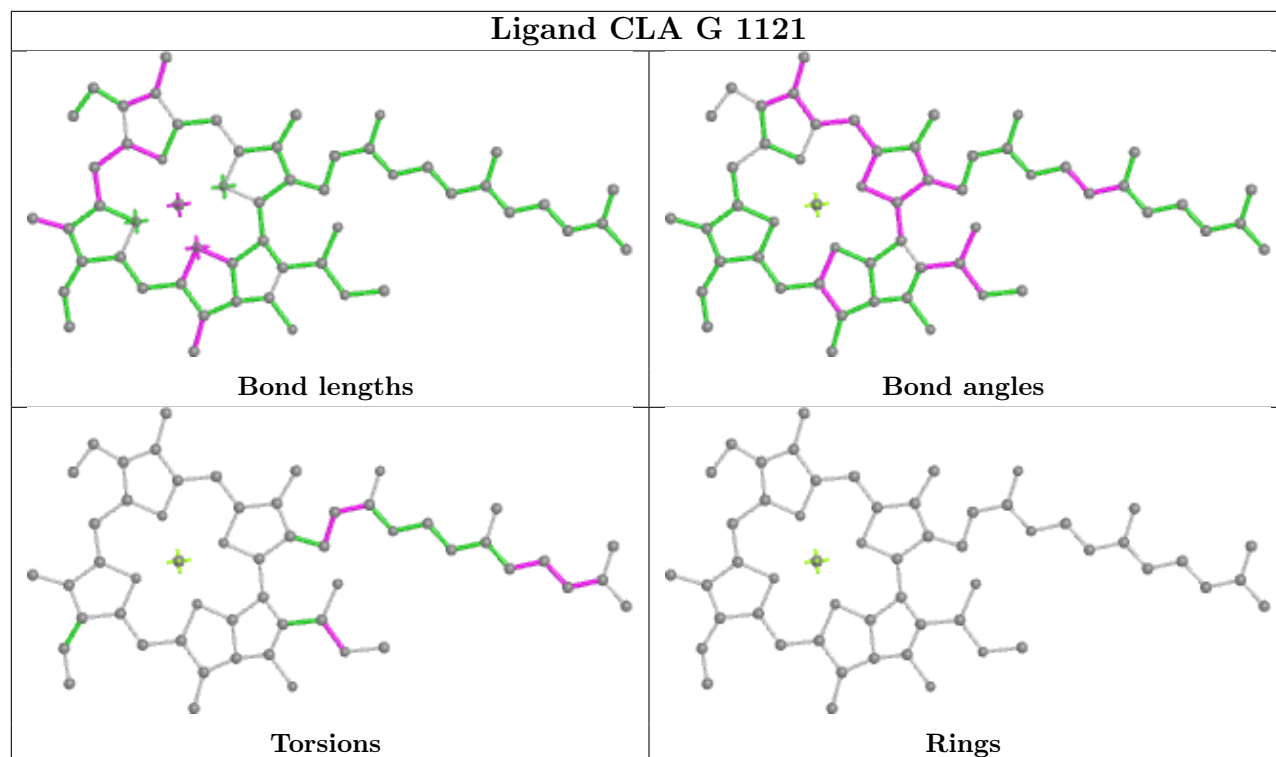
Ligand BCR b 522



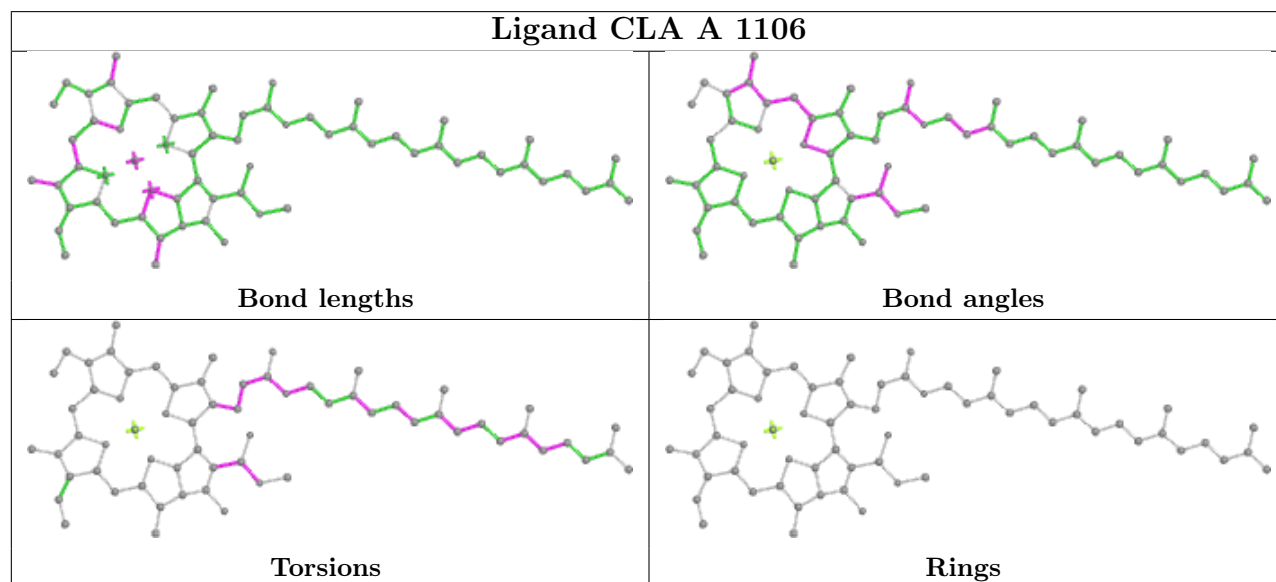


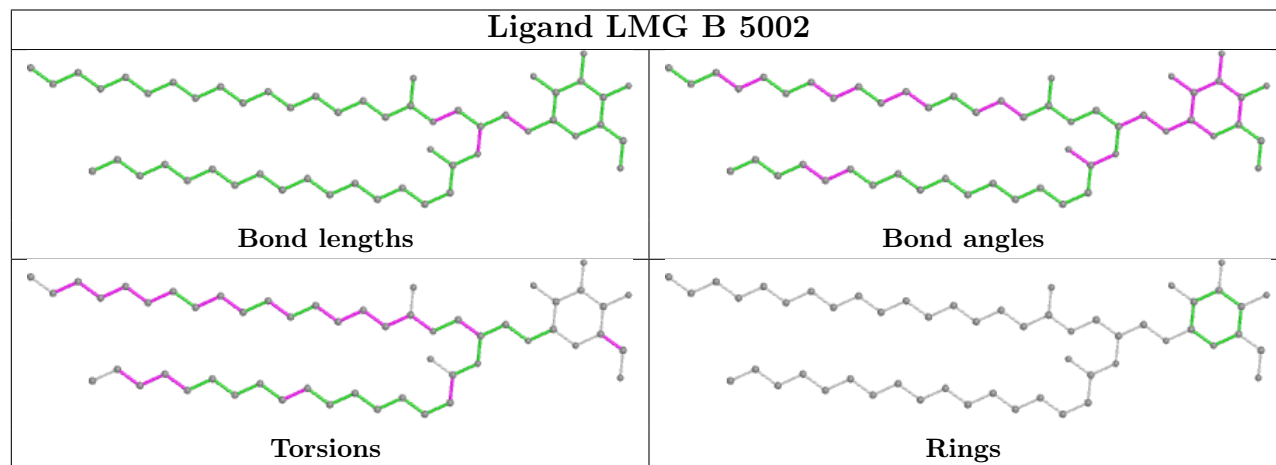
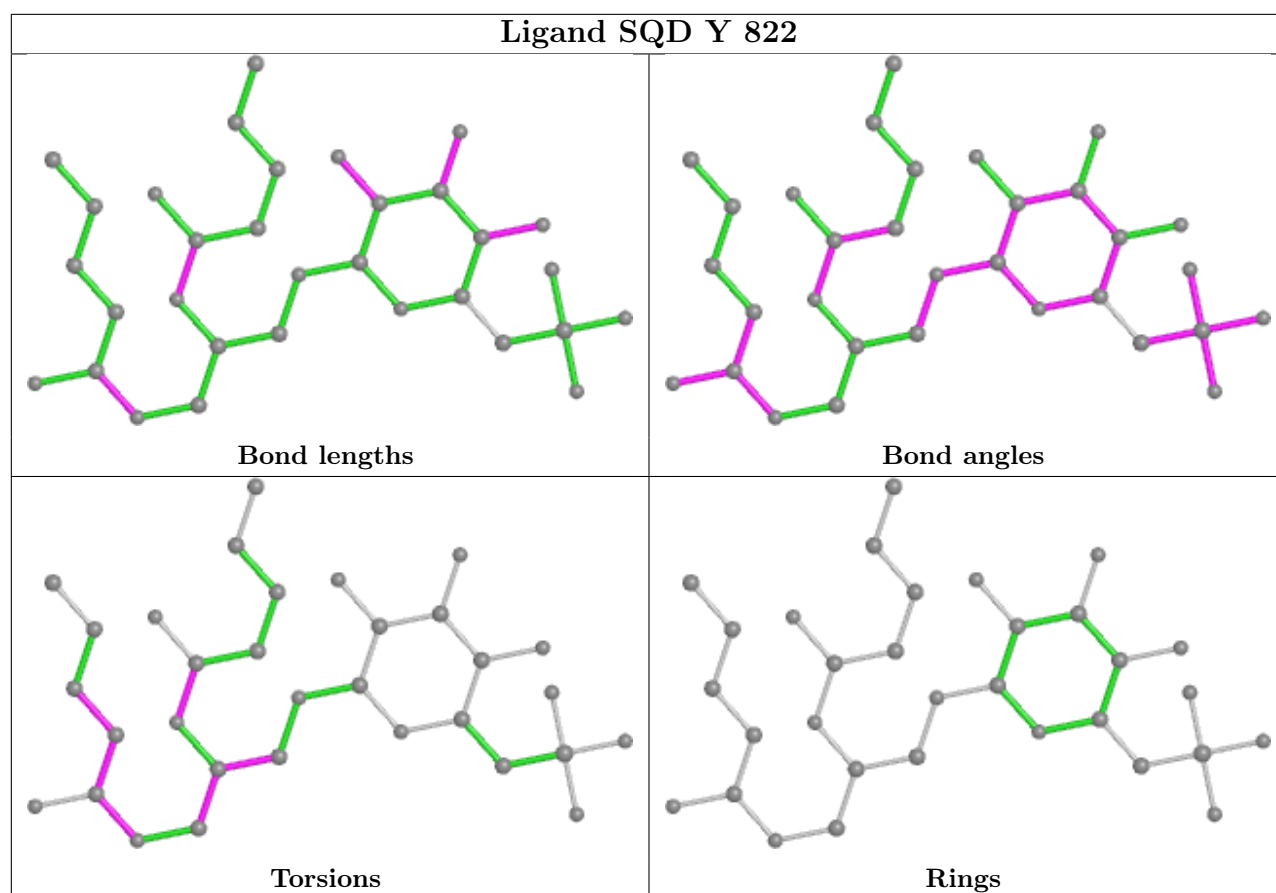


Ligand CLA G 1121

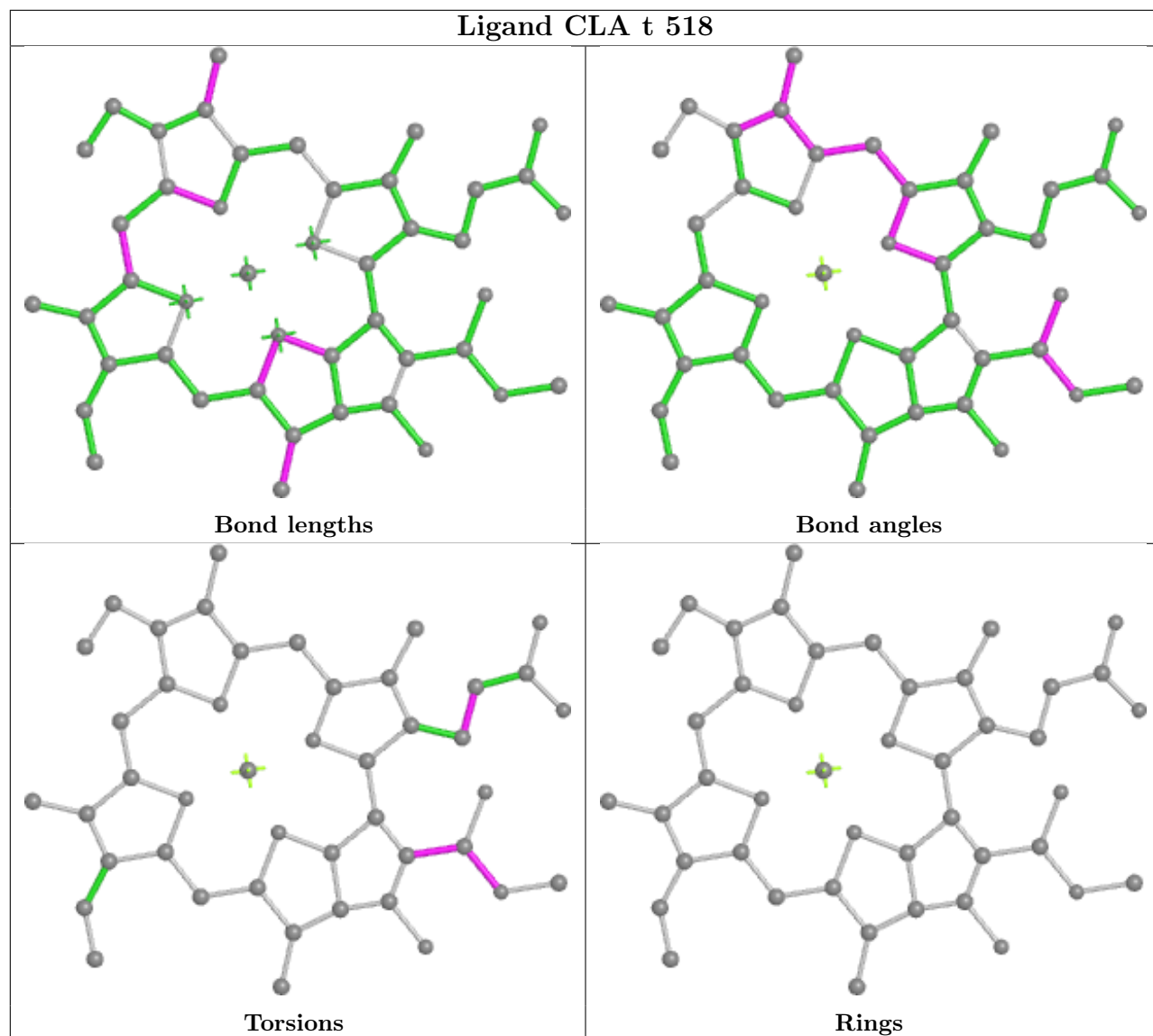


Ligand CLA A 1106

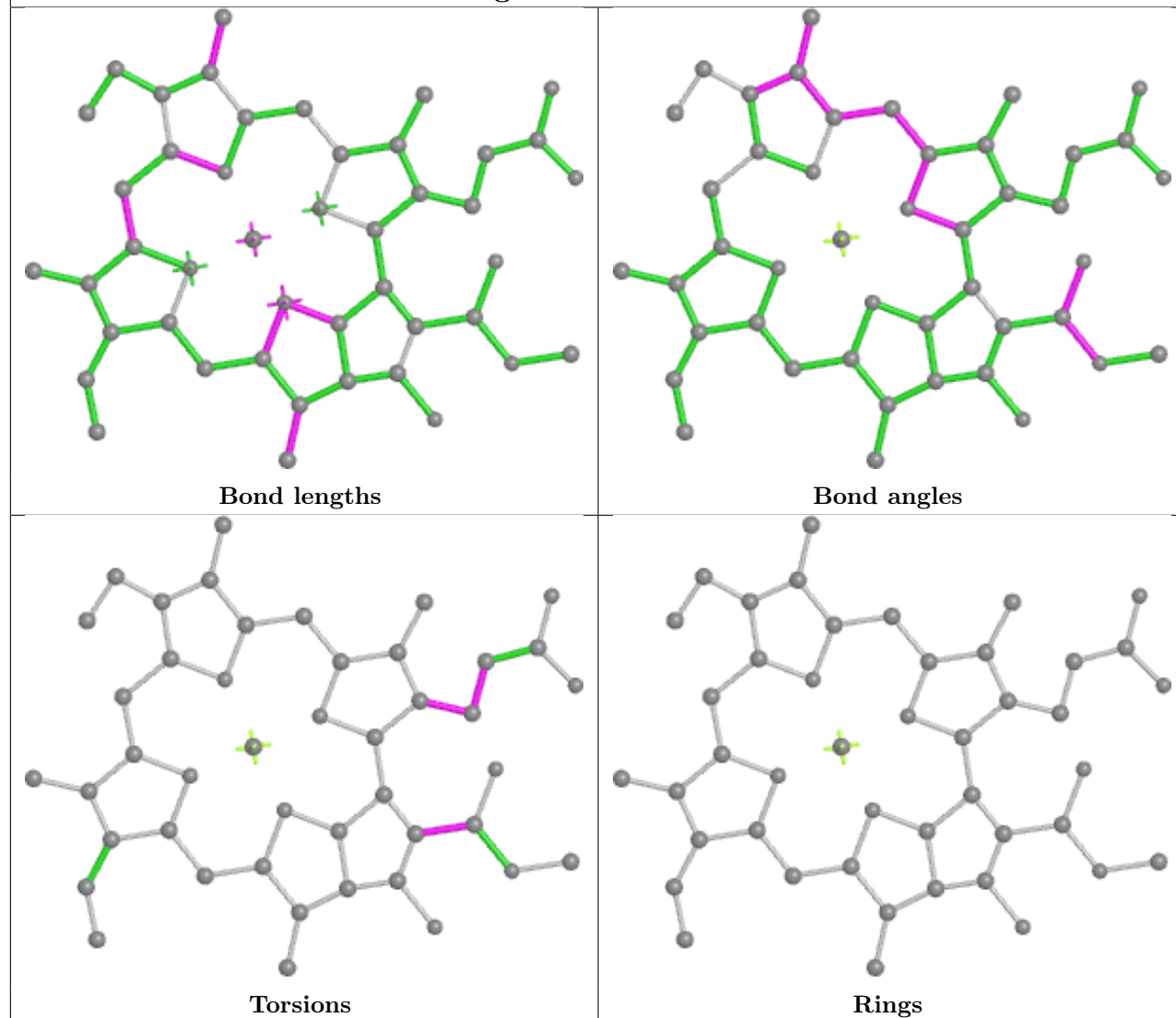




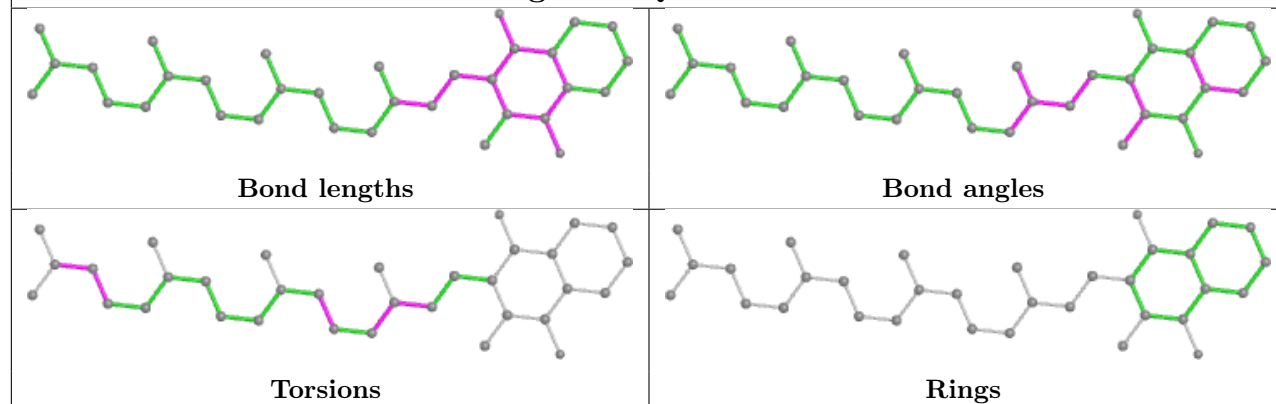
Ligand CLA t 518

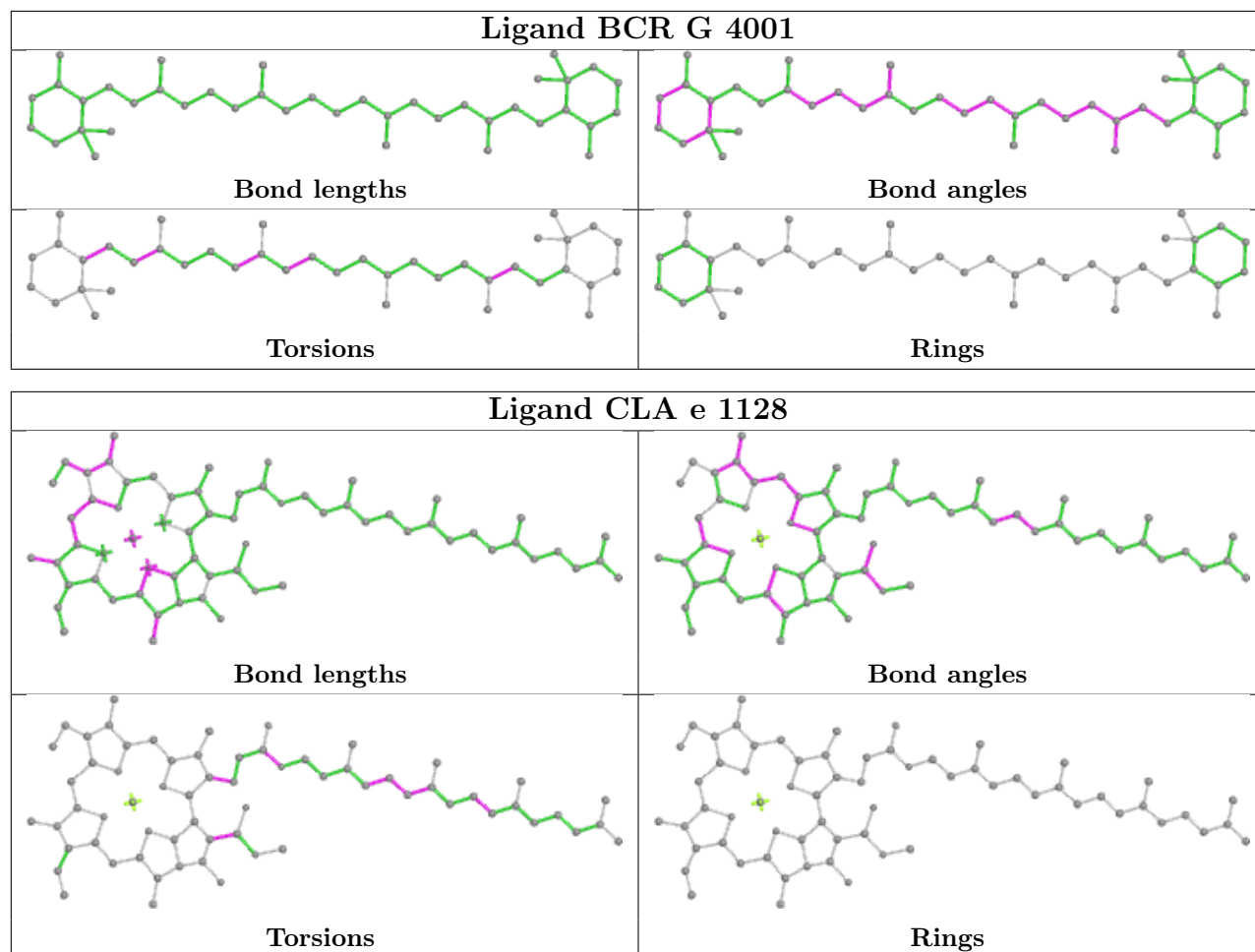


Ligand CLA 5 505

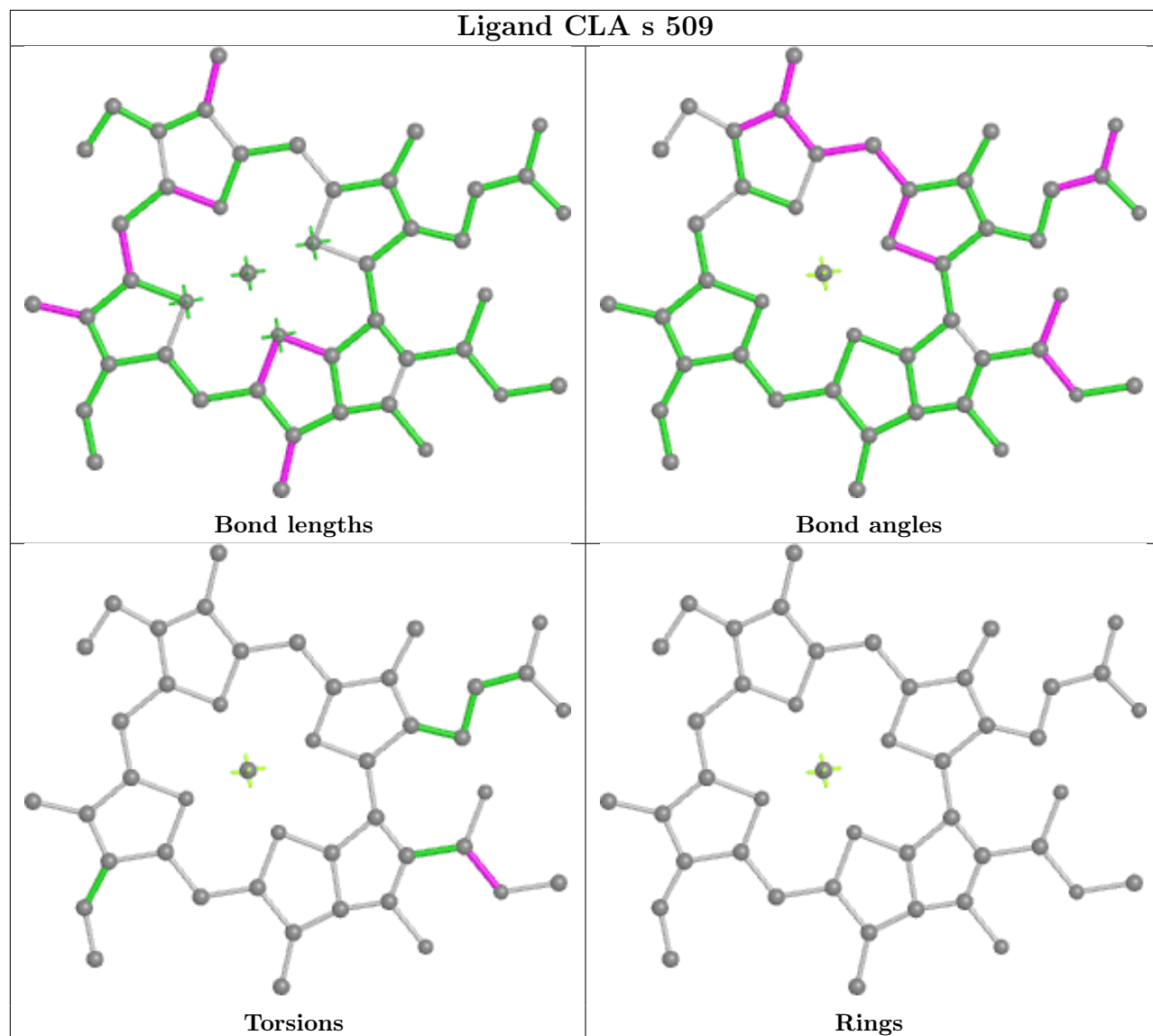


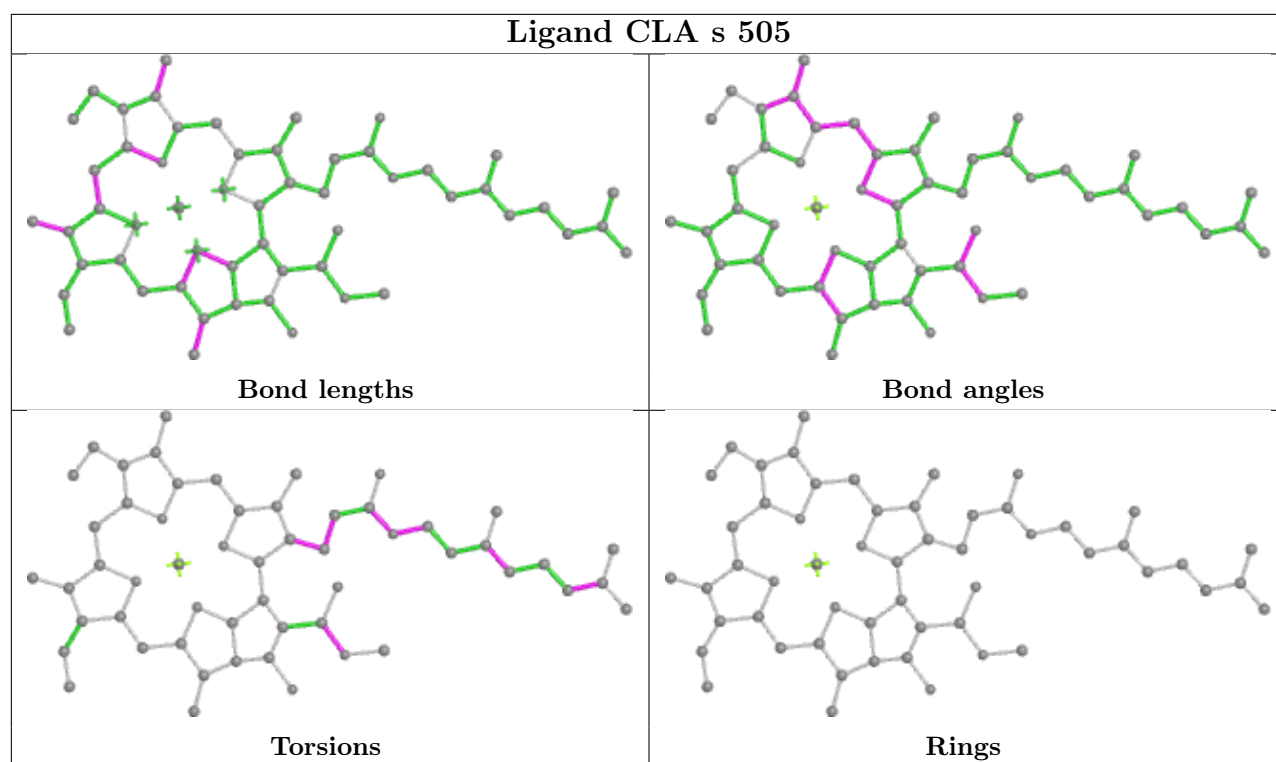
Ligand PQN f 2002



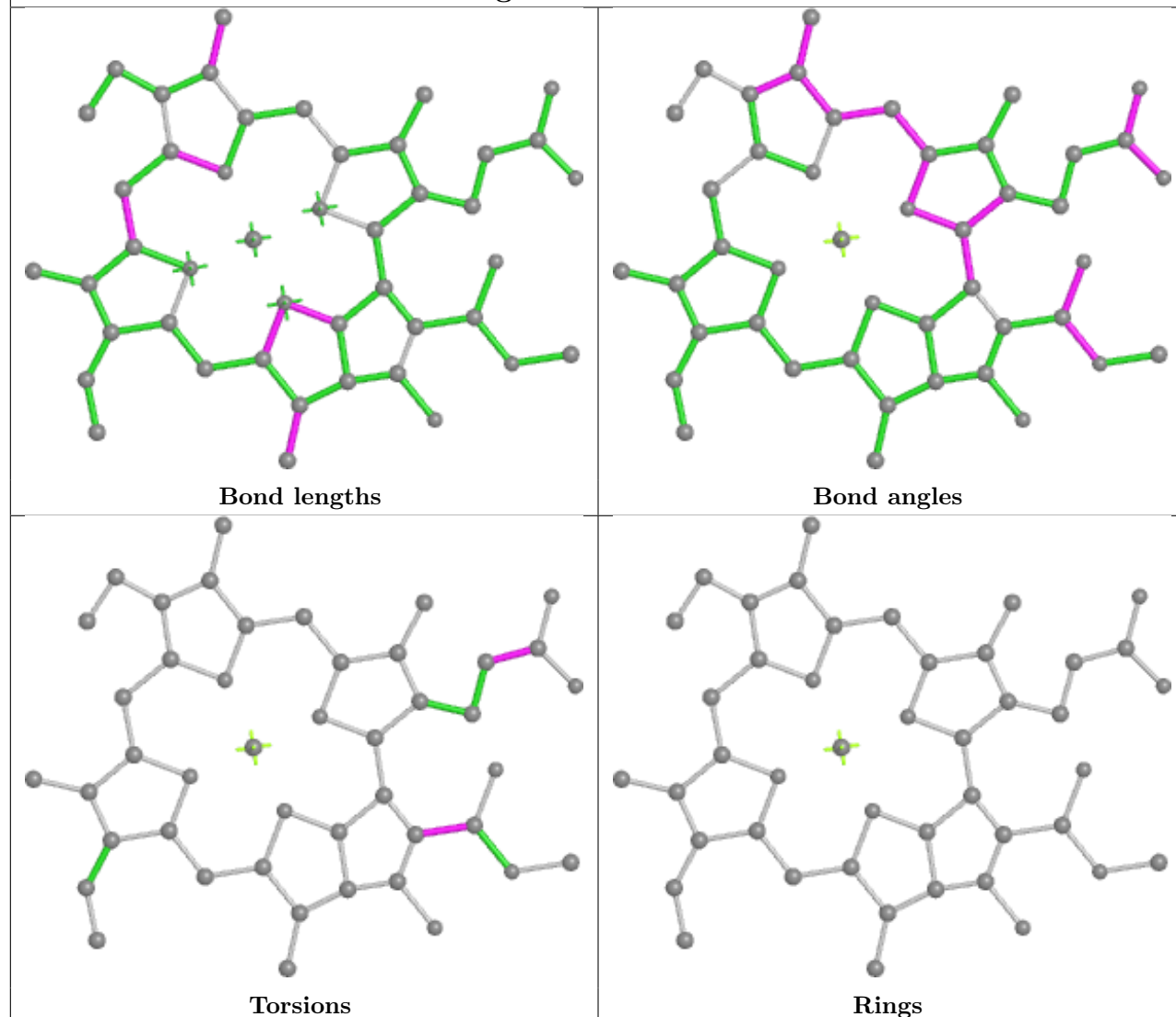


Ligand CLA s 509

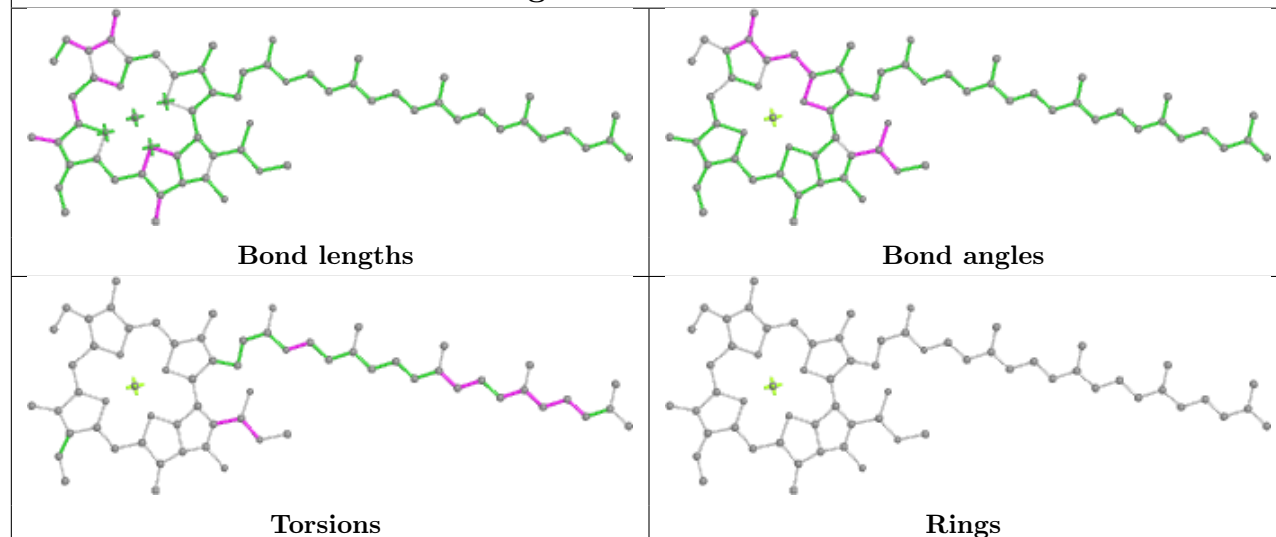




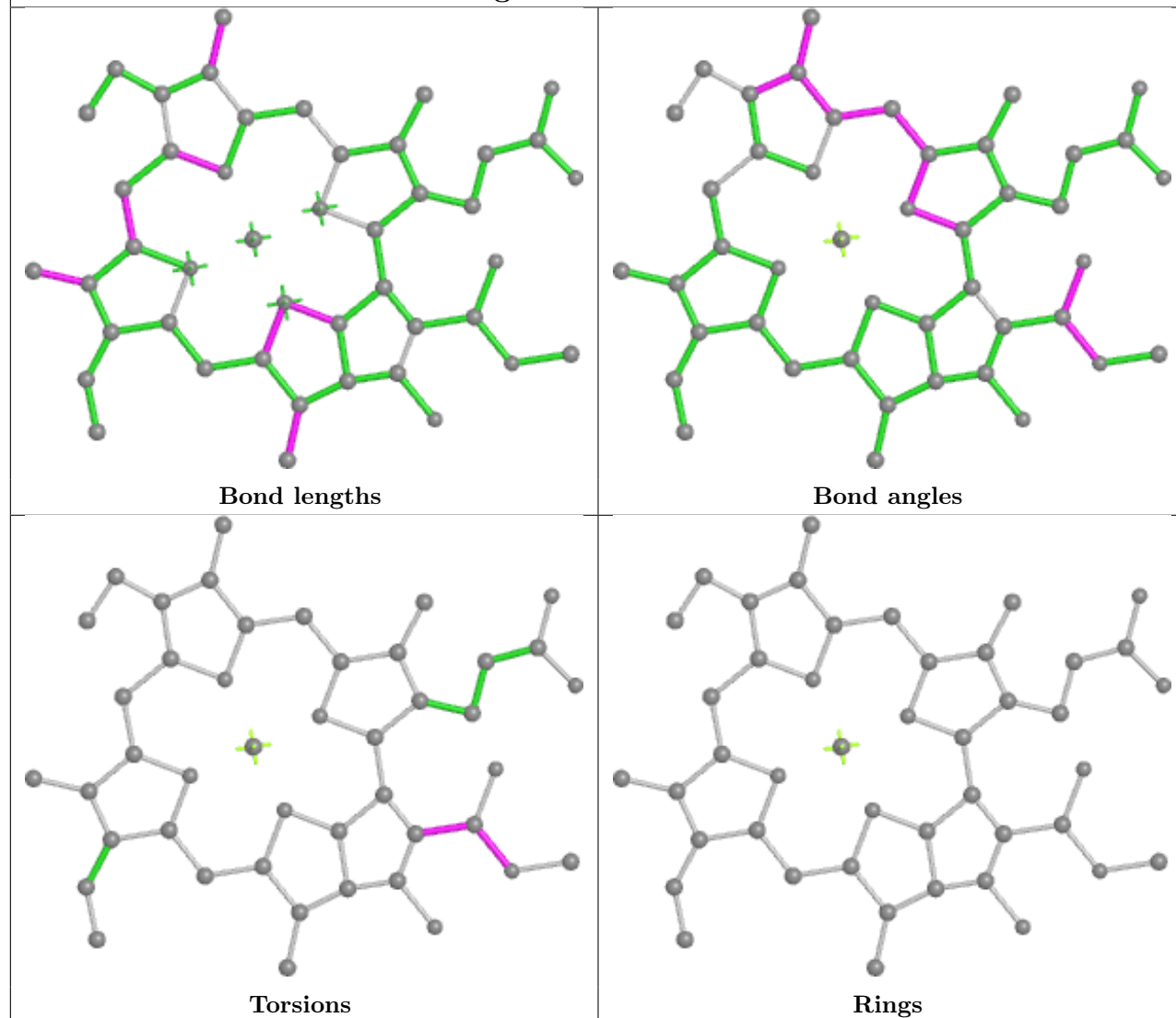
Ligand CLA s 507



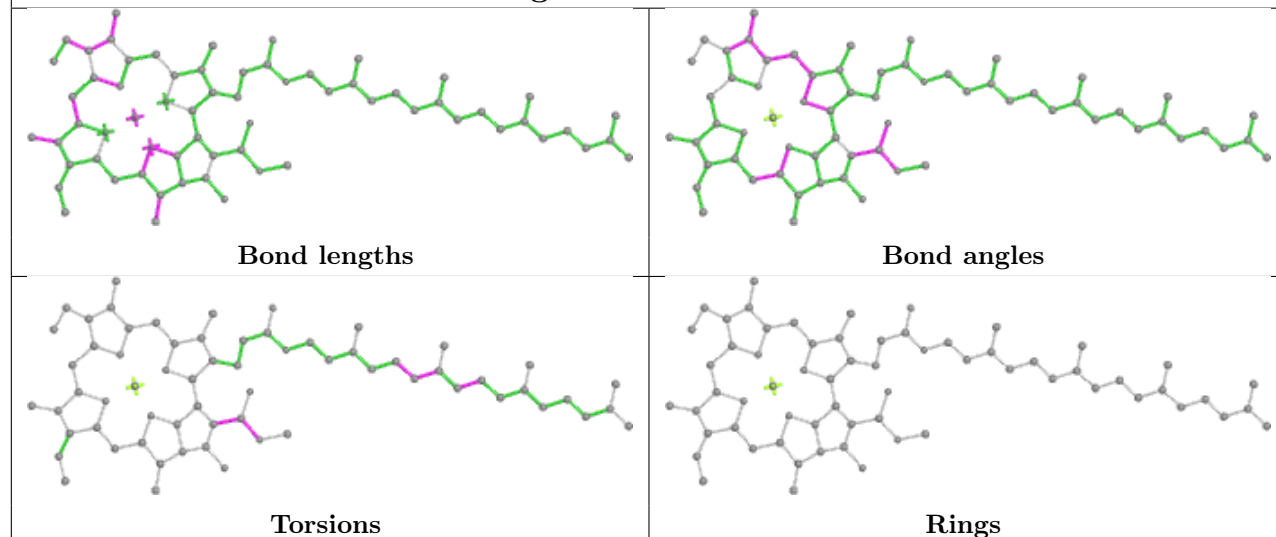
Ligand CLA e 1138



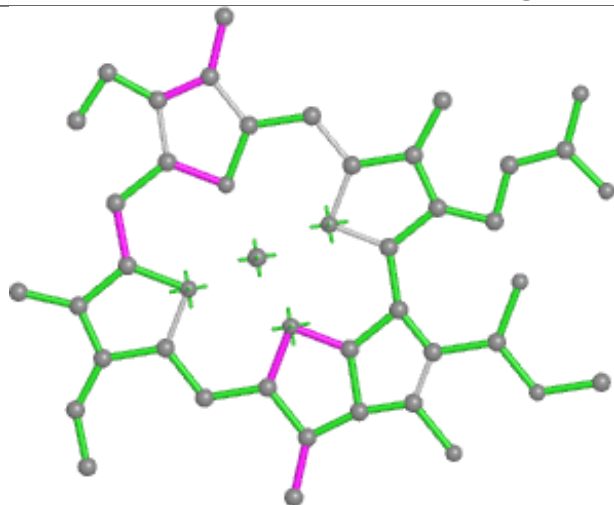
Ligand CLA 6 506



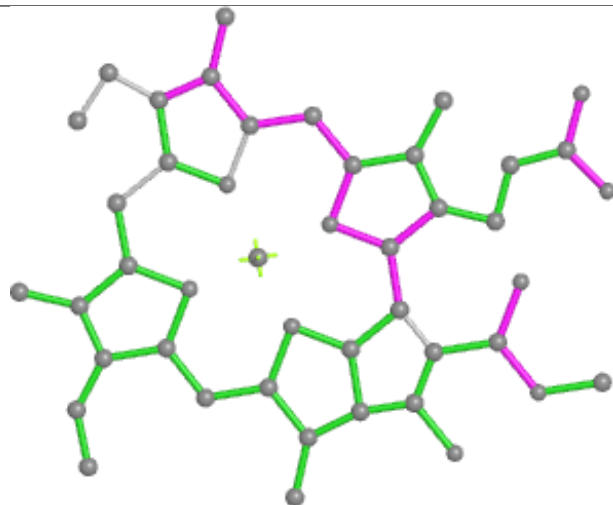
Ligand CLA f 1235



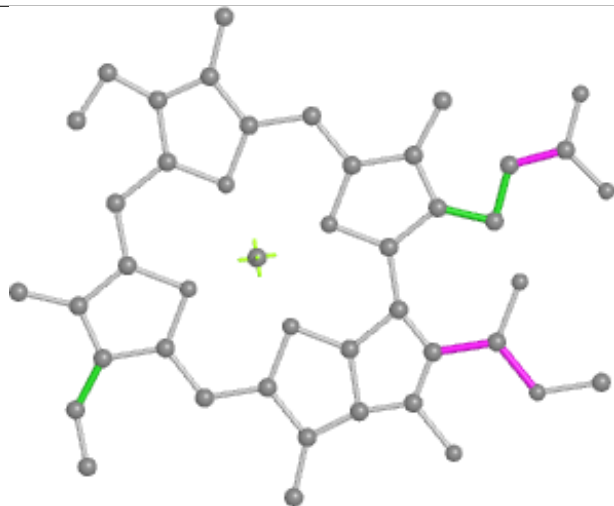
Ligand CLA v 507



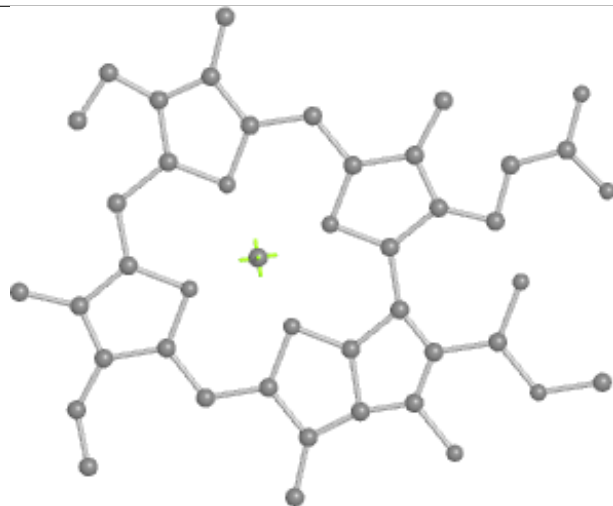
Bond lengths



Bond angles

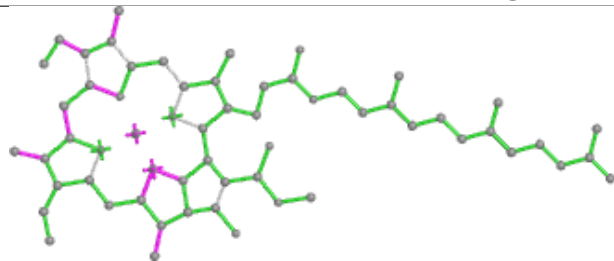


Torsions

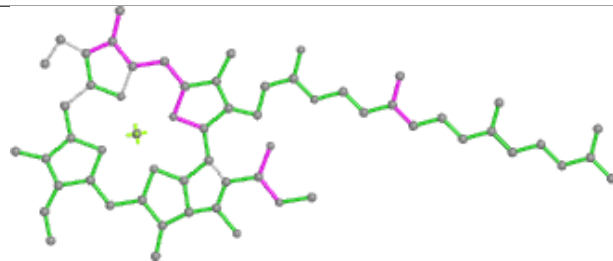


Rings

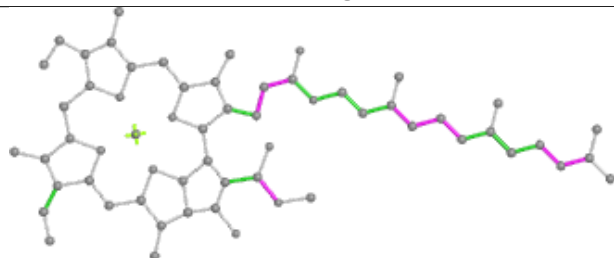
Ligand CLA G 1115



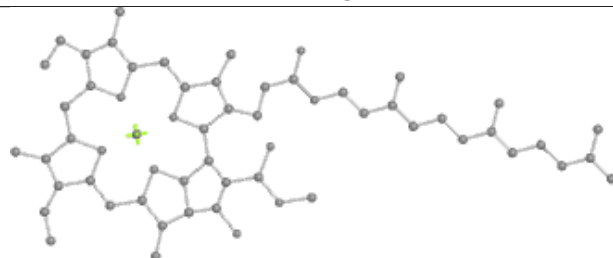
Bond lengths



Bond angles

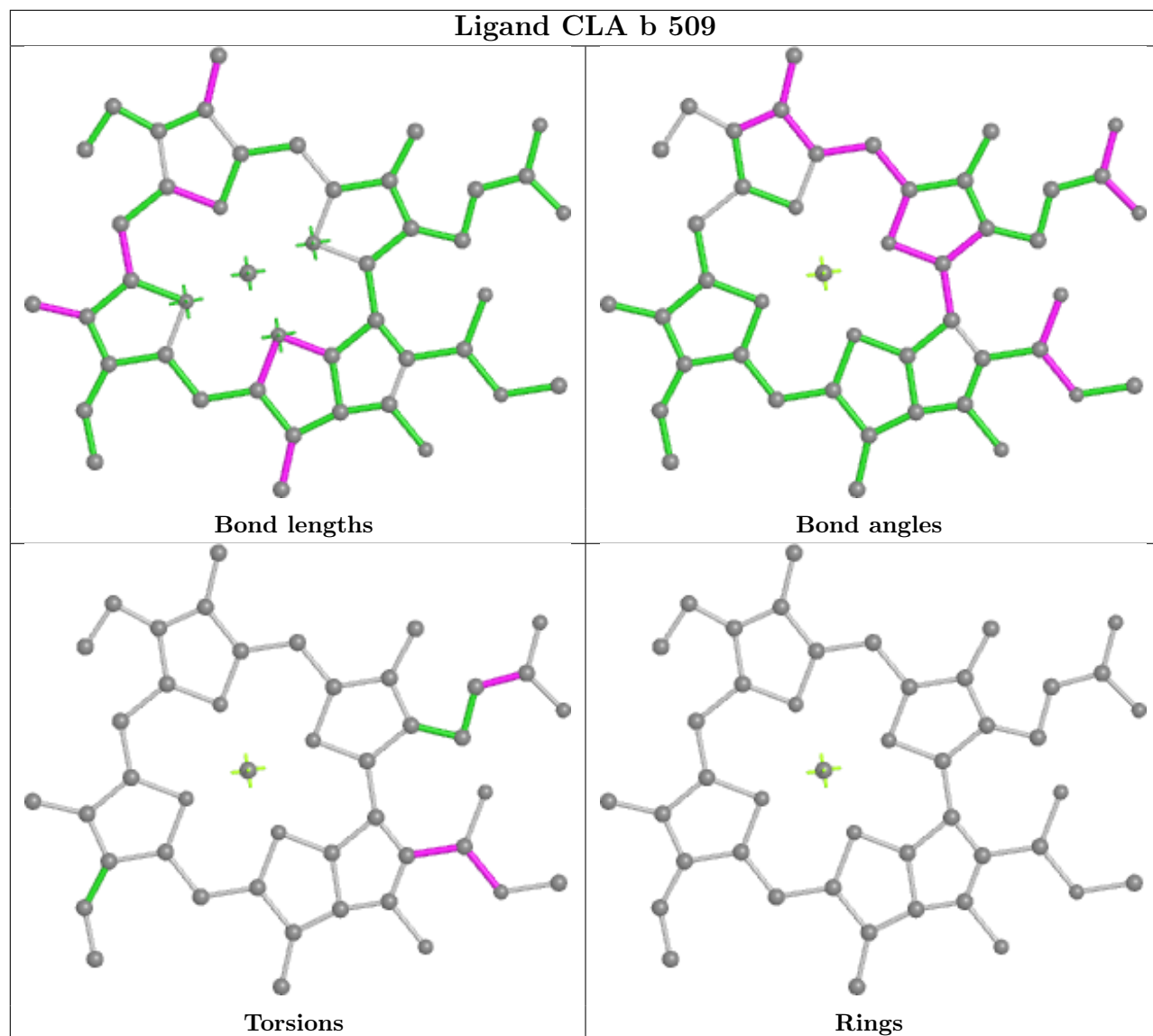


Torsions

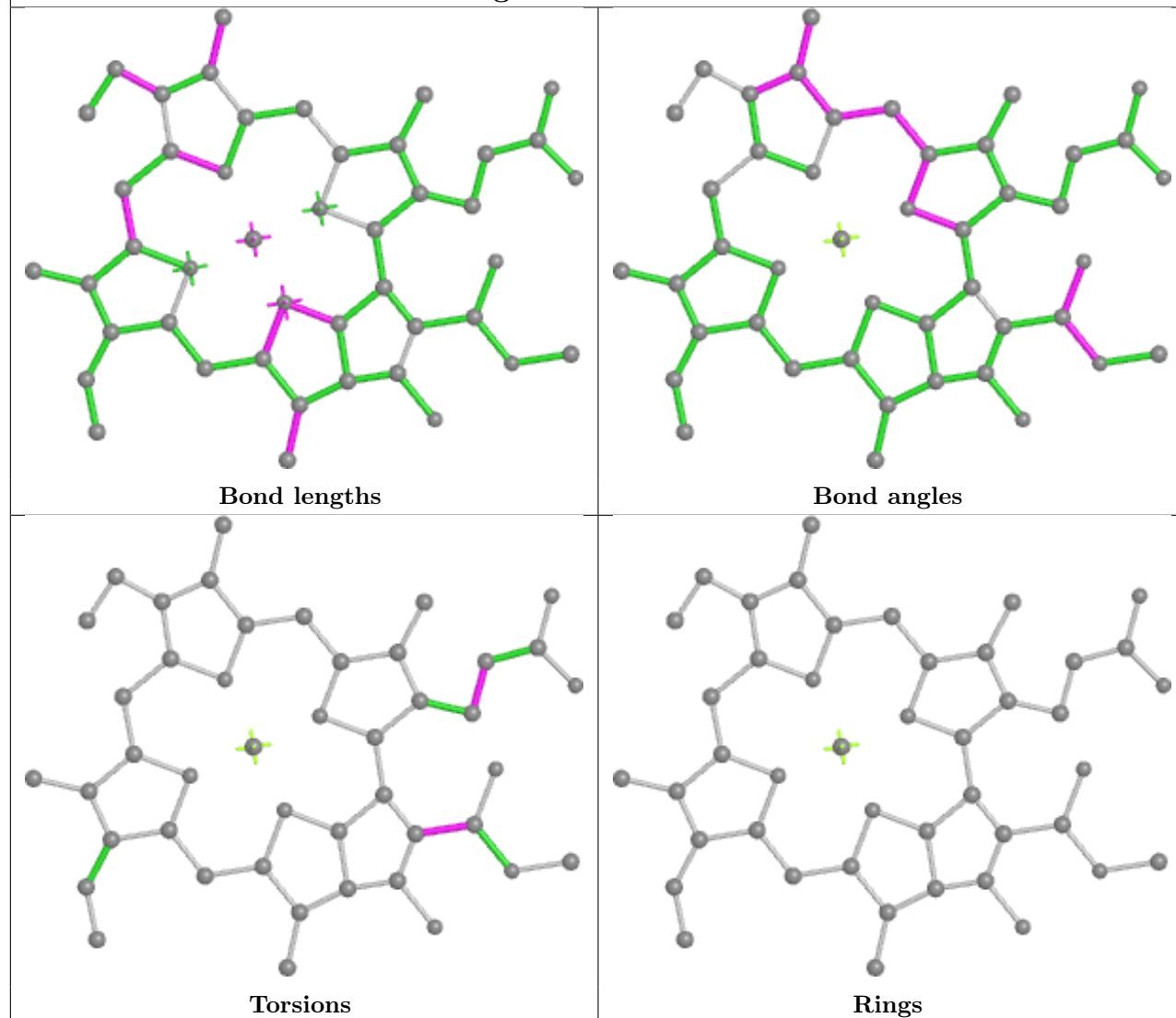


Rings

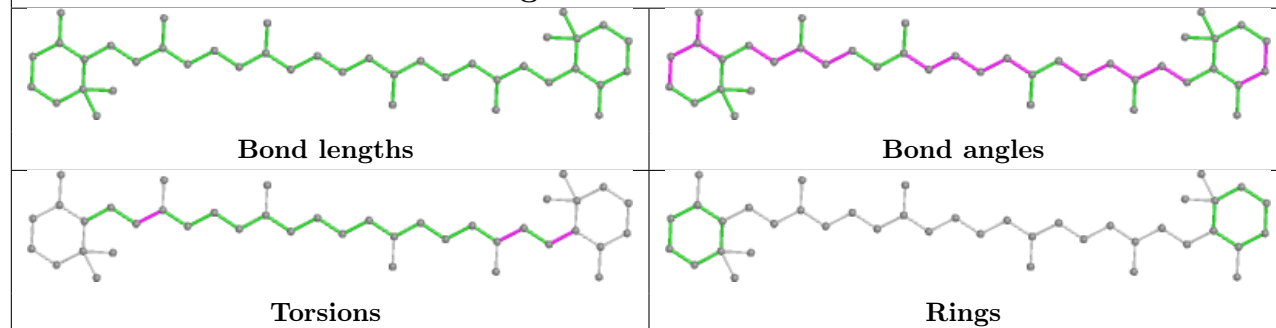
Ligand CLA b 509



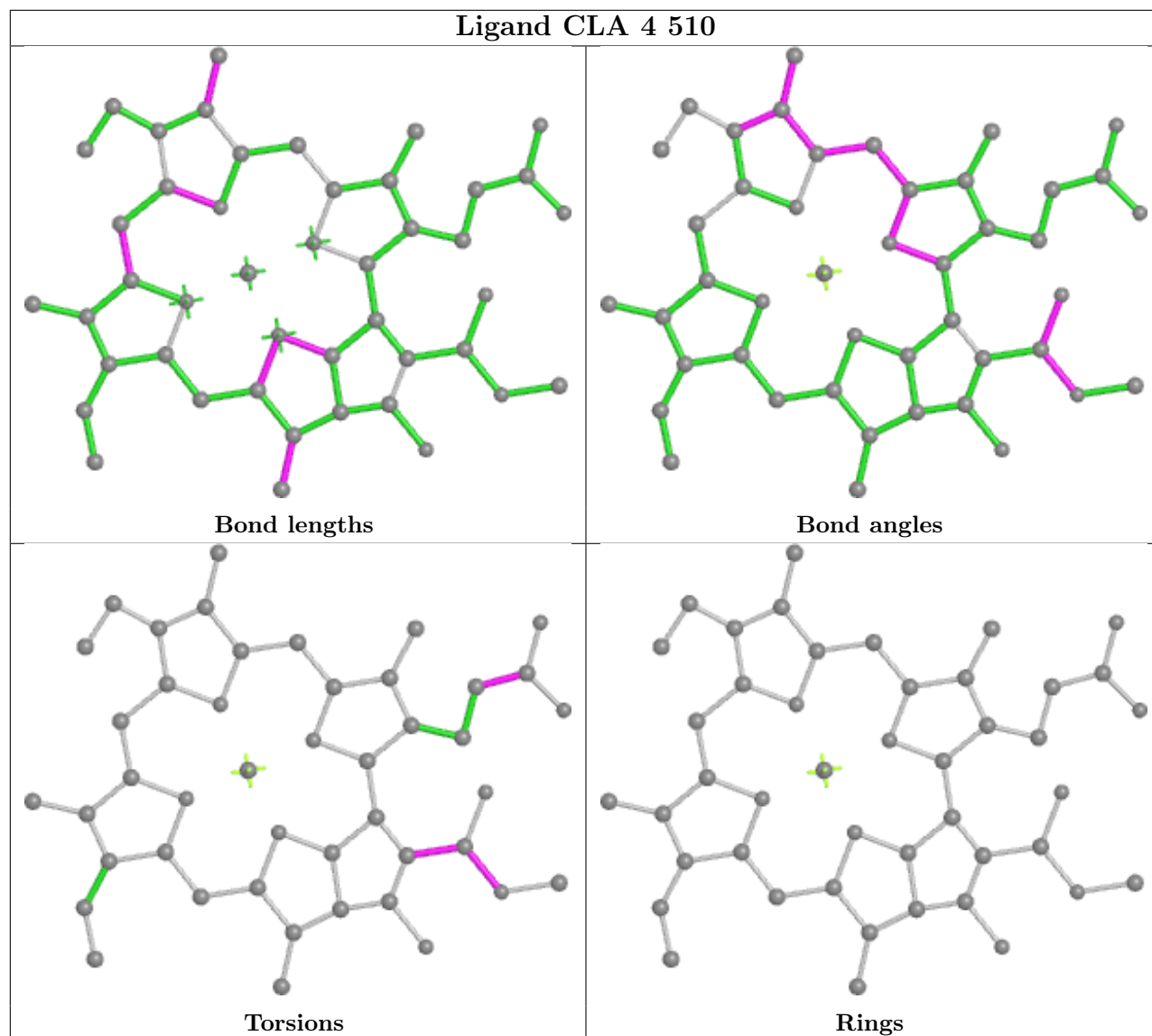
Ligand CLA b 505

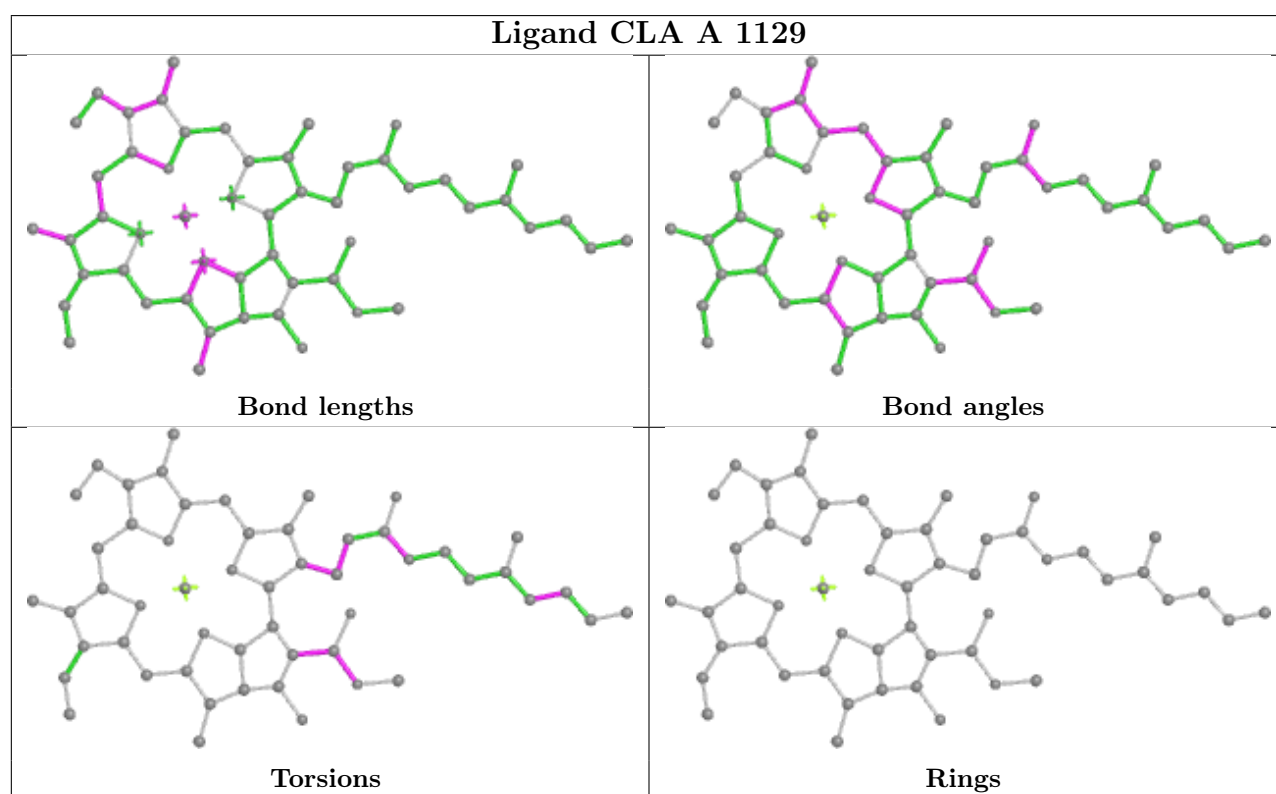
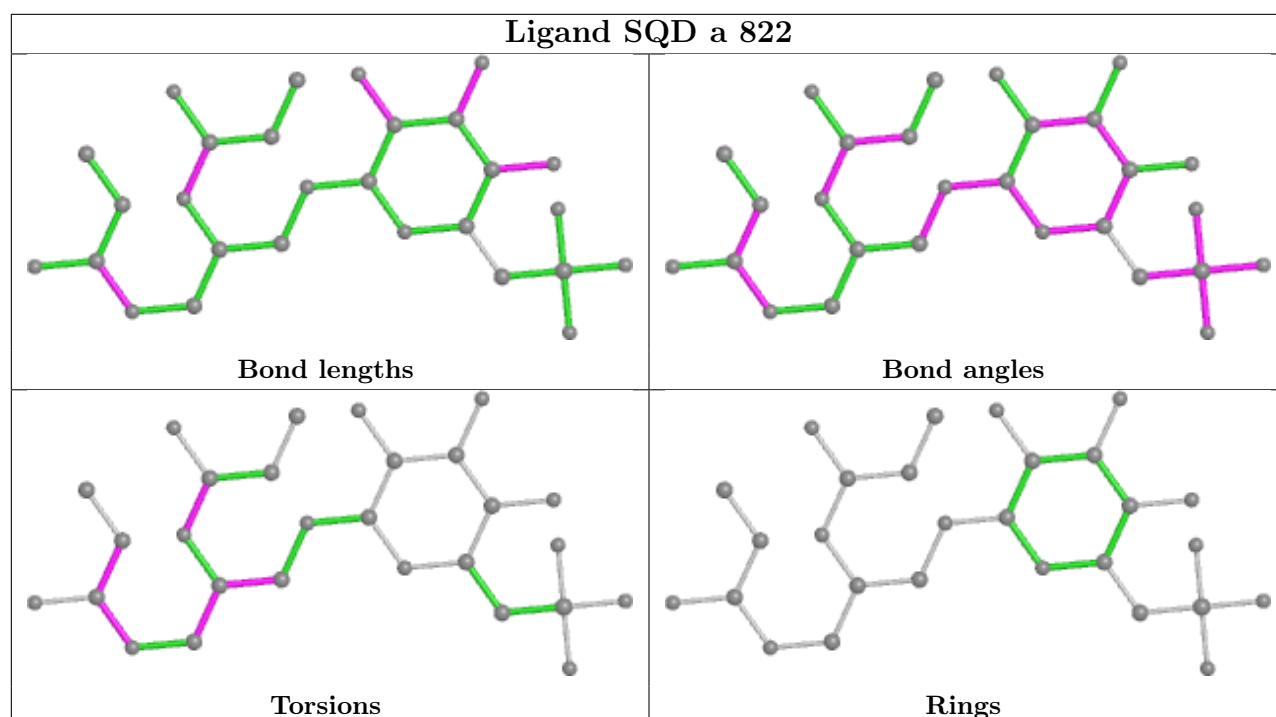


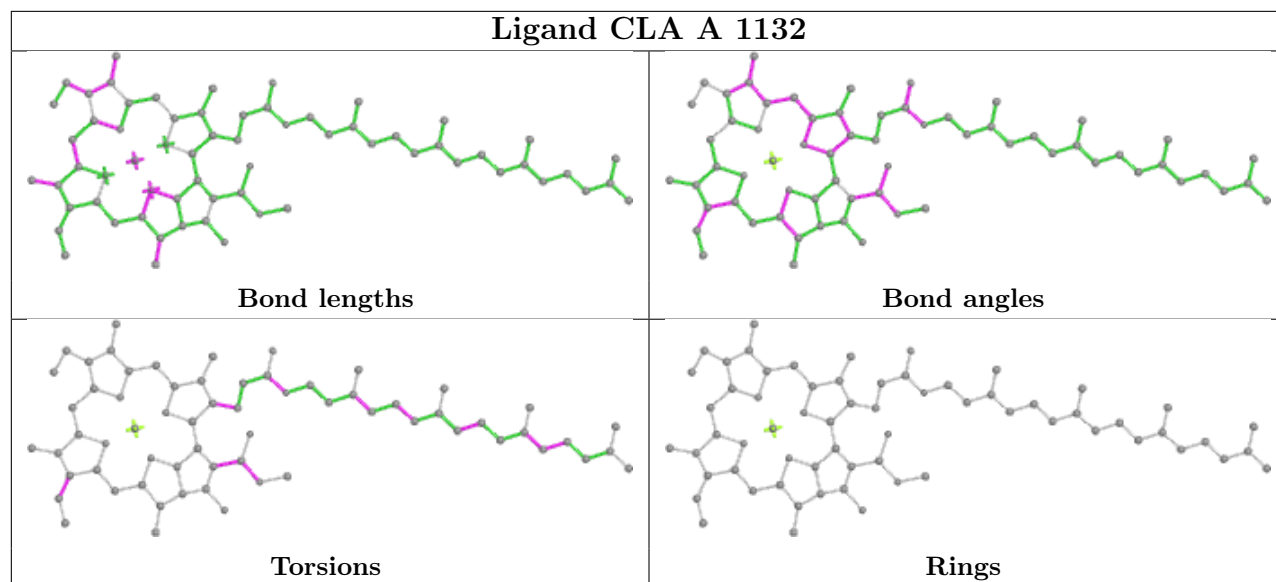
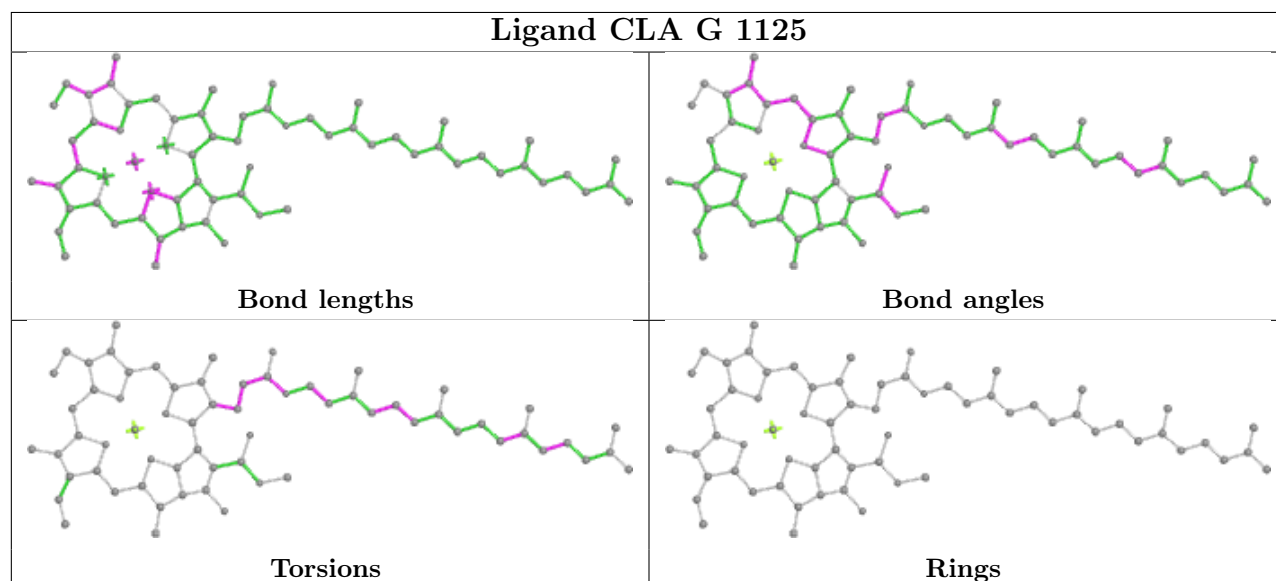
Ligand BCR H 4005



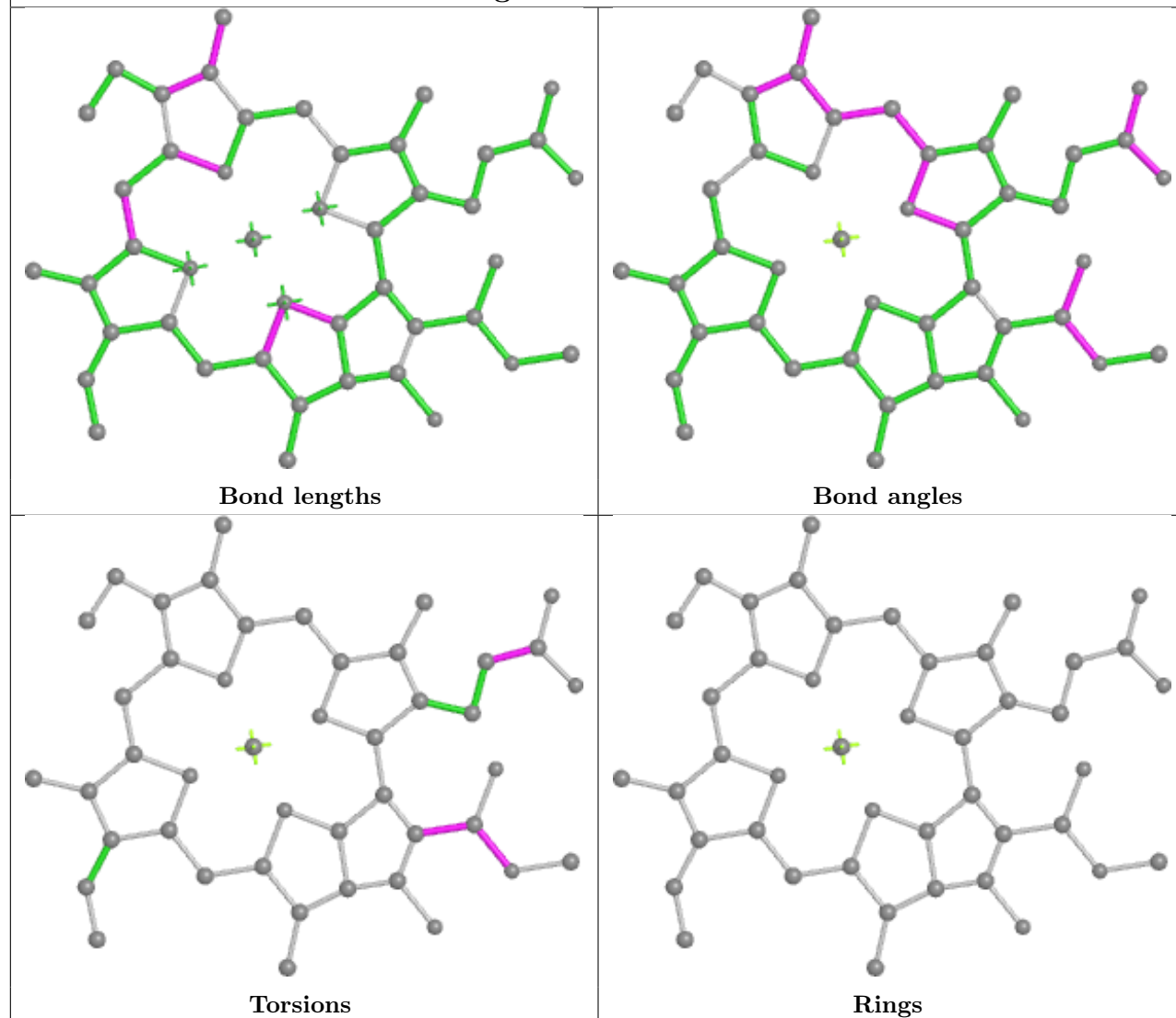
Ligand CLA 4 510



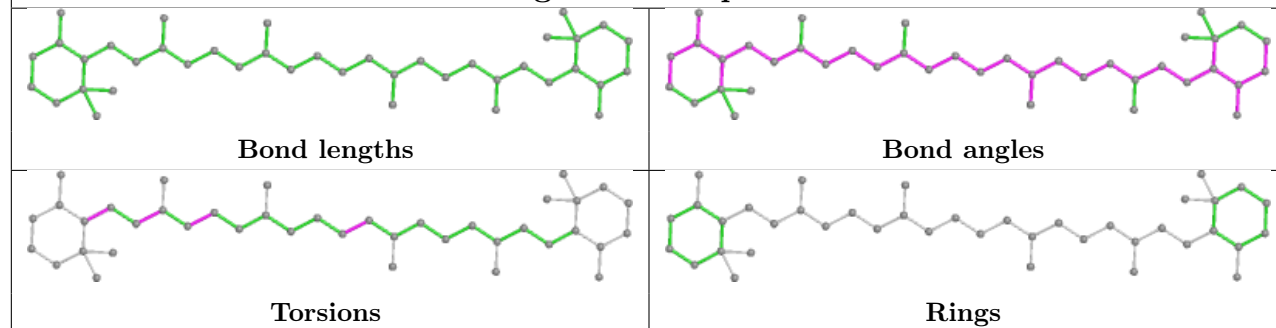


Ligand CLA A 1132**Ligand CLA G 1125**

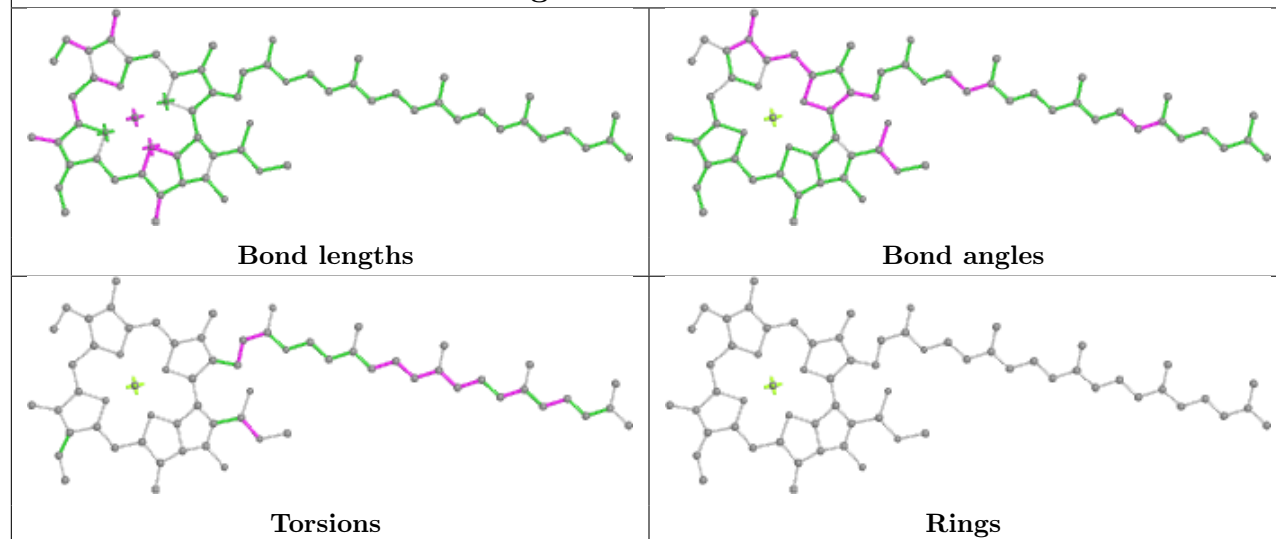
Ligand CLA 5 519



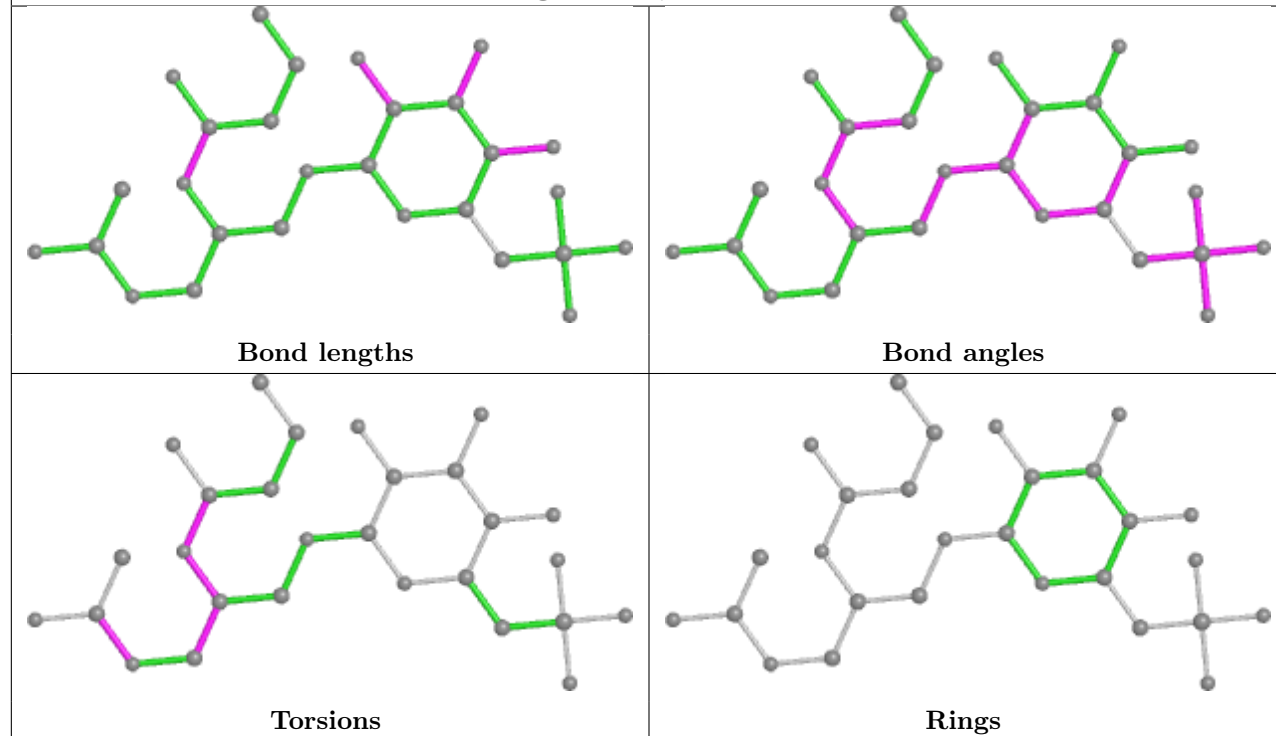
Ligand BCR q 522



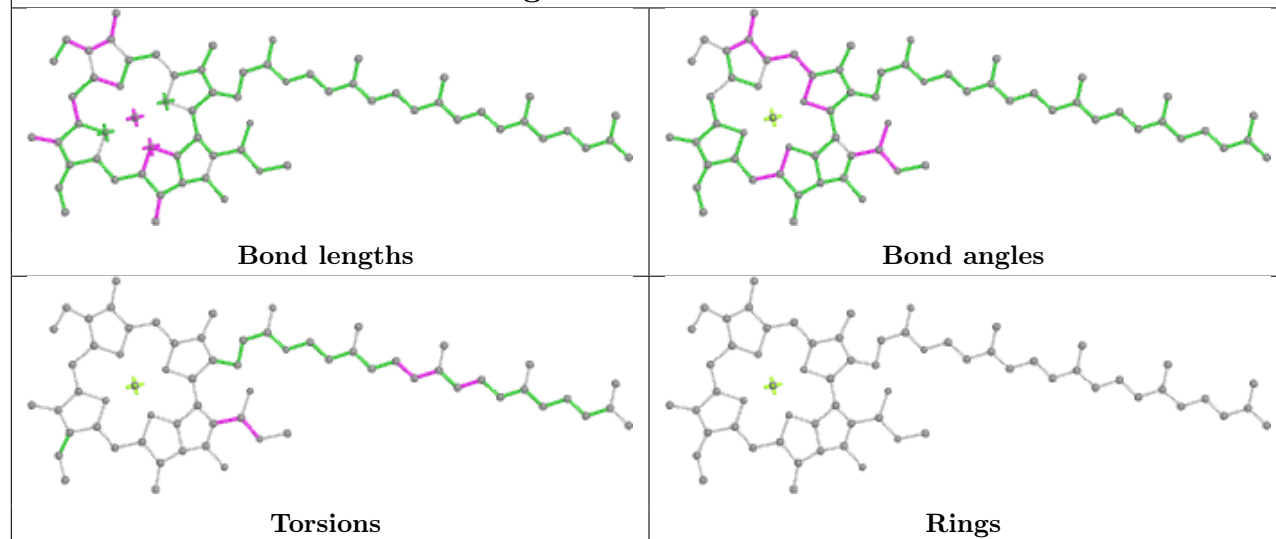
Ligand CLA f 1203



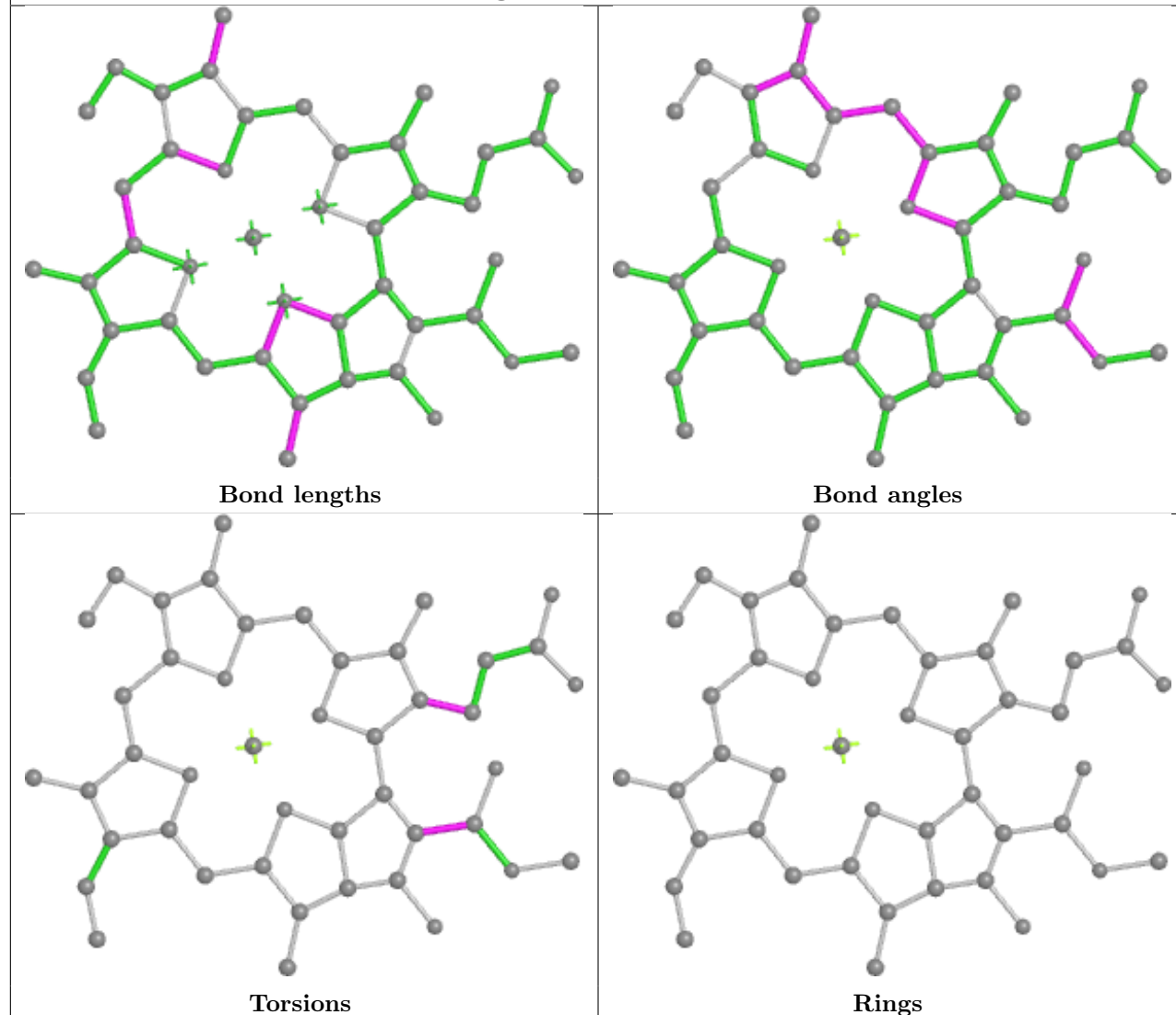
Ligand SQD Z 822



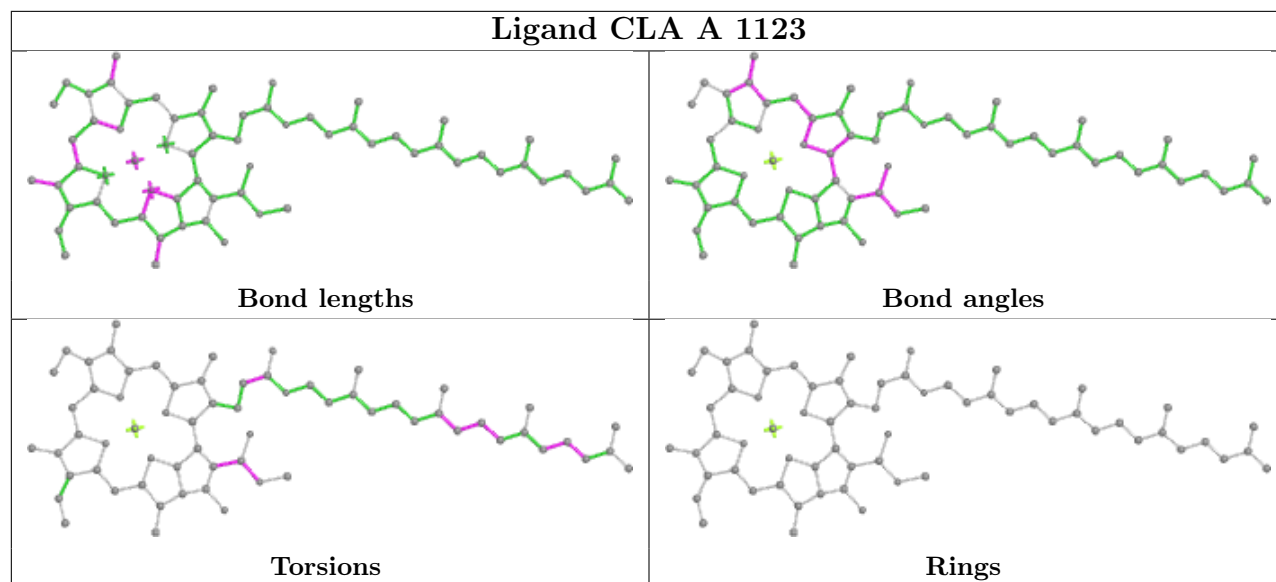
Ligand CLA B 1235



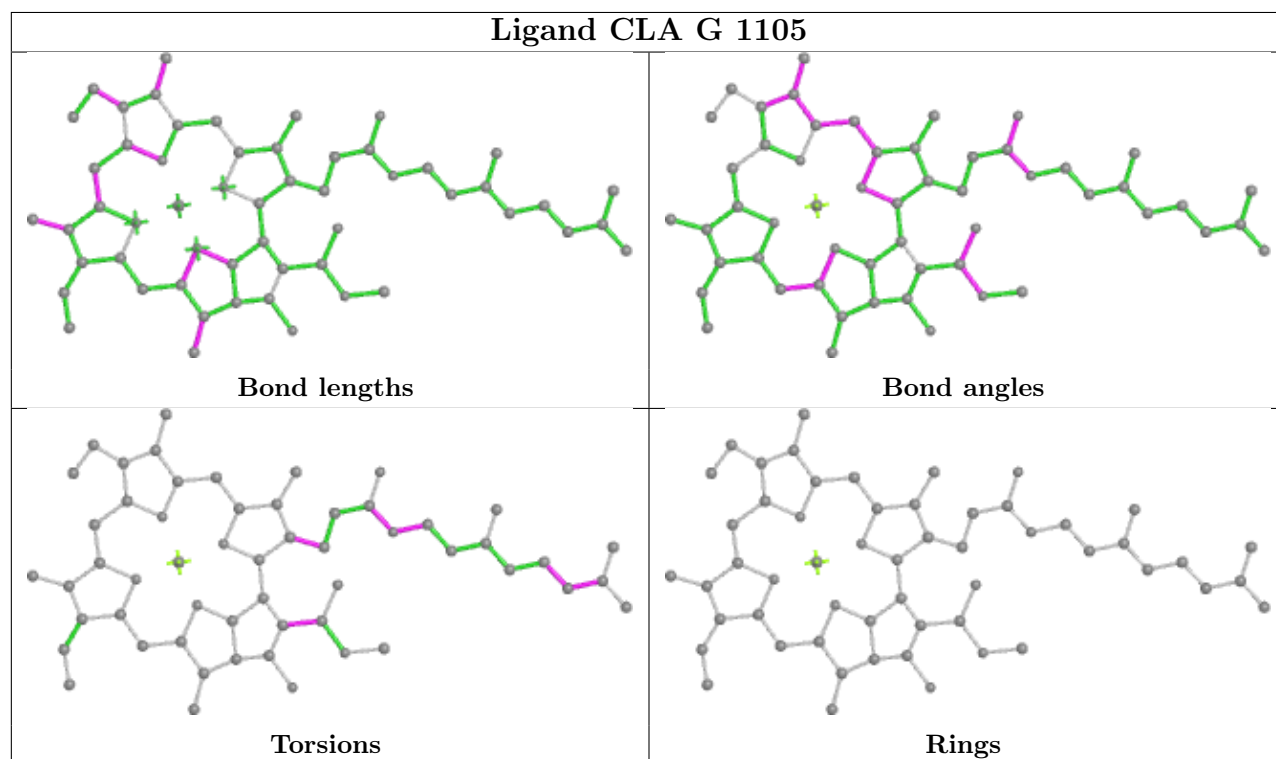
Ligand CLA u 516

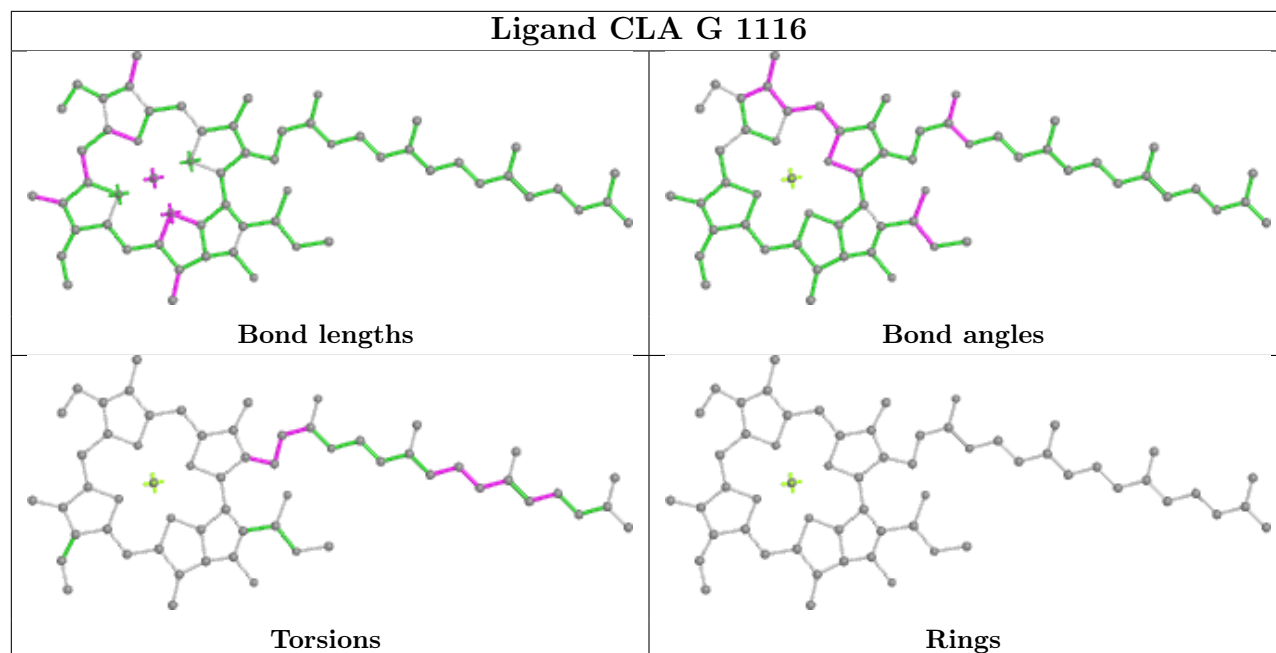
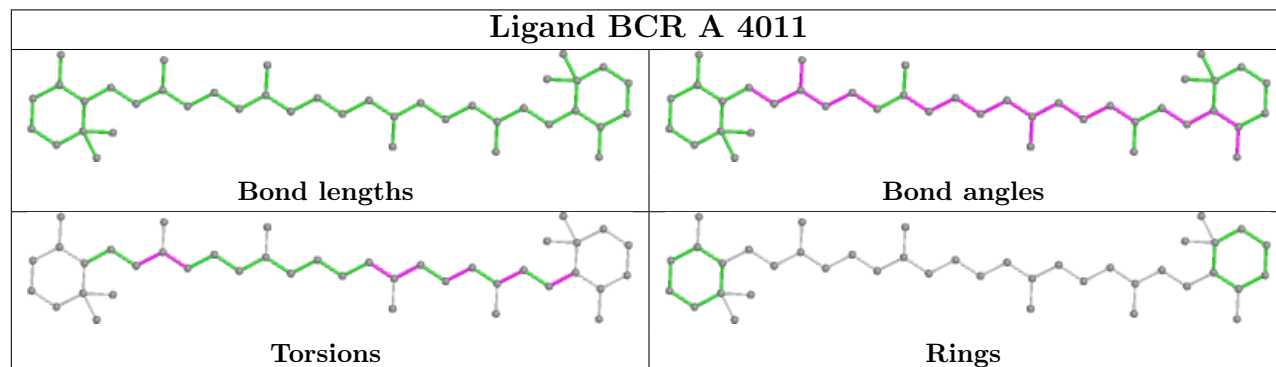


Ligand CLA A 1123

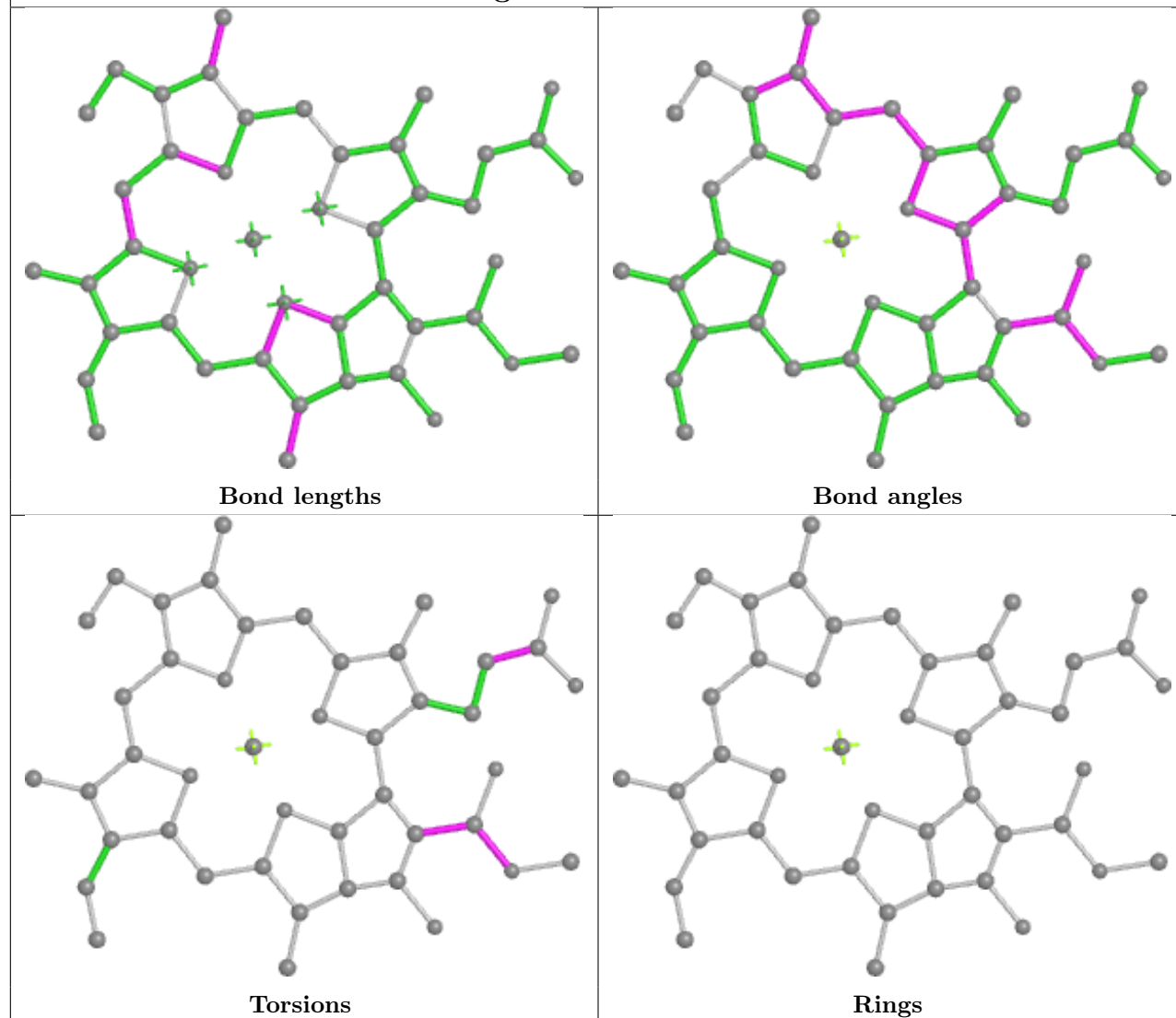


Ligand CLA G 1105

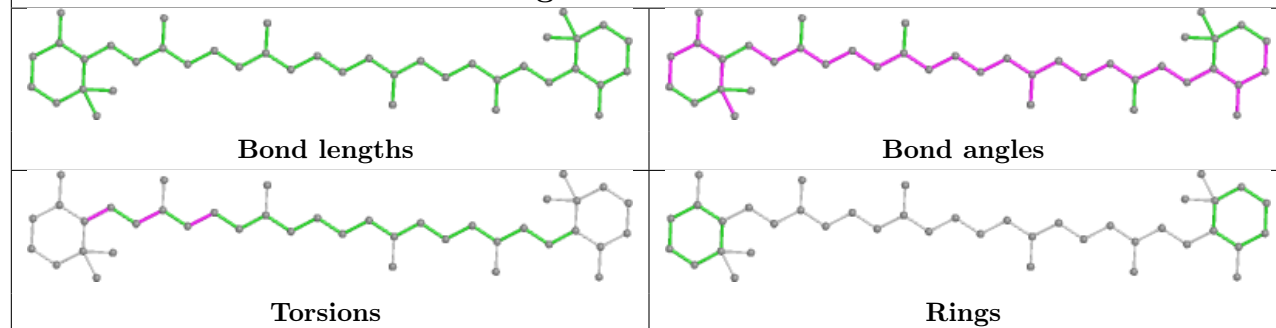


Ligand CLA G 1116**Ligand BCR A 4011**

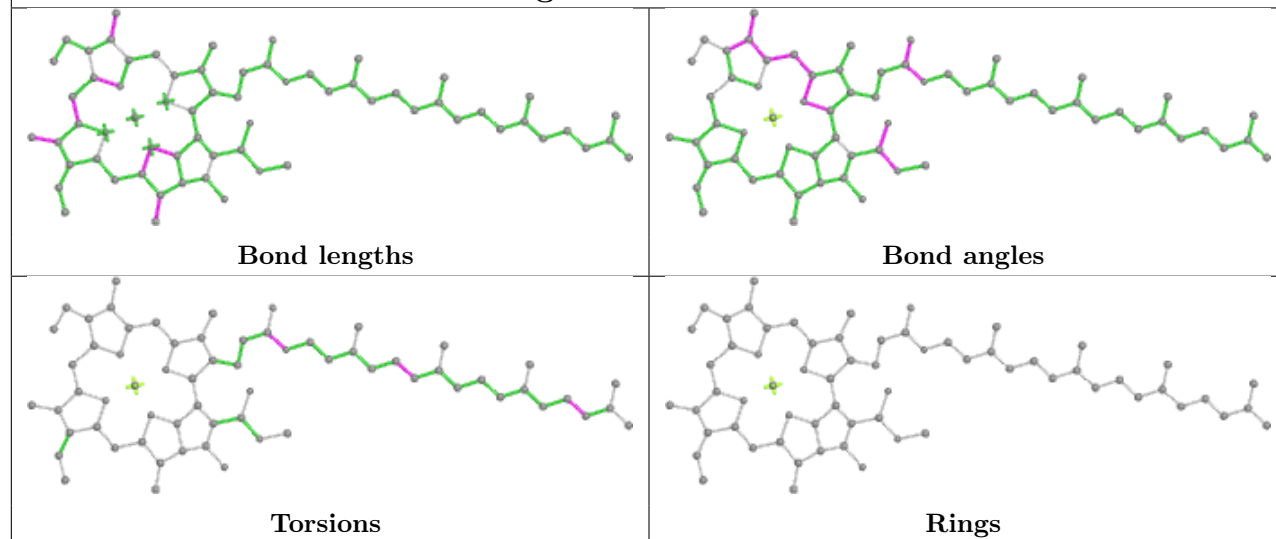
Ligand CLA 4 507



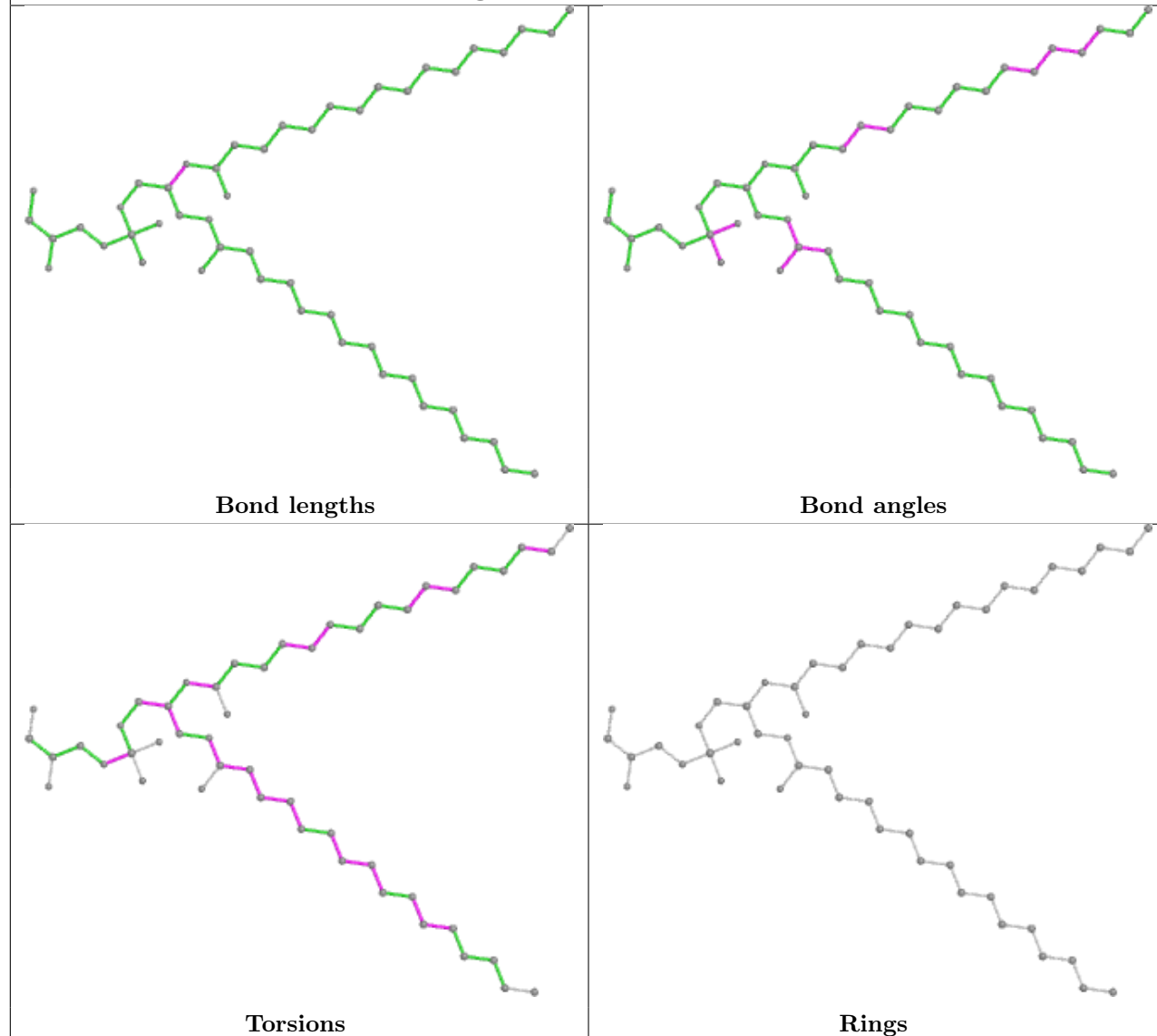
Ligand BCR s 522



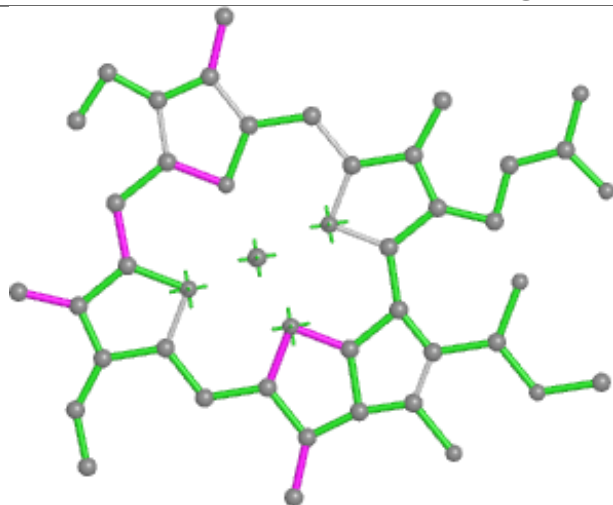
Ligand CLA 2 509



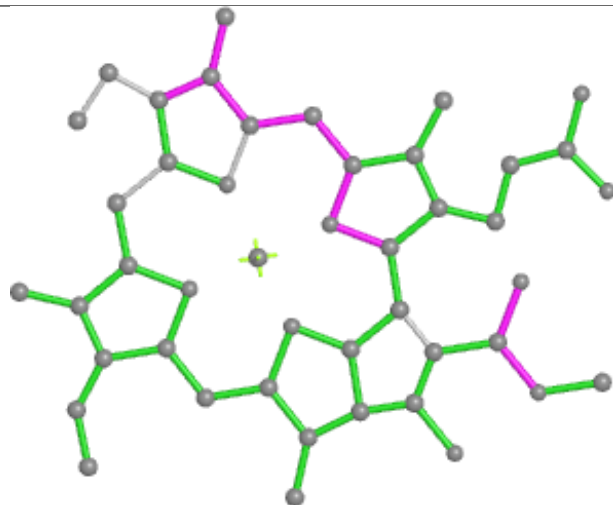
Ligand LHG A 5001



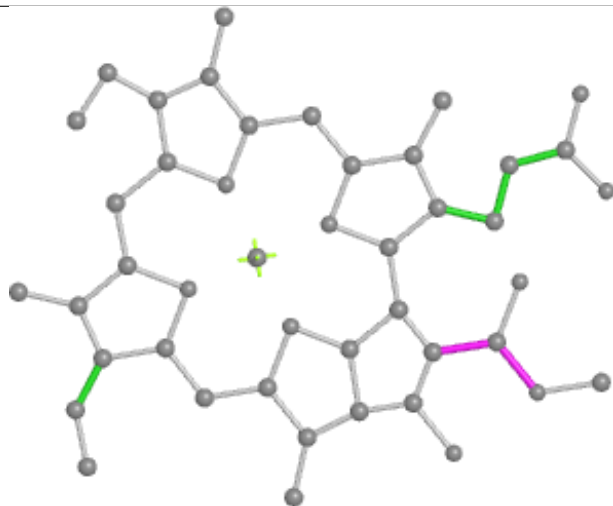
Ligand CLA d 506



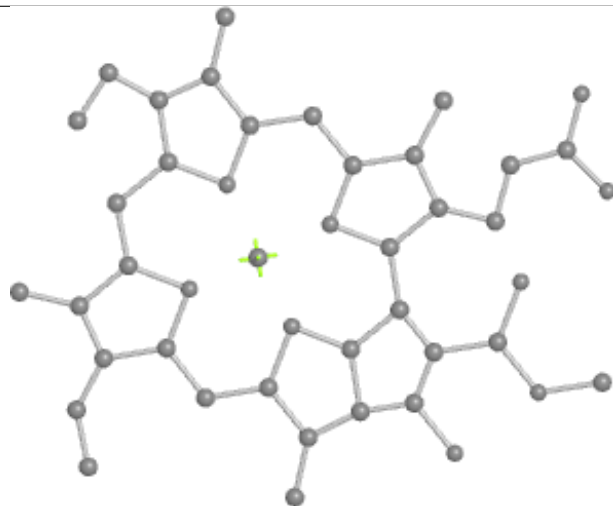
Bond lengths



Bond angles

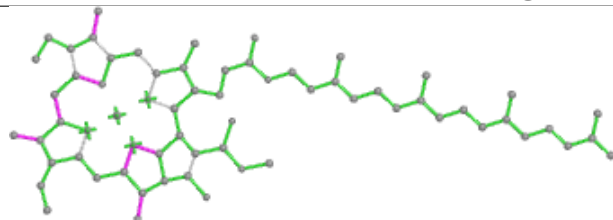


Torsions

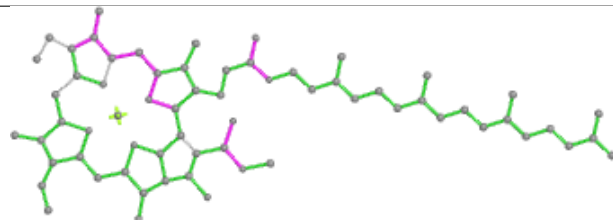


Rings

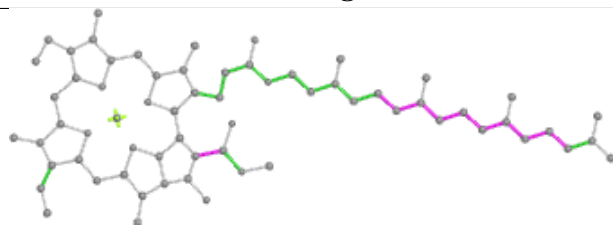
Ligand CLA c 509



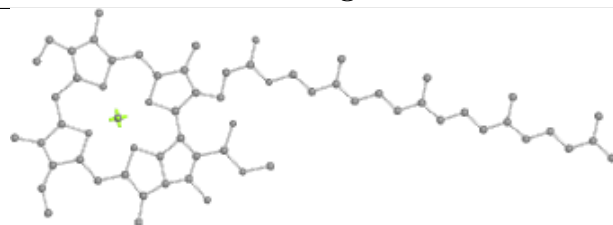
Bond lengths



Bond angles

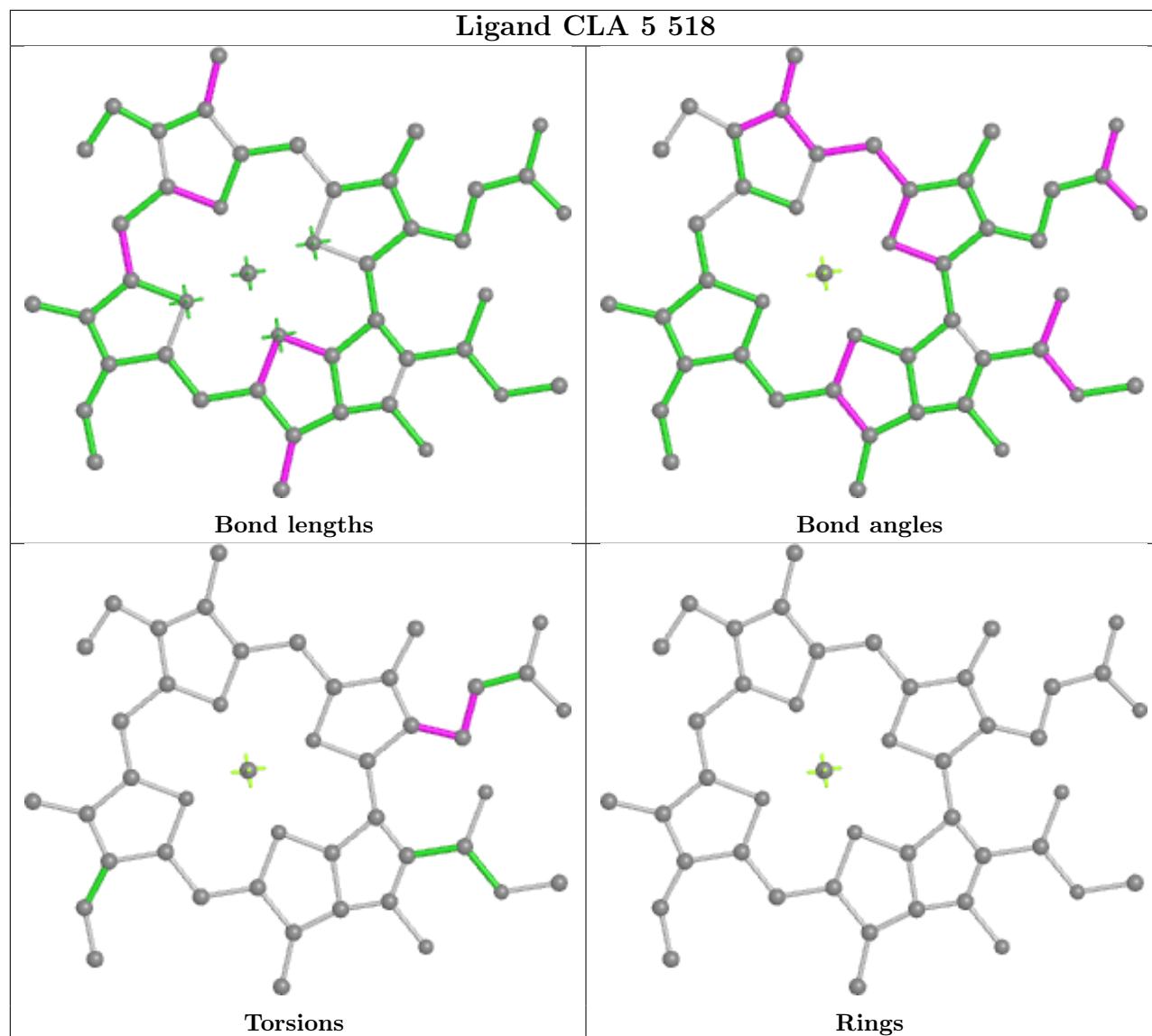


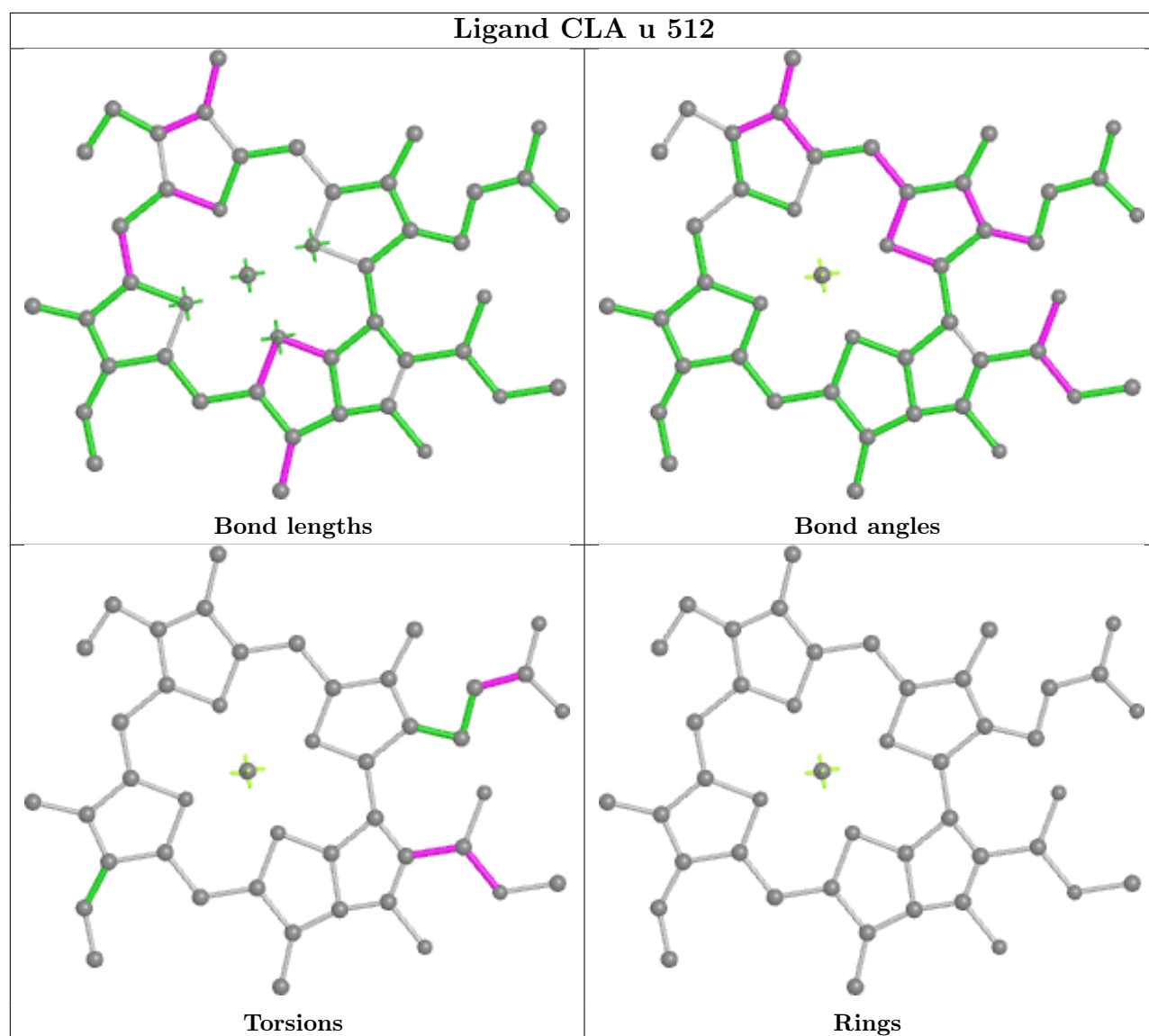
Torsions



Rings

Ligand CLA 5 518





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

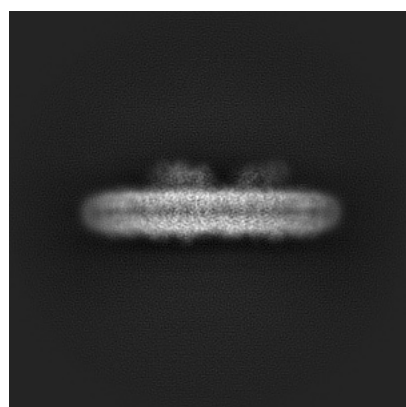
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9994. These allow visual inspection of the internal detail of the map and identification of artifacts.

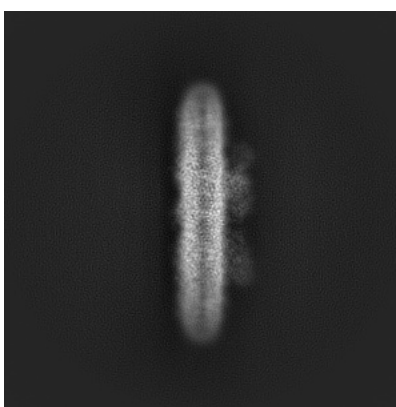
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

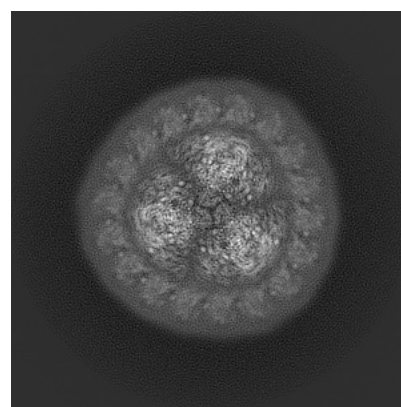
6.1.1 Primary map



X



Y

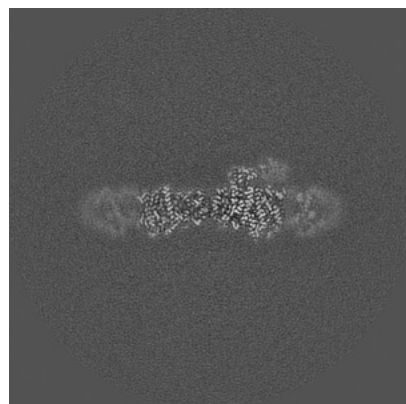


Z

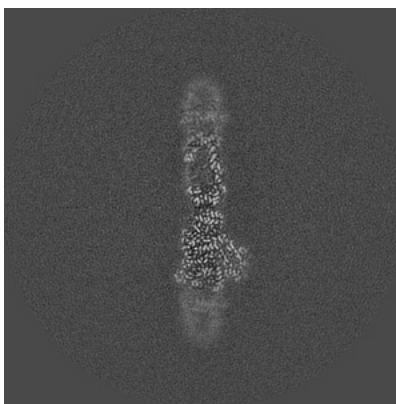
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

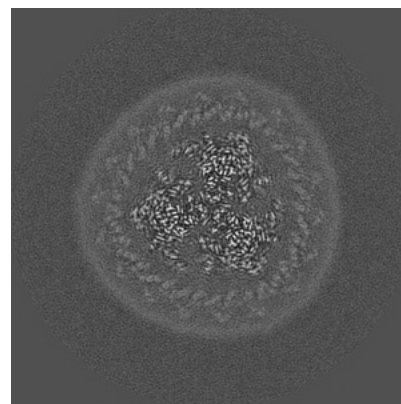
6.2.1 Primary map



X Index: 240



Y Index: 240

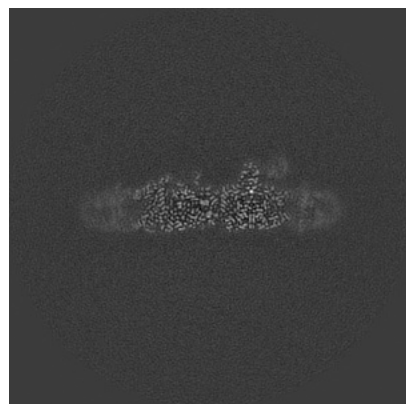


Z Index: 240

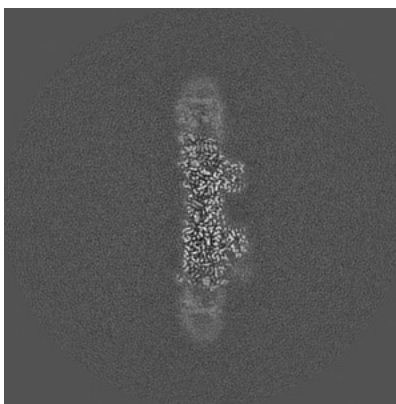
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

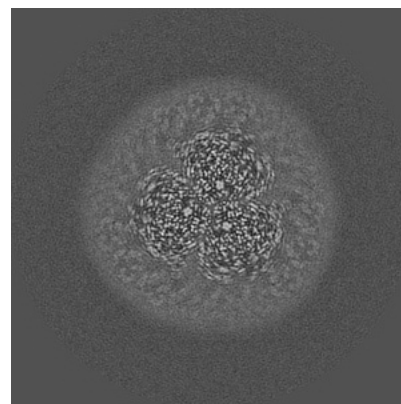
6.3.1 Primary map



X Index: 259



Y Index: 225

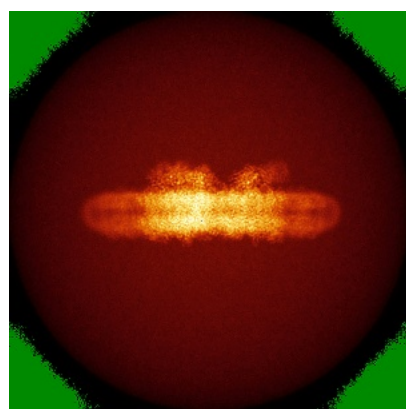


Z Index: 253

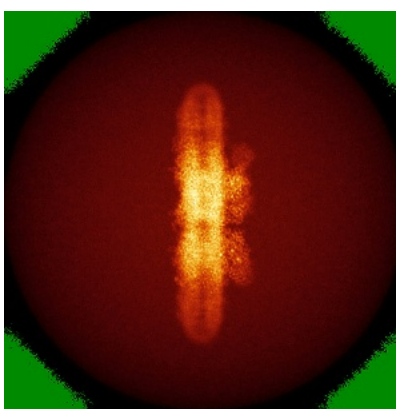
The images above show the largest variance slices of the map in three orthogonal directions.

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

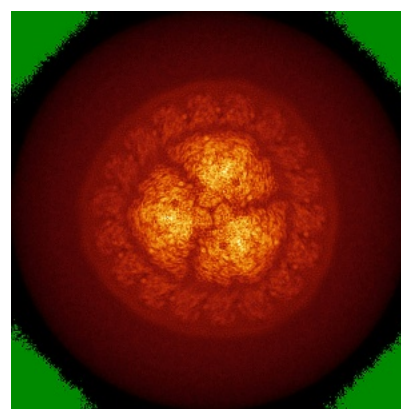
6.4.1 Primary map



X



Y

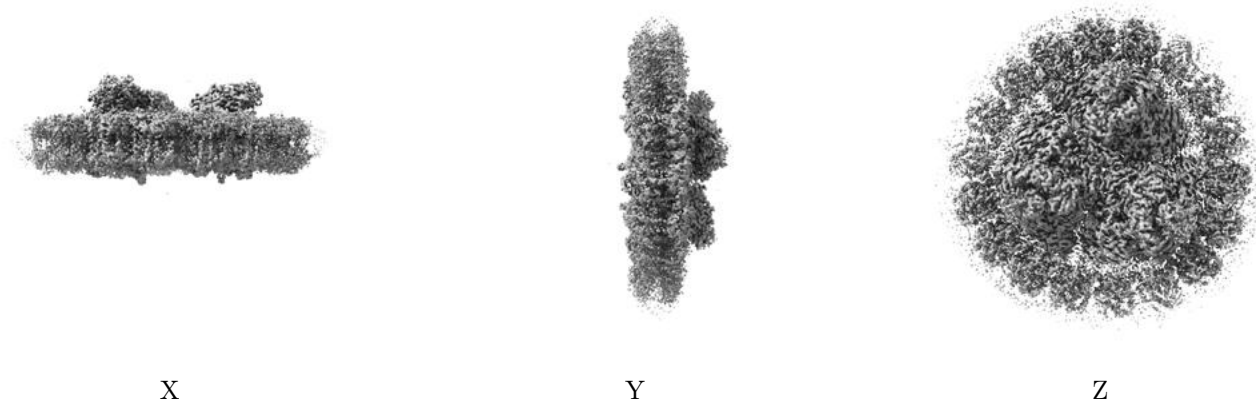


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

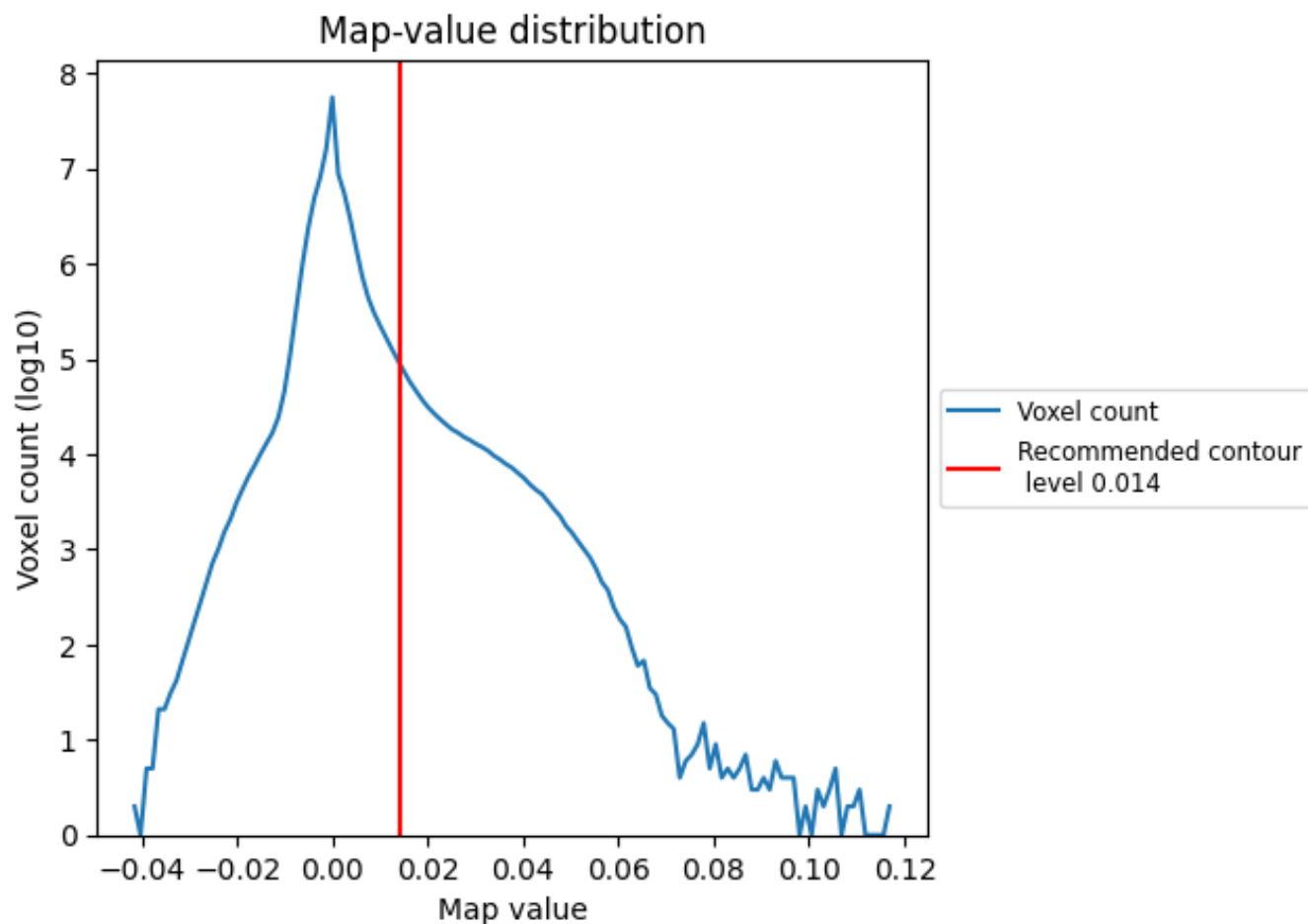
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

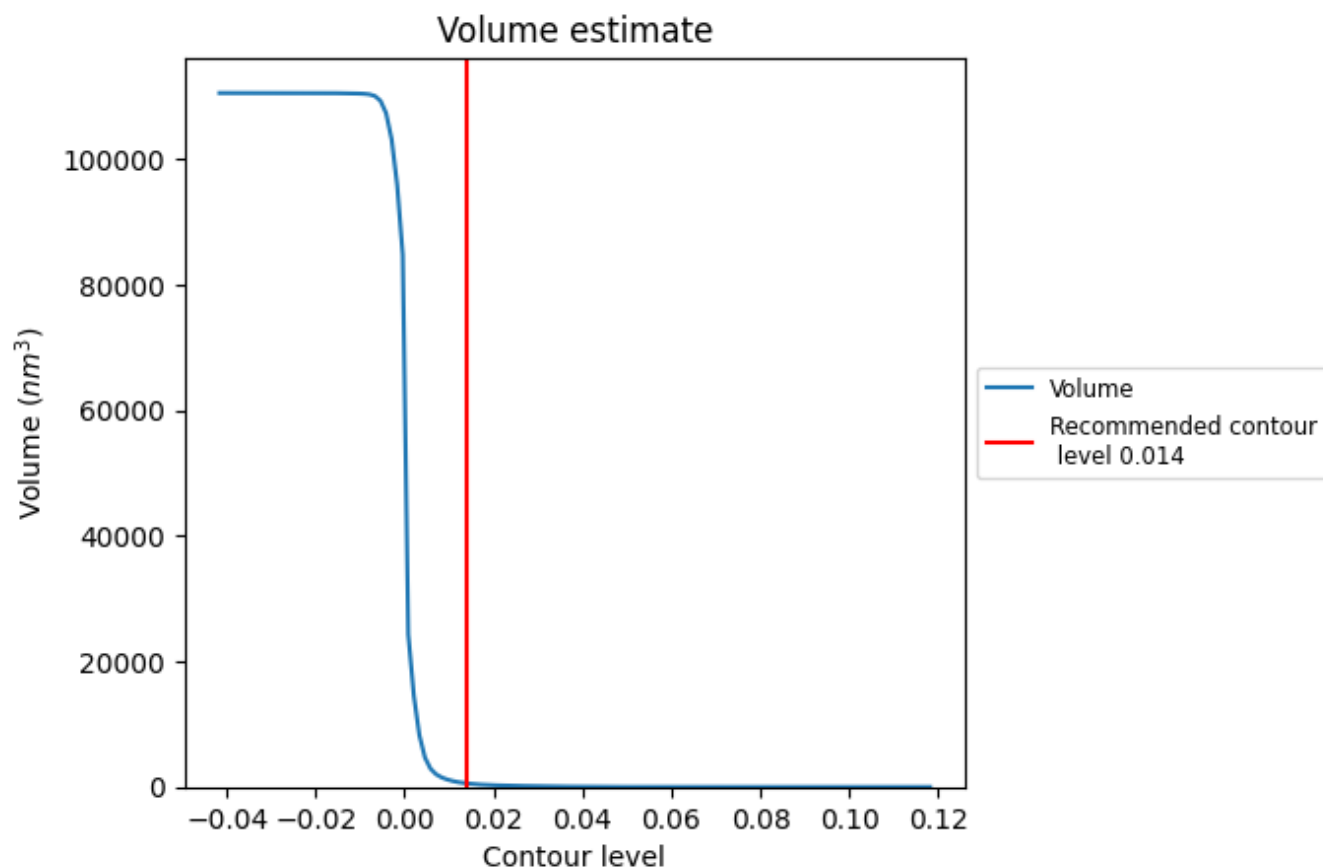
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

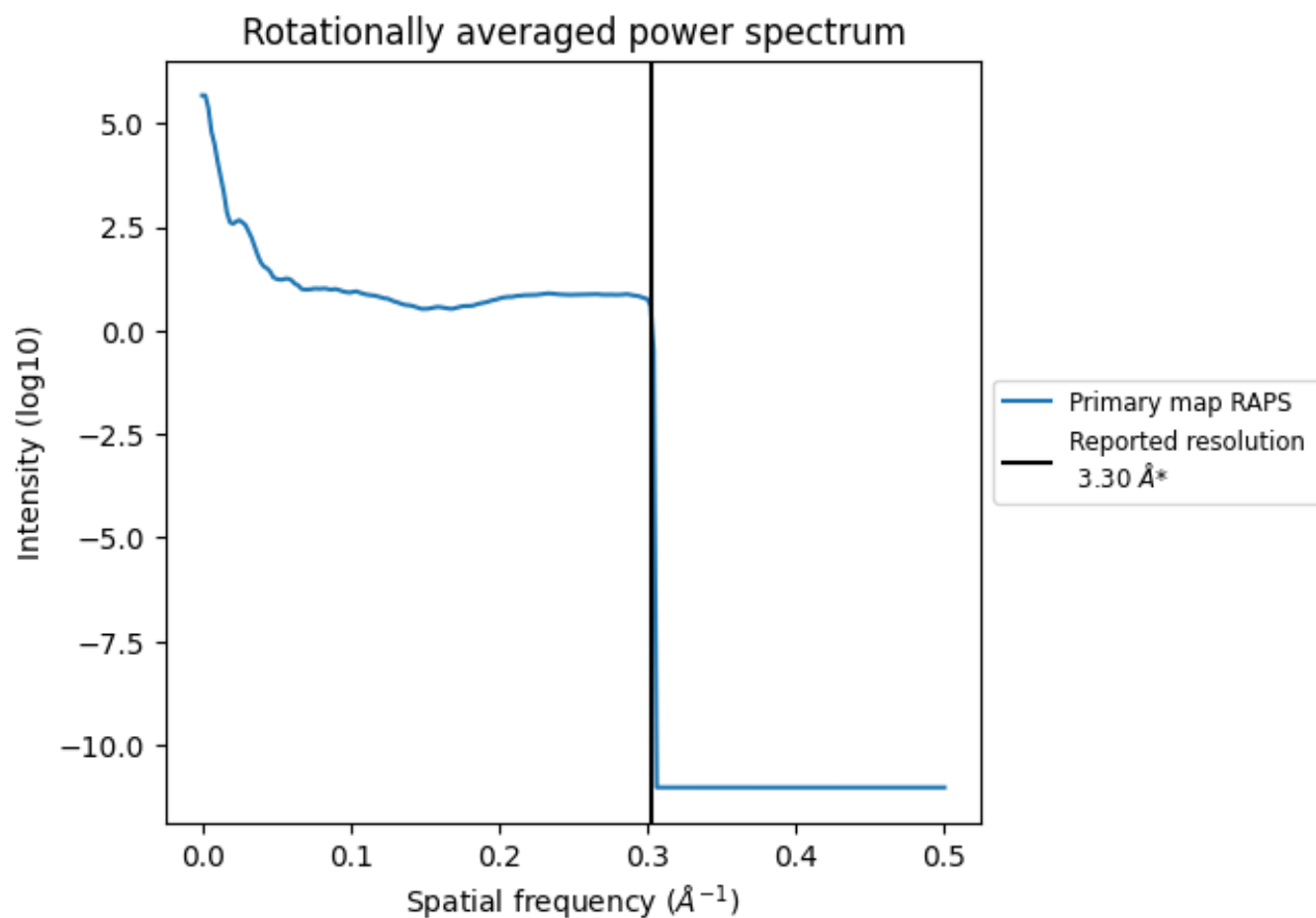
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 567 nm^3 ; this corresponds to an approximate mass of 512 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

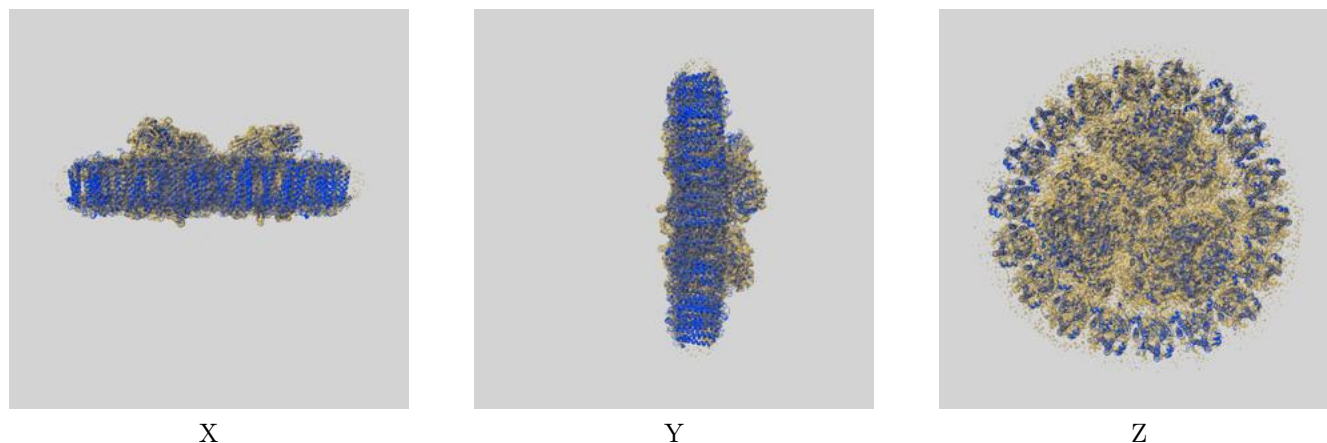
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

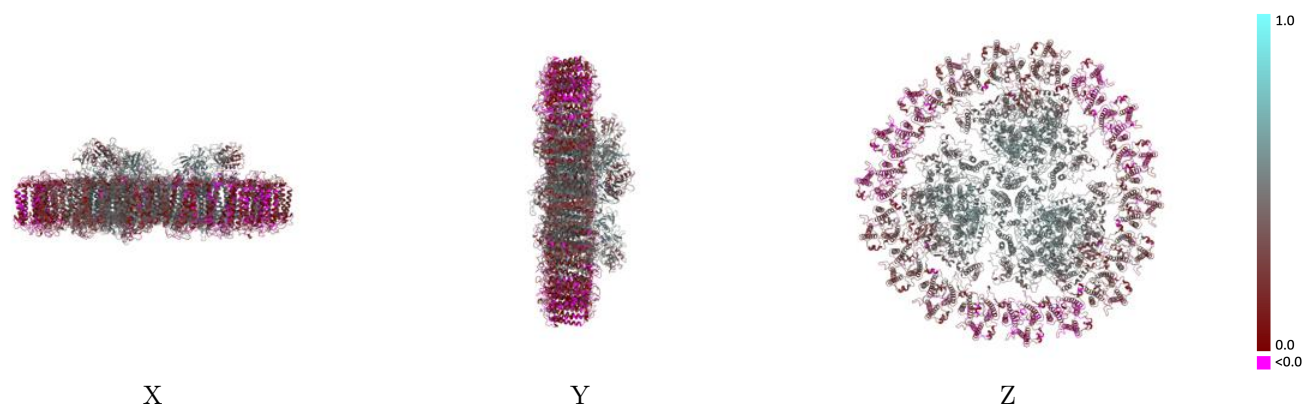
This section contains information regarding the fit between EMDB map EMD-9994 and PDB model 6KIF. Per-residue inclusion information can be found in section [3](#) on page [69](#).

9.1 Map-model overlay [i](#)



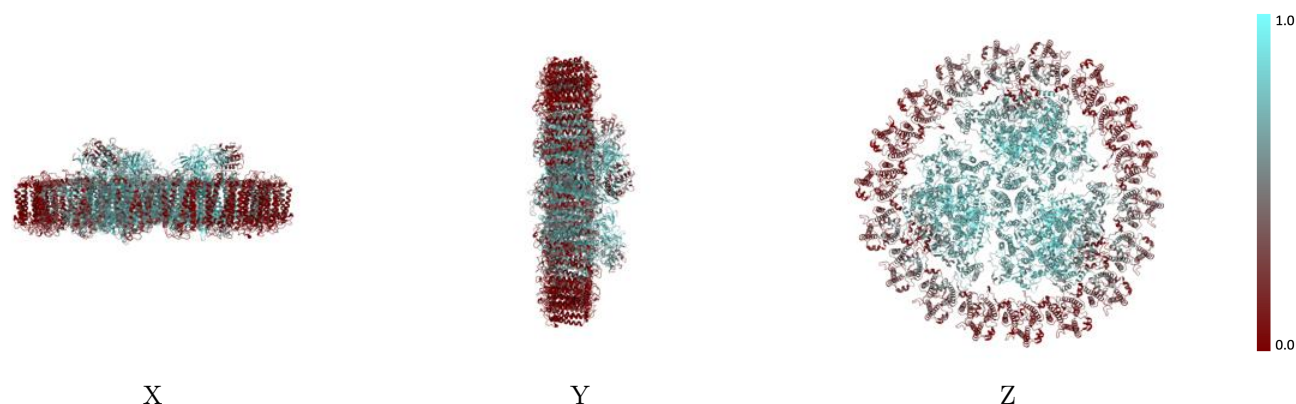
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



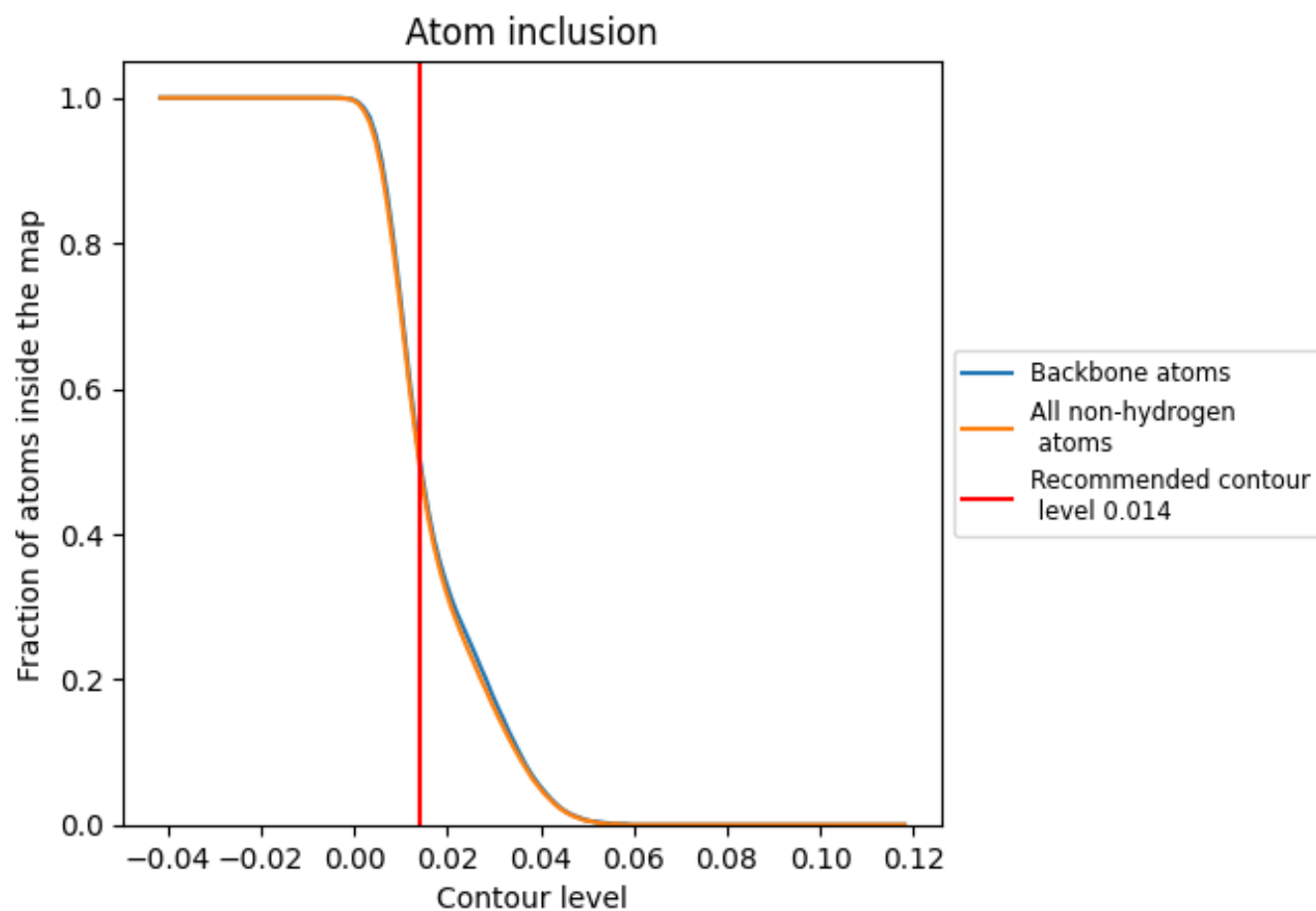
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.014) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.4950 |  0.3600 |
| 1 |  0.3260 |  0.2570 |
| 2 |  0.3300 |  0.2860 |
| 3 |  0.2650 |  0.2560 |
| 4 |  0.0820 |  0.0950 |
| 5 |  0.0790 |  0.1060 |
| 6 |  0.1420 |  0.1610 |
| A |  0.7560 |  0.5190 |
| B |  0.7500 |  0.5000 |
| C |  0.8750 |  0.5350 |
| D |  0.7920 |  0.5270 |
| E |  0.7270 |  0.4830 |
| F |  0.6900 |  0.4570 |
| G |  0.7550 |  0.5150 |
| H |  0.7500 |  0.5000 |
| I |  0.7510 |  0.5410 |
| J |  0.6790 |  0.4920 |
| K |  0.5300 |  0.3470 |
| L |  0.7810 |  0.5400 |
| M |  0.7060 |  0.5080 |
| N |  0.8720 |  0.5370 |
| O |  0.7930 |  0.5260 |
| P |  0.3710 |  0.3350 |
| Q |  0.7210 |  0.4810 |
| R |  0.6900 |  0.4570 |
| S |  0.7590 |  0.5440 |
| T |  0.6690 |  0.4930 |
| U |  0.5180 |  0.3330 |
| V |  0.7830 |  0.5400 |
| W |  0.6990 |  0.5040 |
| X |  0.3680 |  0.3320 |
| Y |  0.3180 |  0.2520 |
| Z |  0.3280 |  0.2790 |
| a |  0.2610 |  0.2510 |
| b |  0.0830 |  0.0900 |



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| Chain | Atom inclusion | Q-score |
|-------|---|---|
| c |  0.0760 |  0.1030 |
| d |  0.1460 |  0.1570 |
| e |  0.7560 |  0.5190 |
| f |  0.7500 |  0.4990 |
| g |  0.8680 |  0.5350 |
| h |  0.7920 |  0.5260 |
| i |  0.7180 |  0.4760 |
| j |  0.6890 |  0.4540 |
| k |  0.7530 |  0.5370 |
| l |  0.6690 |  0.4910 |
| m |  0.5360 |  0.3490 |
| n |  0.7850 |  0.5390 |
| o |  0.7020 |  0.5050 |
| p |  0.3780 |  0.3340 |
| q |  0.3240 |  0.2590 |
| r |  0.3350 |  0.2880 |
| s |  0.2640 |  0.2580 |
| t |  0.0810 |  0.0950 |
| u |  0.0770 |  0.1070 |
| v |  0.1480 |  0.1590 |