



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 06:30 AM UTC

PDB ID : 7BGI / pdb\_00007bgi  
EMDB ID : EMD-12180  
Title : Photosystem I of a temperature sensitive mutant *Chlamydomonas reinhardtii*  
Authors : Caspy, I.; Nelson, N.  
Deposited on : 2021-01-07  
Resolution : 2.54 Å(reported)  
Based on initial model : 6JO5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

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

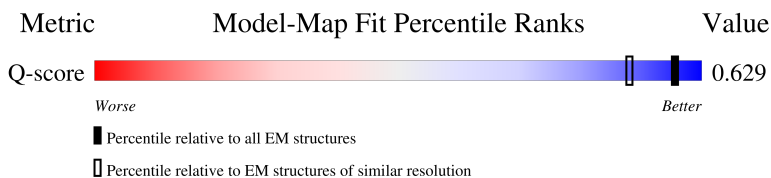
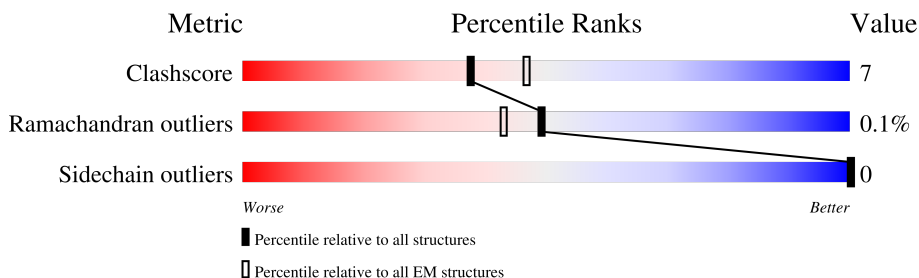
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.54 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.



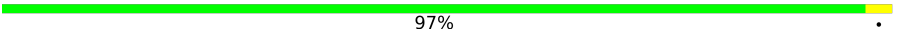
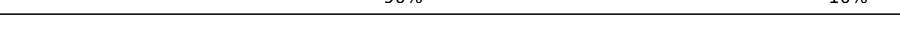
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 7403 ( 2.04 - 3.04 )                                     |

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  $\geq 3$ , 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     | 741    | <br>87% 13%      |
| 2   | B     | 733    | <br>86% 14%      |
| 3   | C     | 80     | <br>95% 5%       |
| 4   | D     | 144    | <br>90% 10%      |

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| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 5   | E     | 63     |  97%       |
| 6   | F     | 165    |  93% 7%    |
| 7   | G     | 91     |  77% 19%   |
| 8   | I     | 37     |  86% 14%   |
| 9   | J     | 39     |  90% 10%   |
| 10  | K     | 84     |  85% 15%   |
| 11  | L     | 138    |  86% 6% 9% |
| 12  | 1     | 194    |  89% 11%   |
| 12  | Z     | 194    |  93% 7%    |
| 13  | 3     | 219    |  90% 10%   |
| 14  | 7     | 213    |  89% 11%   |
| 15  | 8     | 217    |  89% 11%   |
| 16  | 4     | 210    |  85% 15% |
| 17  | 5     | 227    |  89% 11% |
| 18  | 6     | 229    |  90% 10% |
| 19  | 2     | 198    |  81% 19% |
| 20  | 9     | 183    |  86% 14% |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 21  | CL0  | A     | 1011 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 601  | X         | -        | -       | -                |
| 22  | CLA  | 1     | 602  | X         | -        | -       | -                |
| 22  | CLA  | 1     | 603  | X         | -        | -       | -                |
| 22  | CLA  | 1     | 604  | X         | -        | -       | -                |
| 22  | CLA  | 1     | 605  | X         | -        | -       | -                |
| 22  | CLA  | 1     | 606  | X         | -        | -       | -                |
| 22  | CLA  | 1     | 607  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | 1     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 611 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 613 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 615 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 603 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 604 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 605 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 606 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 607 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 615 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 603 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 604 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 605 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 606 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 607 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 610 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 613 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 616 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 618 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 603 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 604 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 605 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 606 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 607 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 609 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 615 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 603 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | 5     | 604 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 605 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 606 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 607 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 609 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 613 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 615 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 618 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 622 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 603 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 604 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 605 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 606 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 607 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 609 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 615 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 618 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 619 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 603 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 604 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 605 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 606 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 607 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 608 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 609 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 611 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 612 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 613 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 615 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 616 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 601 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 602 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 603 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 604 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CLA  | 8     | 605  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 606  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 607  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 608  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 609  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 611  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 612  | X         | -        | -       | -                |
| 22  | CLA  | 8     | 615  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 601  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 602  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 603  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 604  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 606  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 607  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 608  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 609  | X         | -        | -       | -                |
| 22  | CLA  | 9     | 612  | X         | -        | -       | -                |
| 22  | CLA  | A     | 1012 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1013 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1101 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1102 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1103 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1104 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1105 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1106 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1107 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1108 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1109 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1110 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1111 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1112 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1113 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1114 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1115 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1116 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1117 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1118 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1119 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1120 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1121 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1122 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1123 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CLA  | A     | 1124 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1125 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1126 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1127 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1128 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1129 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1130 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1131 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1132 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1133 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1134 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1135 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1136 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1137 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1138 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1139 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1140 | X         | -        | -       | -                |
| 22  | CLA  | A     | 1141 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1021 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1022 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1023 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1201 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1202 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1203 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1204 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1205 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1206 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1207 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1208 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1209 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1210 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1211 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1212 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1213 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1214 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1215 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1216 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1217 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1218 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1219 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1220 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1221 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | CLA  | B     | 1222 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1223 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1224 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1225 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1226 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1227 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1228 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1229 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1230 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1231 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1232 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1234 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1235 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1236 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1237 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1238 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1239 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1240 | X         | -        | -       | -                |
| 22  | CLA  | B     | 1241 | X         | -        | -       | -                |
| 22  | CLA  | F     | 1301 | X         | -        | -       | -                |
| 22  | CLA  | F     | 1302 | X         | -        | -       | -                |
| 22  | CLA  | G     | 1601 | X         | -        | -       | -                |
| 22  | CLA  | G     | 1602 | X         | -        | -       | -                |
| 22  | CLA  | J     | 1901 | X         | -        | -       | -                |
| 22  | CLA  | K     | 1401 | X         | -        | -       | -                |
| 22  | CLA  | K     | 1402 | X         | -        | -       | -                |
| 22  | CLA  | K     | 1403 | X         | -        | -       | -                |
| 22  | CLA  | K     | 1404 | X         | -        | -       | -                |
| 22  | CLA  | L     | 1502 | X         | -        | -       | -                |
| 22  | CLA  | L     | 1503 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 601  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 602  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 603  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 604  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 605  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 606  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 607  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 608  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 611  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 612  | X         | -        | -       | -                |
| 22  | CLA  | Z     | 615  | X         | -        | -       | -                |
| 36  | RRX  | F     | 4001 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 37  | C7Z  | 1     | 503  | X         | -        | -       | -                |
| 37  | C7Z  | 5     | 505  | X         | -        | -       | -                |
| 37  | C7Z  | J     | 4002 | X         | -        | -       | -                |
| 39  | LUT  | 2     | 501  | X         | -        | -       | -                |
| 39  | LUT  | 2     | 503  | X         | -        | -       | -                |
| 40  | CHL  | 1     | 609  | X         | -        | -       | -                |
| 40  | CHL  | 1     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 2     | 609  | X         | -        | -       | -                |
| 40  | CHL  | 2     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 2     | 613  | X         | -        | -       | -                |
| 40  | CHL  | 3     | 611  | X         | -        | -       | -                |
| 40  | CHL  | 4     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 4     | 611  | X         | -        | -       | -                |
| 40  | CHL  | 4     | 613  | X         | -        | -       | -                |
| 40  | CHL  | 4     | 617  | X         | -        | -       | -                |
| 40  | CHL  | 5     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 5     | 611  | X         | -        | -       | -                |
| 40  | CHL  | 5     | 617  | X         | -        | -       | -                |
| 40  | CHL  | 6     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 6     | 611  | X         | -        | -       | -                |
| 40  | CHL  | 6     | 613  | X         | -        | -       | -                |
| 40  | CHL  | 6     | 617  | X         | -        | -       | -                |
| 40  | CHL  | 7     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 8     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 8     | 613  | X         | -        | -       | -                |
| 40  | CHL  | 9     | 610  | X         | -        | -       | -                |
| 40  | CHL  | 9     | 613  | X         | -        | -       | -                |
| 40  | CHL  | Z     | 609  | X         | -        | -       | -                |
| 40  | CHL  | Z     | 610  | X         | -        | -       | -                |
| 40  | CHL  | Z     | 613  | X         | -        | -       | -                |
| 42  | QTB  | Z     | 504  | X         | -        | -       | -                |

## 2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 52213 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     | 741      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5820  | 3805 | 993 | 1000 | 22 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | B     | 733      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5825  | 3825 | 977 | 1005 | 18 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 601   | 369 | 103 | 117 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1135  | 725 | 201 | 202 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | E     | 63       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 497   | 316 | 87 | 94 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1266  | 817 | 213 | 233 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 7   | G     | 74       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 550   | 354 | 94 | 102 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | I     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 282   | 195 | 39 | 47 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | J     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 321   | 219 | 45 | 56 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 10  | K     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 571   | 362 | 98 | 109 | 2 |         |       |

- Molecule 11 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | L     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 595 | 148 | 168 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | 1     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1445  | 941 | 240 | 261 | 3 |         |       |
| 12  | Z     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1445  | 941 | 240 | 261 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | 3     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1674  | 1092 | 270 | 304 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | 7     | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1072 | 274 | 298 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | 8     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1073 | 280 | 293 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 4     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1628  | 1068 | 262 | 293 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | 5     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1775  | 1154 | 297 | 316 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | 6     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1766  | 1164 | 292 | 304 | 6 |         |       |

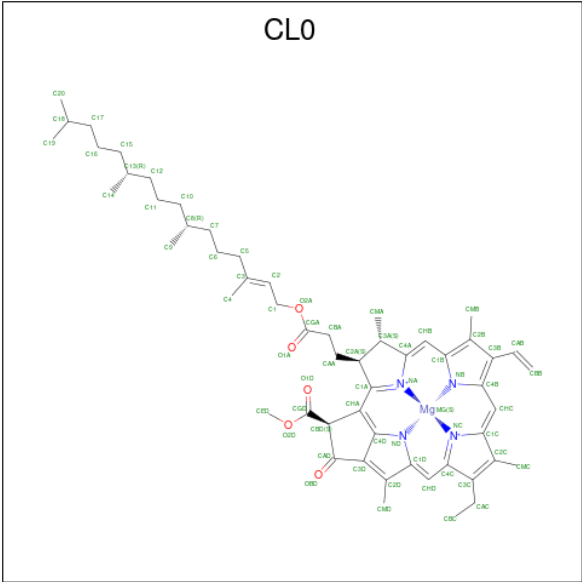
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 19  | 2     | 198      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1518  | 983 | 249 | 276 | 10 |         |       |

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

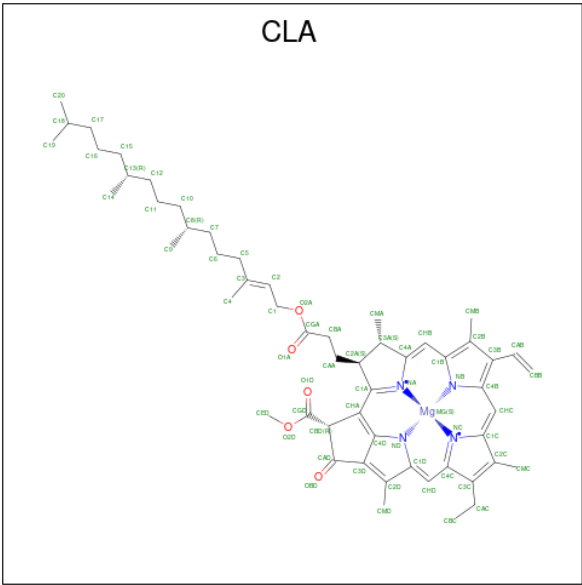
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | 9     | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1406  | 910 | 235 | 254 | 7 |         |       |

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | F     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | G     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 22  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | K     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | K     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | K     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | L     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>43 | C<br>35 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 22  | 7     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 22  | 7     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 7     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 8     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 4     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 22  | 4     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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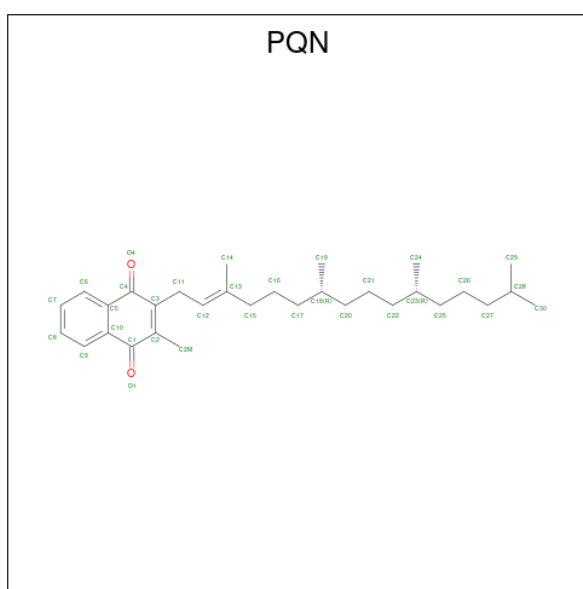
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 9     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 9     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 9     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 9     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 9     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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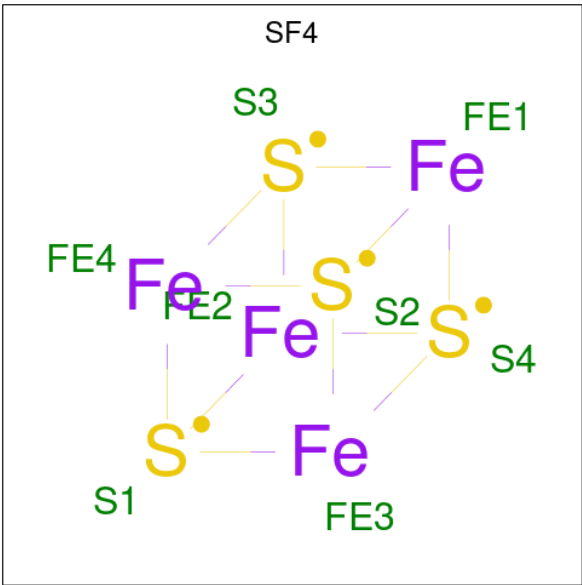
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



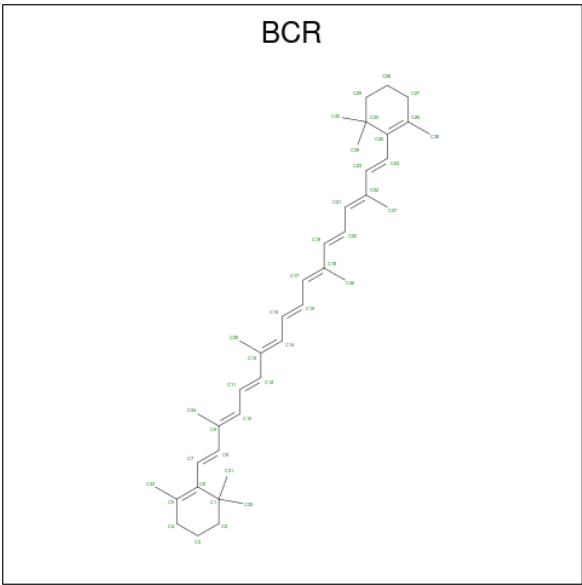
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 23  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 23  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33 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

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 24  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 24  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 25  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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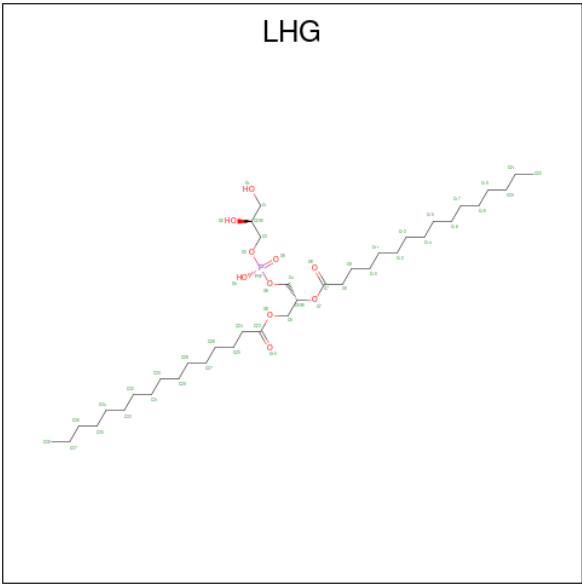
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 25  | A     | 1        | Total C<br>40 40 | 0       |
| 25  | A     | 1        | Total C<br>40 40 | 0       |
| 25  | A     | 1        | Total C<br>40 40 | 0       |
| 25  | A     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | B     | 1        | Total C<br>40 40 | 0       |
| 25  | G     | 1        | Total C<br>40 40 | 0       |
| 25  | I     | 1        | Total C<br>40 40 | 0       |
| 25  | J     | 1        | Total C<br>40 40 | 0       |
| 25  | K     | 1        | Total C<br>40 40 | 0       |
| 25  | K     | 1        | Total C<br>40 40 | 0       |
| 25  | L     | 1        | Total C<br>40 40 | 0       |
| 25  | L     | 1        | Total C<br>40 40 | 0       |
| 25  | 3     | 1        | Total C<br>40 40 | 0       |
| 25  | 3     | 1        | Total C<br>40 40 | 0       |
| 25  | 3     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 25  | 3     | 1        | Total C<br>40 40 | 0       |
| 25  | 7     | 1        | Total C<br>40 40 | 0       |
| 25  | 7     | 1        | Total C<br>40 40 | 0       |
| 25  | 8     | 1        | Total C<br>40 40 | 0       |
| 25  | 4     | 1        | Total C<br>40 40 | 0       |
| 25  | 5     | 1        | Total C<br>40 40 | 0       |
| 25  | 5     | 1        | Total C<br>40 40 | 0       |
| 25  | 6     | 1        | Total C<br>40 40 | 0       |
| 25  | 6     | 1        | Total C<br>40 40 | 0       |

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



| Mol | Chain | Residues | Atoms                     | AltConf |
|-----|-------|----------|---------------------------|---------|
| 26  | A     | 1        | Total C O P<br>35 24 10 1 | 0       |
| 26  | A     | 1        | Total C O P<br>49 38 10 1 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 23    | 12 | 10 | 1 |         |
| 26  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 20    | 9  | 10 | 1 |         |
| 26  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 33    | 22 | 10 | 1 |         |
| 26  | 1     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 26  | Z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 26  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 20    | 9  | 10 | 1 |         |
| 26  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 26  | 8     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 26  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | 4     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |
| 26  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 26  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 34    | 23 | 10 | 1 |         |
| 26  | 9     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 33    | 22 | 10 | 1 |         |

- Molecule 27 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: C<sub>21</sub>H<sub>41</sub>O<sub>7</sub>P).



| Mol | Chain | Residues | Atoms       |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 27  | A     | 1        | Total<br>29 | C<br>21 | O<br>7 | P<br>1 | 0       |
| 27  | 3     | 1        | Total<br>16 | C<br>8  | O<br>7 | P<br>1 | 0       |
| 27  | 8     | 1        | Total<br>29 | C<br>21 | O<br>7 | P<br>1 | 0       |

- Molecule 28 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



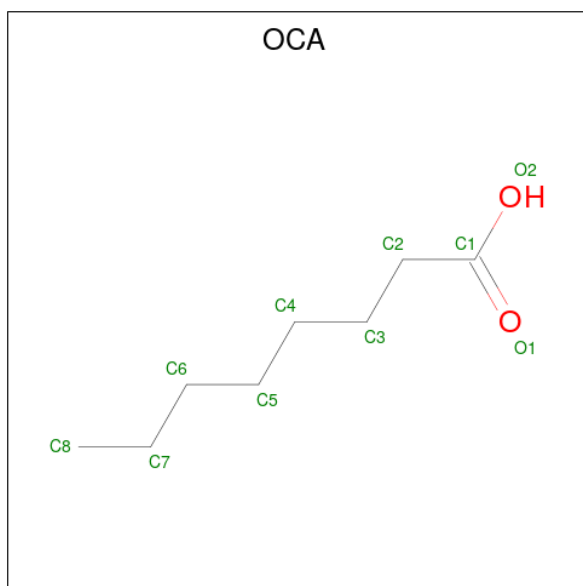
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 28  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

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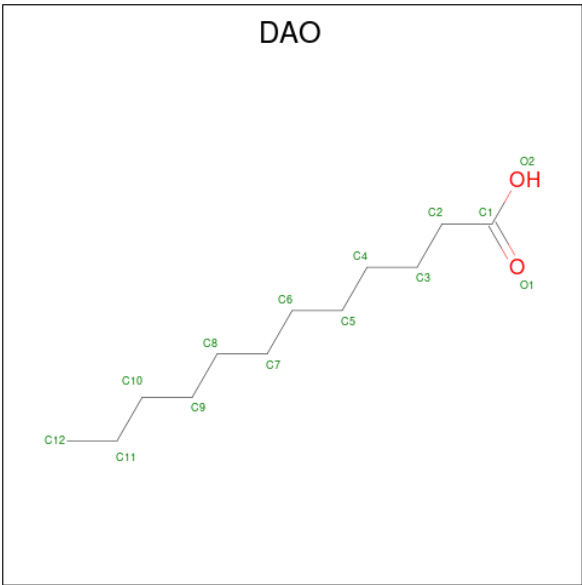
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 28  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 28  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 28  | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 28  | 1     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 28  | 8     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 28  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 28  | 9     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 29 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula:  $C_8H_{16}O_2$ ).



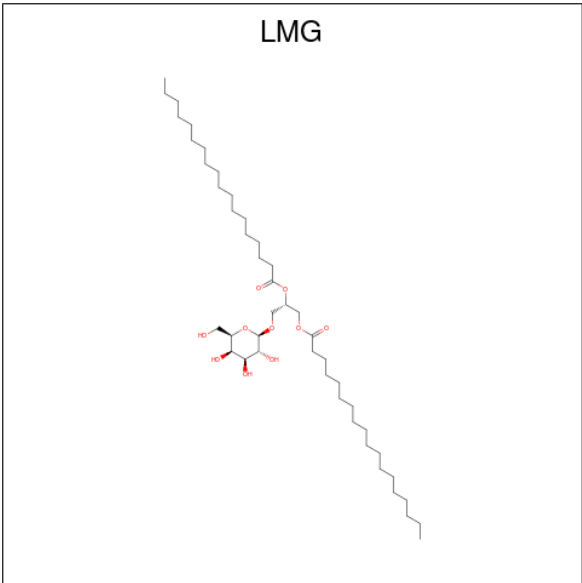
| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 29  | A     | 1        | Total | C | O | 0       |
|     |       |          | 10    | 8 | 2 |         |

- Molecule 30 is LAURIC ACID (CCD ID: DAO) (formula:  $C_{12}H_{24}O_2$ ).



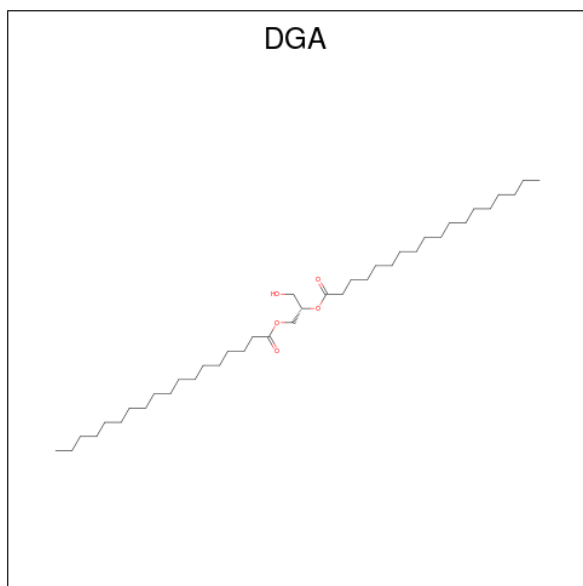
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 30  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 14    | 12 | 2 |         |

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



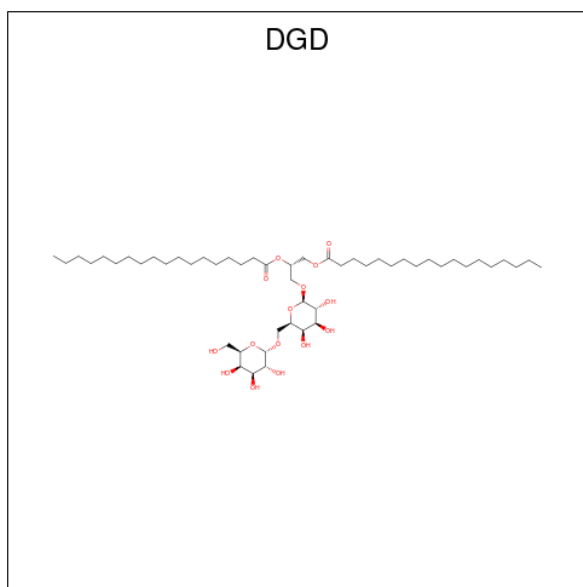
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 31  | A     | 1        | Total | C  | O  | 0       |
|     |       |          | 29    | 19 | 10 |         |
| 31  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 25 | 10 |         |

- Molecule 32 is DIACYL GLYCEROL (CCD ID: DGA) (formula:  $C_{39}H_{76}O_5$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 32  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 39 | 5 |         |
| 32  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 39    | 34 | 5 |         |

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).

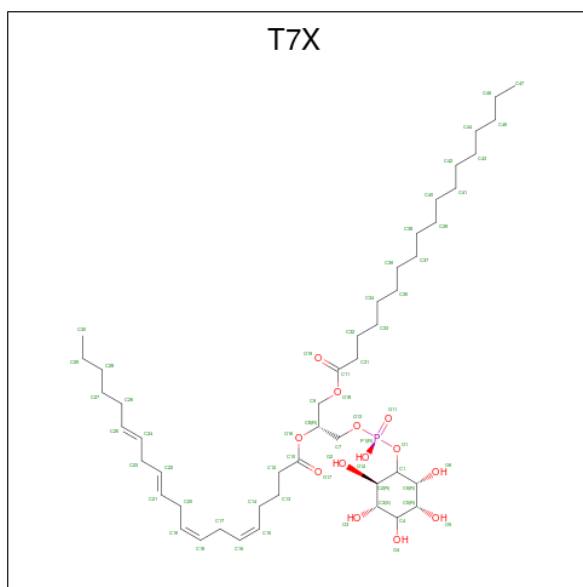


| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 66    | 51 | 15 |         |

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

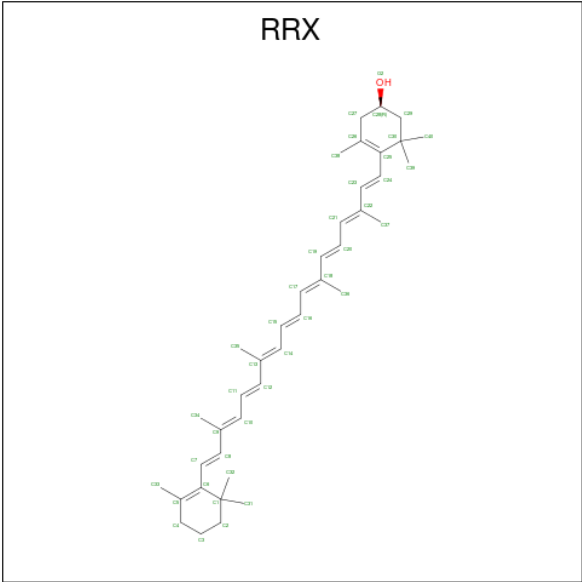
| Mol | Chain | Residues | Atoms |    |  | AltConf |
|-----|-------|----------|-------|----|--|---------|
| 34  | B     | 1        | Total | Ca |  | 0       |
|     |       |          | 1     | 1  |  |         |

- Molecule 35 is Phosphatidylinositol (CCD ID: T7X) (formula: C<sub>47</sub>H<sub>83</sub>O<sub>13</sub>P).



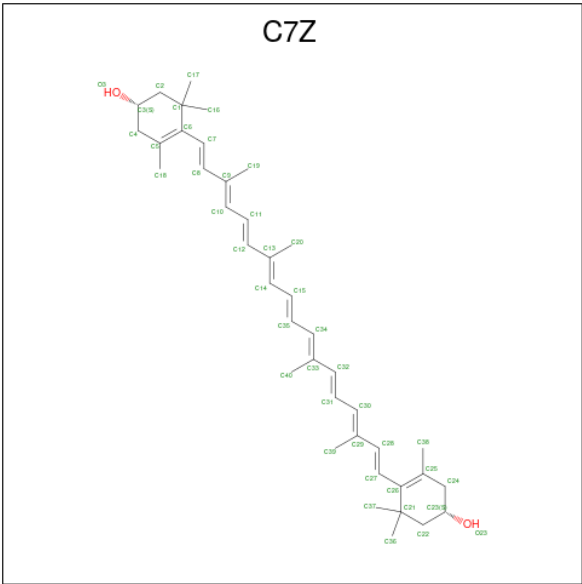
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 35  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 35 | 13 | 1 |         |

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



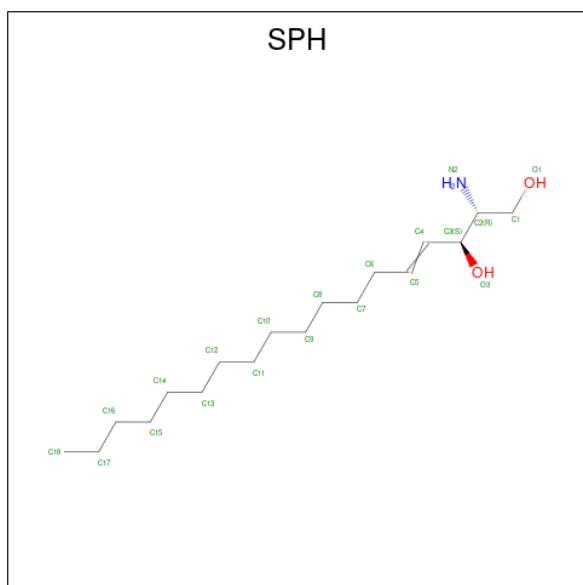
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 37  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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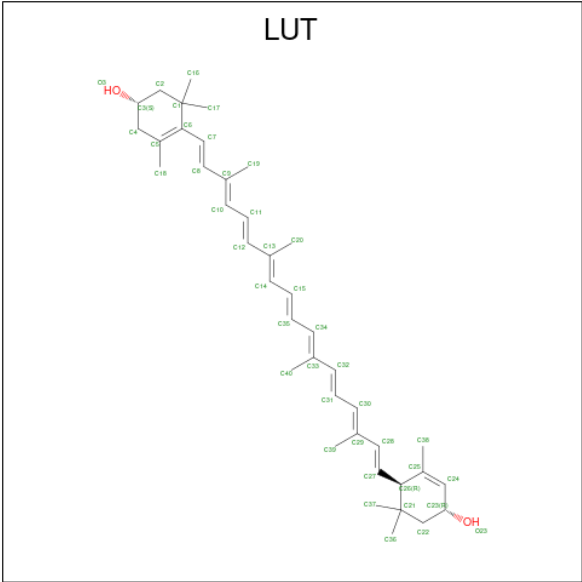
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 37  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 37  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 38 is SPHINGOSINE (CCD ID: SPH) (formula:  $C_{18}H_{37}NO_2$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 38  | K     | 1        | Total | C  | N | O | 0       |
|     |       |          | 21    | 18 | 1 | 2 |         |
| 38  | 7     | 1        | Total | C  | N | O | 0       |
|     |       |          | 21    | 18 | 1 | 2 |         |
| 38  | 7     | 1        | Total | C  | N | O | 0       |
|     |       |          | 21    | 18 | 1 | 2 |         |

- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula:  $C_{40}H_{56}O_2$ ).



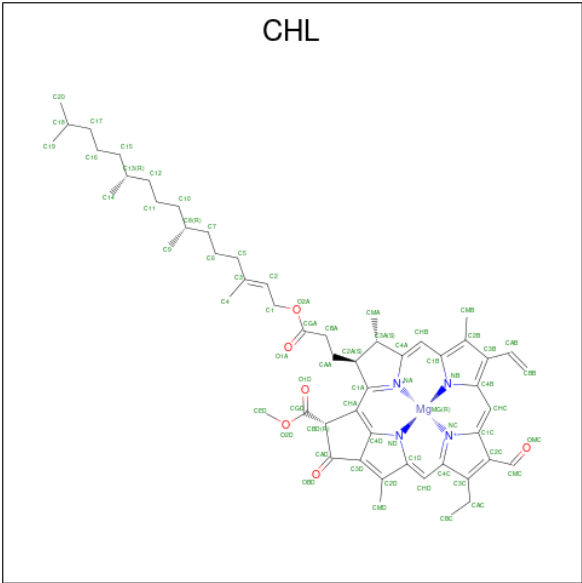
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 39  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 39  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 39  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 40 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 40  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 40  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 40  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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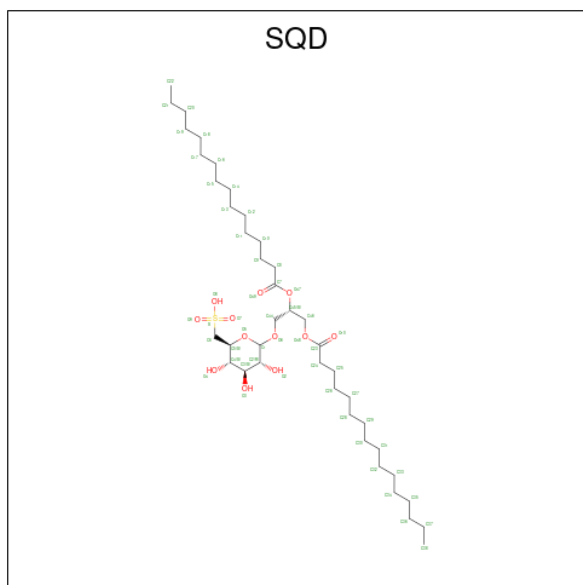
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 40  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 40  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 40  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 40  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 43 | 1  | 4 | 6 |         |
| 40  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 40  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 40  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 40  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 40  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 40  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 40  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 40  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 40  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 40  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 40  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 40  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 40  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 40  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 40  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 40  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 40  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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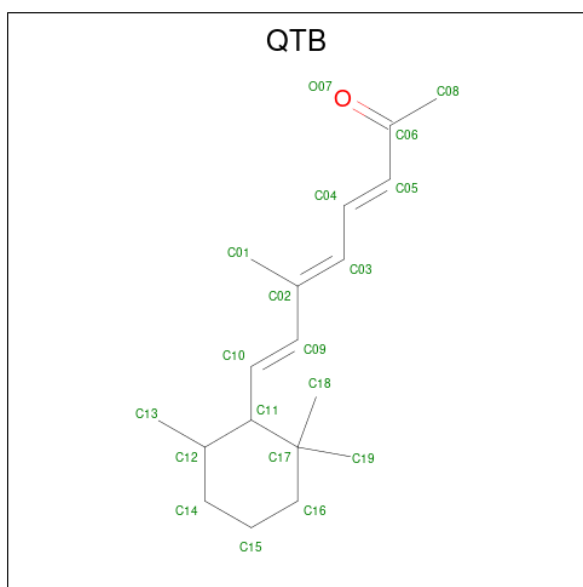
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
|     |       |          | Total | C  | Mg | N | O |         |
| 40  | 9     | 1        | 42    | 33 | 1  | 4 | 4 | 0       |

- Molecule 41 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



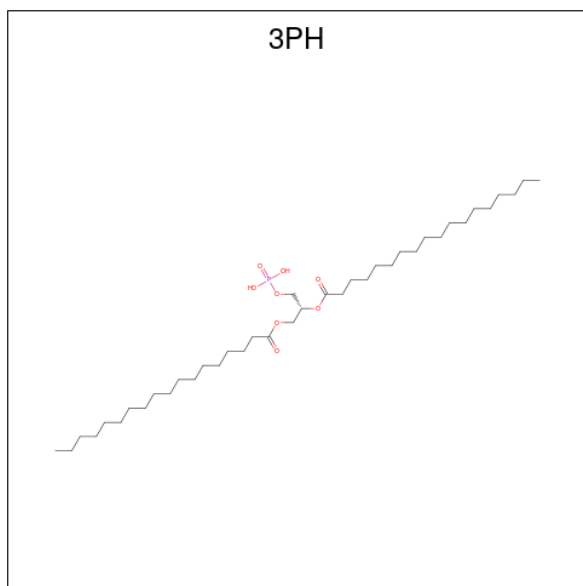
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
|     |       |          | Total | C  | O  | S |         |
| 41  | 1     | 1        | 48    | 35 | 12 | 1 | 0       |
| 41  | 2     | 1        | 43    | 30 | 12 | 1 | 0       |

- Molecule 42 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: C<sub>18</sub>H<sub>28</sub>O).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 42  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 19    | 18 | 1 |         |

- Molecule 43 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



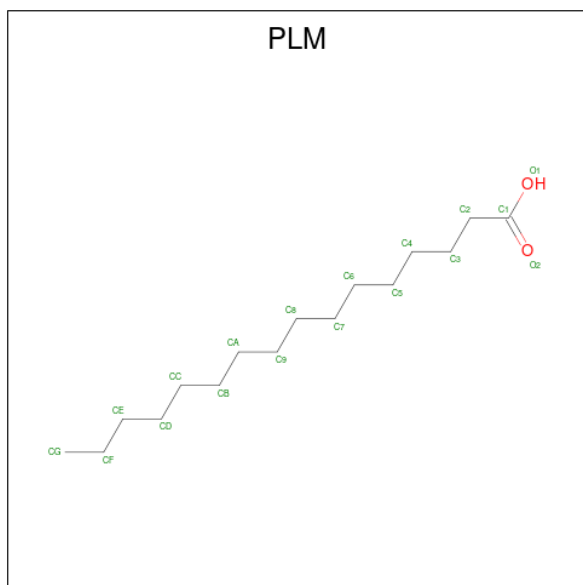
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 43  | 7     | 1        | Total | C  | O | P | 0       |
|     |       |          | 39    | 30 | 8 | 1 |         |
| 43  | 8     | 1        | Total | C  | O | P | 0       |
|     |       |          | 30    | 21 | 8 | 1 |         |

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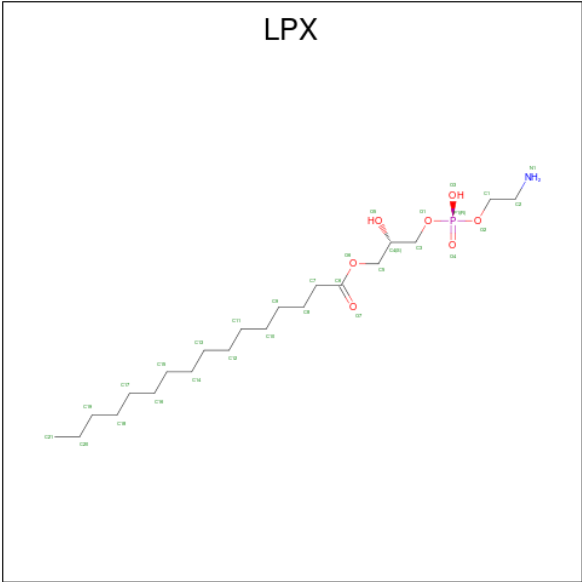
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 43  | 5     | 1        | Total | C  | O | P | 0       |
|     |       |          | 23    | 14 | 8 | 1 |         |
| 43  | 6     | 1        | Total | C  | O | P | 0       |
|     |       |          | 29    | 20 | 8 | 1 |         |
| 43  | 2     | 1        | Total | C  | O | P | 0       |
|     |       |          | 27    | 18 | 8 | 1 |         |

- Molecule 44 is PALMITIC ACID (CCD ID: PLM) (formula:  $C_{16}H_{32}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 44  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 16 | 2 |         |

- Molecule 45 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula:  $C_{21}H_{44}NO_7P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | 8     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 21 | 1 | 7 | 1 |         |

- Molecule 46 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 46  | A     | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 46  | A     | 15       | Total | O  | 0       |
|     |       |          | 15    | 15 |         |
| 46  | A     | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 46  | A     | 6        | Total | O  | 0       |
|     |       |          | 6     | 6  |         |
| 46  | A     | 9        | Total | O  | 0       |
|     |       |          | 9     | 9  |         |
| 46  | A     | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 46  | A     | 7        | Total | O  | 0       |
|     |       |          | 7     | 7  |         |
| 46  | A     | 18       | Total | O  | 0       |
|     |       |          | 18    | 18 |         |
| 46  | A     | 8        | Total | O  | 0       |
|     |       |          | 8     | 8  |         |
| 46  | A     | 14       | Total | O  | 0       |
|     |       |          | 14    | 14 |         |
| 46  | A     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | A     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 2        | Total<br>2  | O<br>2  | 0       |
| 46  | B     | 12       | Total<br>12 | O<br>12 | 0       |
| 46  | B     | 10       | Total<br>10 | O<br>10 | 0       |
| 46  | B     | 16       | Total<br>16 | O<br>16 | 0       |
| 46  | B     | 2        | Total<br>2  | O<br>2  | 0       |
| 46  | B     | 2        | Total<br>2  | O<br>2  | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |
| 46  | B     | 28       | Total<br>28 | O<br>28 | 0       |
| 46  | B     | 1        | Total<br>1  | O<br>1  | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | C     | 12       | Total O<br>12 12 | 0       |
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | C     | 1        | Total O<br>1 1   | 0       |
| 46  | D     | 1        | Total O<br>1 1   | 0       |
| 46  | D     | 1        | Total O<br>1 1   | 0       |
| 46  | D     | 1        | Total O<br>1 1   | 0       |
| 46  | D     | 2        | Total O<br>2 2   | 0       |
| 46  | D     | 1        | Total O<br>1 1   | 0       |
| 46  | D     | 2        | Total O<br>2 2   | 0       |
| 46  | D     | 1        | Total O<br>1 1   | 0       |
| 46  | D     | 2        | Total O<br>2 2   | 0       |
| 46  | D     | 1        | Total O<br>1 1   | 0       |
| 46  | E     | 1        | Total O<br>1 1   | 0       |
| 46  | E     | 4        | Total O<br>4 4   | 0       |
| 46  | E     | 1        | Total O<br>1 1   | 0       |
| 46  | E     | 1        | Total O<br>1 1   | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 46  | F     | 1        | Total O<br>1 1   | 0       |
| 46  | F     | 1        | Total O<br>1 1   | 0       |
| 46  | F     | 2        | Total O<br>2 2   | 0       |
| 46  | F     | 8        | Total O<br>8 8   | 0       |
| 46  | F     | 1        | Total O<br>1 1   | 0       |
| 46  | F     | 1        | Total O<br>1 1   | 0       |
| 46  | J     | 2        | Total O<br>2 2   | 0       |
| 46  | J     | 1        | Total O<br>1 1   | 0       |
| 46  | K     | 2        | Total O<br>2 2   | 0       |
| 46  | L     | 1        | Total O<br>1 1   | 0       |
| 46  | L     | 1        | Total O<br>1 1   | 0       |
| 46  | L     | 1        | Total O<br>1 1   | 0       |
| 46  | L     | 2        | Total O<br>2 2   | 0       |
| 46  | 1     | 16       | Total O<br>16 16 | 0       |
| 46  | Z     | 1        | Total O<br>1 1   | 0       |
| 46  | Z     | 7        | Total O<br>7 7   | 0       |
| 46  | 3     | 17       | Total O<br>17 17 | 0       |
| 46  | 7     | 18       | Total O<br>18 18 | 0       |
| 46  | 8     | 1        | Total O<br>1 1   | 0       |
| 46  | 8     | 15       | Total O<br>15 15 | 0       |
| 46  | 4     | 7        | Total O<br>7 7   | 0       |

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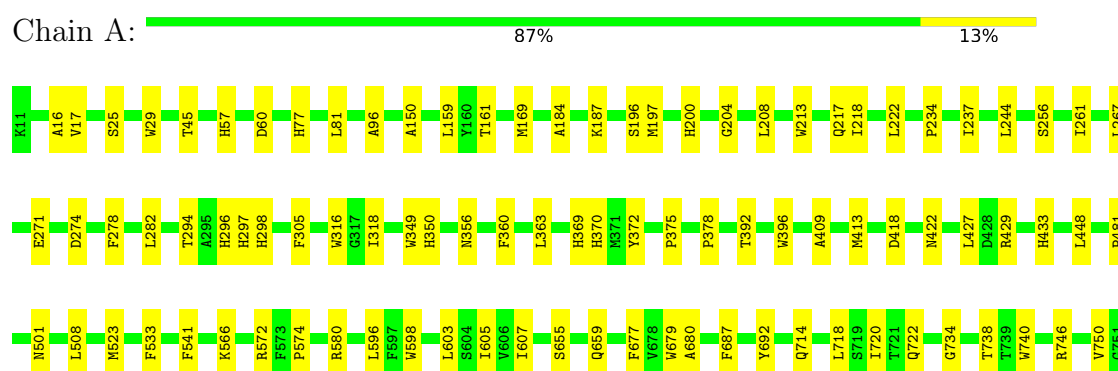
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| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 46  | 5     | 9        | Total<br>9 | O<br>9 | 0       |
| 46  | 6     | 8        | Total<br>8 | O<br>8 | 0       |
| 46  | 2     | 4        | Total<br>4 | O<br>4 | 0       |
| 46  | 9     | 2        | Total<br>2 | O<br>2 | 0       |

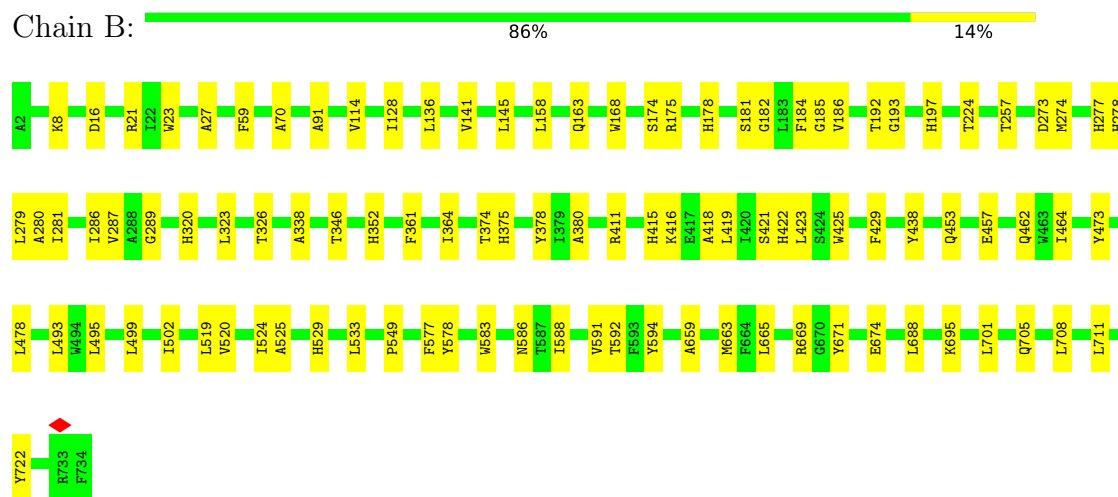
### 3 Residue-property plots

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

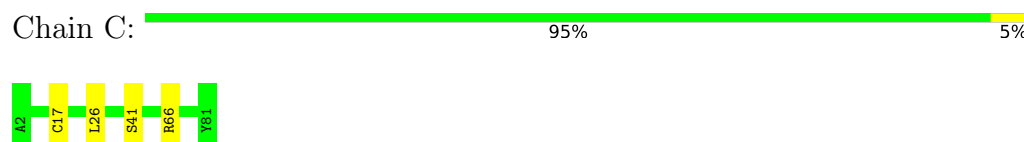
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

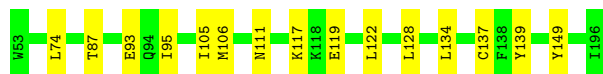


- Molecule 3: Photosystem I iron-sulfur center

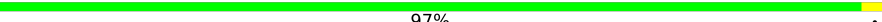


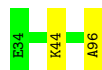
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  90% 10%



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

Chain E:  97% .



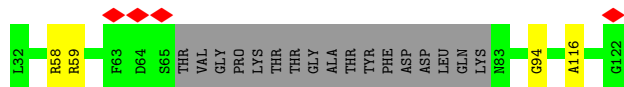
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:  93% 7%



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

Chain G:  77% 19%



- Molecule 8: Photosystem I reaction center subunit VIII

Chain I:  86% 14%



- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  90% 10%



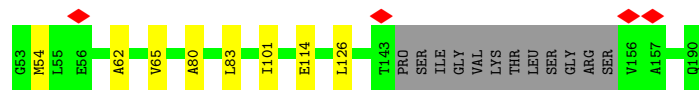
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  85% 15%



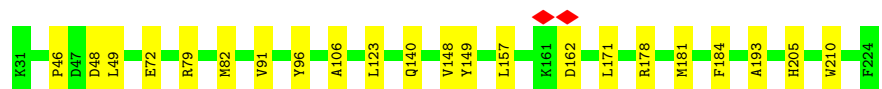
- Molecule 11: PSI subunit V

Chain L:  86% 6% 9%

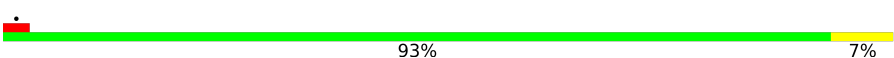


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:  89% 11%



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

Chain Z:  93% 7%



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

Chain 3:  90% 10%



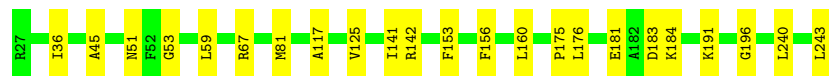
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  89% 11%



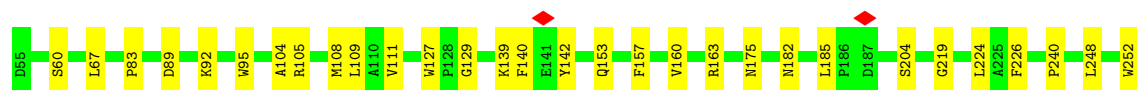
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

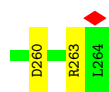
Chain 8:  89% 11%



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

Chain 4:  85% 15%





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

Chain 5: 89% 11%



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

Chain 6: 90% 10%



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

Chain 2: 81% 19%



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

Chain 9: 86% 14%



## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, C1                     | Depositor |
| Number of particles used             | 103082                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method                | NONE                          | Depositor |
| Microscope                           | FEI TITAN KRIOS               | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 46.8                          | Depositor |
| Minimum defocus (nm)                 | Not provided                  |           |
| Maximum defocus (nm)                 | Not provided                  |           |
| Magnification                        | 165000                        | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 0.125                         | Depositor |
| Minimum map value                    | -0.058                        | Depositor |
| Average map value                    | 0.000                         | Depositor |
| Map value standard deviation         | 0.005                         | Depositor |
| Recommended contour level            | 0.01                          | Depositor |
| Map size ( $\text{\AA}$ )            | 264.64, 264.64, 264.64        | wwPDB     |
| Map dimensions                       | 320, 320, 320                 | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.827, 0.827, 0.827           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, SNC, QTB, PLM, CA, PQN, LPX, LMT, C7Z, T7X, LHG, SPH, CLA, DGD, 3PH, DAO, NKP, DGA, SF4, RRX, SQD, CL0, LMG, CHL, OCA, LUT

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     | 0.22         | 0/6016  | 0.48        | 0/8201         |
| 2   | B     | 0.24         | 0/6037  | 0.50        | 1/8242 (0.0%)  |
| 3   | C     | 0.16         | 0/611   | 0.47        | 0/826          |
| 4   | D     | 0.17         | 0/1154  | 0.48        | 0/1556         |
| 5   | E     | 0.14         | 0/507   | 0.36        | 0/689          |
| 6   | F     | 0.20         | 0/1292  | 0.45        | 0/1747         |
| 7   | G     | 0.17         | 0/561   | 0.42        | 0/760          |
| 8   | I     | 0.28         | 0/294   | 0.58        | 0/406          |
| 9   | J     | 0.23         | 0/332   | 0.42        | 0/454          |
| 10  | K     | 0.15         | 0/576   | 0.40        | 0/779          |
| 11  | L     | 0.19         | 0/935   | 0.42        | 0/1277         |
| 12  | 1     | 0.17         | 0/1491  | 0.40        | 0/2028         |
| 12  | Z     | 0.15         | 0/1491  | 0.38        | 0/2028         |
| 13  | 3     | 0.22         | 0/1722  | 0.48        | 0/2336         |
| 14  | 7     | 0.19         | 0/1702  | 0.46        | 0/2310         |
| 15  | 8     | 0.19         | 0/1701  | 0.42        | 0/2315         |
| 16  | 4     | 0.19         | 0/1683  | 0.43        | 0/2296         |
| 17  | 5     | 0.17         | 0/1830  | 0.38        | 0/2492         |
| 18  | 6     | 0.18         | 0/1828  | 0.39        | 0/2497         |
| 19  | 2     | 0.20         | 0/1556  | 0.50        | 0/2109         |
| 20  | 9     | 0.23         | 0/1447  | 0.52        | 0/1967         |
| All | All   | 0.20         | 0/34766 | 0.46        | 1/47315 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | B     | 669 | ARG  | N-CA-C | 5.37 | 117.57      | 111.02   |

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     | 5820  | 0        | 5670     | 74      | 0            |
| 2   | B     | 5825  | 0        | 5579     | 79      | 0            |
| 3   | C     | 601   | 0        | 581      | 3       | 0            |
| 4   | D     | 1135  | 0        | 1148     | 8       | 0            |
| 5   | E     | 497   | 0        | 491      | 1       | 0            |
| 6   | F     | 1266  | 0        | 1301     | 9       | 0            |
| 7   | G     | 550   | 0        | 532      | 3       | 0            |
| 8   | I     | 282   | 0        | 292      | 4       | 0            |
| 9   | J     | 321   | 0        | 322      | 4       | 0            |
| 10  | K     | 571   | 0        | 606      | 11      | 0            |
| 11  | L     | 914   | 0        | 921      | 5       | 0            |
| 12  | 1     | 1445  | 0        | 1396     | 17      | 0            |
| 12  | Z     | 1445  | 0        | 1396     | 12      | 0            |
| 13  | 3     | 1674  | 0        | 1633     | 21      | 0            |
| 14  | 7     | 1650  | 0        | 1589     | 19      | 0            |
| 15  | 8     | 1650  | 0        | 1629     | 17      | 0            |
| 16  | 4     | 1628  | 0        | 1576     | 25      | 0            |
| 17  | 5     | 1775  | 0        | 1746     | 23      | 0            |
| 18  | 6     | 1766  | 0        | 1765     | 21      | 0            |
| 19  | 2     | 1518  | 0        | 1512     | 34      | 0            |
| 20  | 9     | 1406  | 0        | 1386     | 21      | 0            |
| 21  | A     | 65    | 0        | 72       | 5       | 0            |
| 22  | 1     | 712   | 0        | 712      | 24      | 0            |
| 22  | 2     | 500   | 0        | 398      | 10      | 0            |
| 22  | 3     | 748   | 0        | 720      | 28      | 0            |
| 22  | 4     | 613   | 0        | 567      | 19      | 0            |
| 22  | 5     | 799   | 0        | 758      | 28      | 0            |
| 22  | 6     | 759   | 0        | 741      | 28      | 0            |
| 22  | 7     | 790   | 0        | 752      | 24      | 0            |
| 22  | 8     | 694   | 0        | 671      | 27      | 0            |
| 22  | 9     | 531   | 0        | 464      | 16      | 0            |
| 22  | A     | 2699  | 0        | 2865     | 115     | 0            |
| 22  | B     | 2680  | 0        | 2837     | 109     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | F     | 110   | 0        | 105      | 5       | 0            |
| 22  | G     | 96    | 0        | 72       | 0       | 0            |
| 22  | J     | 42    | 0        | 31       | 3       | 0            |
| 22  | K     | 205   | 0        | 168      | 7       | 0            |
| 22  | L     | 115   | 0        | 110      | 1       | 0            |
| 22  | Z     | 622   | 0        | 584      | 17      | 0            |
| 23  | A     | 33    | 0        | 46       | 1       | 0            |
| 23  | B     | 33    | 0        | 46       | 0       | 0            |
| 24  | A     | 8     | 0        | 0        | 0       | 0            |
| 24  | C     | 16    | 0        | 0        | 1       | 0            |
| 25  | 3     | 160   | 0        | 211      | 9       | 0            |
| 25  | 4     | 40    | 0        | 53       | 2       | 0            |
| 25  | 5     | 80    | 0        | 105      | 6       | 0            |
| 25  | 6     | 80    | 0        | 106      | 4       | 0            |
| 25  | 7     | 80    | 0        | 106      | 4       | 0            |
| 25  | 8     | 40    | 0        | 53       | 1       | 0            |
| 25  | A     | 200   | 0        | 264      | 14      | 0            |
| 25  | B     | 280   | 0        | 370      | 18      | 0            |
| 25  | G     | 40    | 0        | 53       | 1       | 0            |
| 25  | I     | 40    | 0        | 52       | 3       | 0            |
| 25  | J     | 40    | 0        | 53       | 4       | 0            |
| 25  | K     | 80    | 0        | 106      | 5       | 0            |
| 25  | L     | 80    | 0        | 106      | 3       | 0            |
| 26  | 1     | 43    | 0        | 56       | 1       | 0            |
| 26  | 2     | 34    | 0        | 38       | 2       | 0            |
| 26  | 3     | 20    | 0        | 12       | 0       | 0            |
| 26  | 4     | 81    | 0        | 108      | 1       | 0            |
| 26  | 5     | 37    | 0        | 44       | 0       | 0            |
| 26  | 6     | 49    | 0        | 74       | 4       | 0            |
| 26  | 7     | 37    | 0        | 44       | 2       | 0            |
| 26  | 8     | 38    | 0        | 46       | 0       | 0            |
| 26  | 9     | 33    | 0        | 36       | 0       | 0            |
| 26  | A     | 84    | 0        | 114      | 7       | 0            |
| 26  | B     | 76    | 0        | 64       | 2       | 0            |
| 26  | Z     | 43    | 0        | 56       | 1       | 0            |
| 27  | 3     | 16    | 0        | 12       | 0       | 0            |
| 27  | 8     | 29    | 0        | 39       | 0       | 0            |
| 27  | A     | 29    | 0        | 39       | 0       | 0            |
| 28  | 1     | 35    | 0        | 45       | 2       | 0            |
| 28  | 4     | 35    | 0        | 44       | 1       | 0            |
| 28  | 8     | 35    | 0        | 46       | 1       | 0            |
| 28  | 9     | 35    | 0        | 45       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | A     | 35    | 0        | 46       | 1       | 0            |
| 28  | B     | 70    | 0        | 90       | 5       | 0            |
| 28  | F     | 35    | 0        | 45       | 0       | 0            |
| 29  | A     | 10    | 0        | 15       | 0       | 0            |
| 30  | A     | 14    | 0        | 23       | 0       | 0            |
| 31  | A     | 29    | 0        | 28       | 1       | 0            |
| 31  | J     | 35    | 0        | 40       | 1       | 0            |
| 32  | 9     | 39    | 0        | 63       | 4       | 0            |
| 32  | A     | 44    | 0        | 76       | 5       | 0            |
| 33  | B     | 66    | 0        | 96       | 4       | 0            |
| 34  | B     | 1     | 0        | 0        | 0       | 0            |
| 35  | B     | 49    | 0        | 0        | 0       | 0            |
| 36  | F     | 41    | 0        | 56       | 1       | 0            |
| 37  | 1     | 42    | 0        | 0        | 0       | 0            |
| 37  | 5     | 42    | 0        | 0        | 0       | 0            |
| 37  | J     | 42    | 0        | 0        | 0       | 0            |
| 38  | 7     | 42    | 0        | 74       | 2       | 0            |
| 38  | K     | 21    | 0        | 37       | 1       | 0            |
| 39  | 1     | 84    | 0        | 110      | 6       | 0            |
| 39  | 2     | 126   | 0        | 165      | 6       | 0            |
| 39  | 3     | 84    | 0        | 110      | 7       | 0            |
| 39  | 4     | 84    | 0        | 110      | 11      | 0            |
| 39  | 5     | 84    | 0        | 110      | 8       | 0            |
| 39  | 6     | 84    | 0        | 110      | 4       | 0            |
| 39  | 7     | 84    | 0        | 110      | 3       | 0            |
| 39  | 8     | 84    | 0        | 110      | 6       | 0            |
| 39  | 9     | 84    | 0        | 110      | 6       | 0            |
| 39  | Z     | 126   | 0        | 165      | 8       | 0            |
| 40  | 1     | 106   | 0        | 82       | 2       | 0            |
| 40  | 2     | 150   | 0        | 105      | 6       | 0            |
| 40  | 3     | 66    | 0        | 69       | 3       | 0            |
| 40  | 4     | 201   | 0        | 146      | 5       | 0            |
| 40  | 5     | 160   | 0        | 134      | 7       | 0            |
| 40  | 6     | 206   | 0        | 156      | 3       | 0            |
| 40  | 7     | 54    | 0        | 42       | 3       | 0            |
| 40  | 8     | 122   | 0        | 115      | 4       | 0            |
| 40  | 9     | 108   | 0        | 97       | 2       | 0            |
| 40  | Z     | 178   | 0        | 168      | 9       | 0            |
| 41  | 1     | 48    | 0        | 62       | 1       | 0            |
| 41  | 2     | 43    | 0        | 49       | 1       | 0            |
| 42  | Z     | 19    | 0        | 0        | 0       | 0            |
| 43  | 2     | 27    | 0        | 27       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | 5     | 23    | 0        | 19       | 0       | 0            |
| 43  | 6     | 29    | 0        | 31       | 0       | 0            |
| 43  | 7     | 39    | 0        | 51       | 1       | 0            |
| 43  | 8     | 30    | 0        | 33       | 0       | 0            |
| 44  | 7     | 18    | 0        | 31       | 0       | 0            |
| 45  | 8     | 30    | 0        | 43       | 1       | 0            |
| 46  | 1     | 16    | 0        | 0        | 0       | 0            |
| 46  | 2     | 4     | 0        | 0        | 0       | 0            |
| 46  | 3     | 17    | 0        | 0        | 0       | 0            |
| 46  | 4     | 7     | 0        | 0        | 0       | 0            |
| 46  | 5     | 9     | 0        | 0        | 0       | 0            |
| 46  | 6     | 8     | 0        | 0        | 0       | 0            |
| 46  | 7     | 18    | 0        | 0        | 0       | 0            |
| 46  | 8     | 16    | 0        | 0        | 0       | 0            |
| 46  | 9     | 2     | 0        | 0        | 0       | 0            |
| 46  | A     | 91    | 0        | 0        | 1       | 0            |
| 46  | B     | 79    | 0        | 0        | 1       | 0            |
| 46  | C     | 19    | 0        | 0        | 0       | 0            |
| 46  | D     | 12    | 0        | 0        | 0       | 0            |
| 46  | E     | 7     | 0        | 0        | 0       | 0            |
| 46  | F     | 14    | 0        | 0        | 0       | 0            |
| 46  | J     | 3     | 0        | 0        | 0       | 0            |
| 46  | K     | 2     | 0        | 0        | 0       | 0            |
| 46  | L     | 5     | 0        | 0        | 0       | 0            |
| 46  | Z     | 8     | 0        | 0        | 0       | 0            |
| All | All   | 52213 | 0        | 51749    | 775     | 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 7.

All (775) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:2:117:VAL:O     | 19:2:121:LEU:HD13  | 1.73                     | 0.88              |
| 1:A:396:TRP:CD1    | 22:A:1126:CLA:HAB  | 2.15                     | 0.82              |
| 22:A:1138:CLA:H121 | 22:A:1138:CLA:HAB  | 1.64                     | 0.79              |
| 22:B:1240:CLA:HBB1 | 22:1:605:CLA:H12   | 1.68                     | 0.74              |
| 22:F:1301:CLA:HBB1 | 36:F:4001:RRX:H11  | 1.67                     | 0.74              |
| 22:B:1238:CLA:H2   | 22:B:1239:CLA:H142 | 1.72                     | 0.71              |
| 22:A:1012:CLA:H2   | 25:A:4005:BCR:H362 | 1.72                     | 0.70              |
| 1:A:204:GLY:O      | 1:A:208:LEU:HB2    | 1.91                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1203:CLA:H151 | 22:B:1225:CLA:HBB2 | 1.73                     | 0.70              |
| 2:B:141:VAL:O      | 2:B:145:LEU:HD23   | 1.93                     | 0.68              |
| 16:4:153:GLN:NE2   | 40:4:610:CHL:OMC   | 2.26                     | 0.68              |
| 39:2:501:LUT:H361  | 39:2:501:LUT:H393  | 1.74                     | 0.68              |
| 22:A:1127:CLA:H2   | 25:A:4002:BCR:HC7  | 1.76                     | 0.68              |
| 2:B:352:HIS:ND1    | 22:B:1214:CLA:OBD  | 2.27                     | 0.68              |
| 22:A:1124:CLA:H61  | 22:A:1133:CLA:HAB  | 1.75                     | 0.67              |
| 22:A:1110:CLA:H161 | 22:A:1118:CLA:HBB1 | 1.76                     | 0.67              |
| 39:6:501:LUT:H30   | 22:6:601:CLA:H72   | 1.77                     | 0.66              |
| 1:A:370:HIS:ND1    | 22:A:1116:CLA:OBD  | 2.29                     | 0.66              |
| 19:2:117:VAL:O     | 19:2:121:LEU:CD1   | 2.42                     | 0.66              |
| 22:2:604:CLA:HHD   | 40:2:609:CHL:HBB2  | 1.78                     | 0.65              |
| 22:B:1220:CLA:HAB  | 22:B:1227:CLA:HMD2 | 1.78                     | 0.65              |
| 22:A:1104:CLA:H151 | 22:A:1127:CLA:HBB2 | 1.77                     | 0.65              |
| 25:3:504:BCR:HC21  | 22:5:609:CLA:H112  | 1.78                     | 0.65              |
| 22:A:1012:CLA:HAB  | 2:B:583:TRP:CH2    | 2.31                     | 0.65              |
| 1:A:305:PHE:HE1    | 22:A:1119:CLA:HAB  | 1.60                     | 0.65              |
| 22:A:1126:CLA:H191 | 25:J:4001:BCR:H19C | 1.79                     | 0.65              |
| 22:B:1023:CLA:H152 | 25:B:4007:BCR:H16C | 1.79                     | 0.64              |
| 15:8:181:GLU:OE1   | 15:8:184:LYS:NZ    | 2.30                     | 0.64              |
| 22:1:603:CLA:H111  | 22:1:603:CLA:HAB   | 1.77                     | 0.64              |
| 13:3:198:MET:HE2   | 39:3:502:LUT:H10   | 1.80                     | 0.63              |
| 1:A:413:MET:HE1    | 1:A:427:LEU:HD11   | 1.80                     | 0.63              |
| 2:B:27:ALA:HA      | 22:B:1226:CLA:H42  | 1.80                     | 0.62              |
| 14:7:109:VAL:HG21  | 22:7:606:CLA:HAA2  | 1.80                     | 0.62              |
| 12:1:82:MET:SD     | 22:1:601:CLA:HAB   | 2.39                     | 0.62              |
| 17:5:82:MET:SD     | 22:5:601:CLA:HAB   | 2.40                     | 0.62              |
| 13:3:65:ALA:HB1    | 13:3:191:GLY:HA3   | 1.82                     | 0.62              |
| 22:A:1121:CLA:H192 | 25:K:4001:BCR:H21C | 1.82                     | 0.61              |
| 22:A:1107:CLA:H42  | 25:J:4001:BCR:H10C | 1.83                     | 0.61              |
| 17:5:85:VAL:HG11   | 39:5:501:LUT:H12   | 1.83                     | 0.61              |
| 15:8:81:MET:SD     | 22:8:601:CLA:HAB   | 2.41                     | 0.60              |
| 18:6:79:MET:SD     | 22:6:601:CLA:HAB   | 2.41                     | 0.60              |
| 2:B:722:TYR:HB2    | 22:B:1021:CLA:HED3 | 1.83                     | 0.60              |
| 39:9:502:LUT:H32   | 22:9:604:CLA:HBB1  | 1.83                     | 0.60              |
| 40:2:609:CHL:HBC3  | 26:2:801:LHG:HC62  | 1.83                     | 0.60              |
| 1:A:196:SER:O      | 1:A:200:HIS:ND1    | 2.25                     | 0.59              |
| 22:B:1209:CLA:HBB2 | 22:B:1217:CLA:H72  | 1.84                     | 0.59              |
| 25:B:4004:BCR:HC41 | 28:B:5005:LMT:H112 | 1.82                     | 0.59              |
| 22:6:609:CLA:H2    | 26:6:801:LHG:H141  | 1.85                     | 0.59              |
| 20:9:157:LYS:HD3   | 22:9:602:CLA:HBD   | 1.83                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F:63:ASP:N       | 6:F:67:LEU:O       | 2.35                     | 0.59              |
| 17:5:78:ALA:HB1    | 17:5:190:GLY:HA3   | 1.83                     | 0.59              |
| 16:4:104:ALA:HB1   | 16:4:219:GLY:HA3   | 1.84                     | 0.59              |
| 25:5:503:BCR:H10C  | 22:6:608:CLA:H52   | 1.85                     | 0.59              |
| 22:A:1106:CLA:H71  | 25:J:4001:BCR:H343 | 1.85                     | 0.58              |
| 2:B:429:PHE:CE2    | 22:B:1235:CLA:HAB  | 2.38                     | 0.58              |
| 12:Z:149:TYR:HB3   | 22:Z:601:CLA:HED3  | 1.86                     | 0.57              |
| 22:A:1112:CLA:H122 | 32:A:5005:DGA:HBW1 | 1.84                     | 0.57              |
| 25:B:4004:BCR:H24C | 25:B:4005:BCR:H24C | 1.86                     | 0.57              |
| 1:A:448:LEU:HB3    | 1:A:541:PHE:HB2    | 1.86                     | 0.57              |
| 13:3:69:MET:SD     | 22:3:601:CLA:HAB   | 2.44                     | 0.57              |
| 39:9:501:LUT:H30   | 22:9:601:CLA:H72   | 1.85                     | 0.57              |
| 22:B:1240:CLA:HBC1 | 28:B:5005:LMT:H6E  | 1.87                     | 0.57              |
| 12:Z:82:MET:SD     | 22:Z:601:CLA:HAB   | 2.44                     | 0.57              |
| 22:7:609:CLA:H162  | 22:7:603:CLA:HBC1  | 1.85                     | 0.57              |
| 2:B:464:ILE:HD11   | 22:B:1234:CLA:H2   | 1.87                     | 0.57              |
| 14:7:165:PRO:HB3   | 22:7:611:CLA:HBC2  | 1.87                     | 0.57              |
| 22:5:605:CLA:H52   | 22:5:622:CLA:HAB   | 1.85                     | 0.57              |
| 25:4:503:BCR:H19C  | 40:4:613:CHL:H11   | 1.87                     | 0.57              |
| 18:6:82:VAL:HG11   | 39:6:501:LUT:H12   | 1.87                     | 0.56              |
| 19:2:213:VAL:HG22  | 32:9:802:DGA:HBS2  | 1.86                     | 0.56              |
| 1:A:508:LEU:HB2    | 1:A:523:MET:HG3    | 1.87                     | 0.56              |
| 22:A:1139:CLA:HBA2 | 26:A:5002:LHG:H161 | 1.87                     | 0.56              |
| 25:A:4005:BCR:H24C | 22:B:1230:CLA:HMC2 | 1.87                     | 0.56              |
| 2:B:70:ALA:HB2     | 2:B:136:LEU:HB2    | 1.86                     | 0.56              |
| 18:6:91:VAL:HG12   | 18:6:92:ARG:HG2    | 1.86                     | 0.56              |
| 13:3:100:VAL:HG21  | 39:3:502:LUT:H22   | 1.87                     | 0.56              |
| 22:B:1237:CLA:HMC2 | 22:B:1238:CLA:H11  | 1.88                     | 0.56              |
| 39:1:502:LUT:H382  | 22:1:604:CLA:H2    | 1.86                     | 0.56              |
| 22:7:602:CLA:HBB1  | 22:7:607:CLA:H143  | 1.88                     | 0.56              |
| 1:A:45:THR:HG22    | 1:A:714:GLN:HB2    | 1.87                     | 0.56              |
| 22:A:1117:CLA:HAB  | 22:A:1117:CLA:H8   | 1.87                     | 0.56              |
| 2:B:184:PHE:HZ     | 22:B:1221:CLA:H12  | 1.71                     | 0.56              |
| 2:B:525:ALA:O      | 2:B:529:HIS:ND1    | 2.35                     | 0.56              |
| 14:7:189:LYS:HG3   | 22:7:607:CLA:HED2  | 1.87                     | 0.56              |
| 4:D:95:ILE:HG12    | 4:D:105:ILE:HG12   | 1.87                     | 0.56              |
| 22:8:605:CLA:H122  | 22:8:604:CLA:H91   | 1.88                     | 0.56              |
| 22:8:601:CLA:H71   | 22:8:602:CLA:HMA3  | 1.88                     | 0.56              |
| 22:Z:605:CLA:H192  | 40:8:613:CHL:H11   | 1.86                     | 0.55              |
| 22:A:1119:CLA:H122 | 22:A:1122:CLA:H93  | 1.87                     | 0.55              |
| 3:C:17:CYS:HB3     | 24:C:3003:SF4:S4   | 2.47                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:Z:609:CHL:HHC   | 40:Z:609:CHL:HBB1  | 1.88                     | 0.55              |
| 16:4:127:TRP:NE1   | 16:4:129:GLY:O     | 2.39                     | 0.55              |
| 2:B:274:MET:O      | 2:B:278:HIS:ND1    | 2.40                     | 0.55              |
| 22:A:1104:CLA:H2   | 22:A:1104:CLA:HED2 | 1.89                     | 0.55              |
| 2:B:174:SER:O      | 2:B:178:HIS:ND1    | 2.26                     | 0.55              |
| 22:5:612:CLA:H43   | 22:6:619:CLA:H92   | 1.89                     | 0.55              |
| 22:B:1234:CLA:H142 | 22:B:1236:CLA:H62  | 1.89                     | 0.55              |
| 12:1:46:PRO:HG2    | 12:1:49:LEU:HB2    | 1.89                     | 0.55              |
| 22:8:609:CLA:H41   | 22:8:608:CLA:H42   | 1.88                     | 0.55              |
| 17:5:109:LEU:HD21  | 22:5:613:CLA:HAC1  | 1.89                     | 0.55              |
| 20:9:28:ARG:NH1    | 20:9:48:ASP:OD1    | 2.40                     | 0.55              |
| 16:4:108:MET:SD    | 22:4:601:CLA:HAB   | 2.46                     | 0.54              |
| 17:5:202:LEU:HD12  | 22:5:603:CLA:HAC2  | 1.88                     | 0.54              |
| 1:A:197:MET:HB2    | 22:A:1111:CLA:HBC2 | 1.89                     | 0.54              |
| 1:A:429:ARG:O      | 1:A:433:HIS:ND1    | 2.41                     | 0.54              |
| 1:A:596:LEU:HD21   | 22:A:1128:CLA:HBC1 | 1.88                     | 0.54              |
| 13:3:147:PHE:CE2   | 40:3:611:CHL:HBB2  | 2.42                     | 0.54              |
| 25:3:504:BCR:H10C  | 40:3:611:CHL:HBA1  | 1.89                     | 0.54              |
| 22:3:616:CLA:H8    | 22:3:616:CLA:HBB1  | 1.88                     | 0.54              |
| 18:6:205:LEU:HD12  | 39:6:501:LUT:H163  | 1.89                     | 0.54              |
| 19:2:209:VAL:HG13  | 32:9:802:DGA:HBT2  | 1.90                     | 0.54              |
| 20:9:126:ARG:HA    | 20:9:142:PHE:HZ    | 1.71                     | 0.54              |
| 8:I:96:PHE:HB2     | 25:L:4001:BCR:H14C | 1.90                     | 0.54              |
| 22:B:1205:CLA:HAB  | 22:B:1206:CLA:HAA1 | 1.90                     | 0.54              |
| 1:A:396:TRP:HD1    | 22:A:1126:CLA:HAB  | 1.70                     | 0.54              |
| 22:A:1115:CLA:H91  | 22:K:1402:CLA:HBC3 | 1.90                     | 0.54              |
| 14:7:123:ILE:HG12  | 22:8:608:CLA:HAA2  | 1.89                     | 0.54              |
| 1:A:305:PHE:CE1    | 22:A:1119:CLA:HAB  | 2.40                     | 0.54              |
| 25:5:504:BCR:H361  | 40:5:610:CHL:HBA2  | 1.90                     | 0.54              |
| 6:F:201:GLY:HA3    | 15:8:59:LEU:HD21   | 1.89                     | 0.54              |
| 26:Z:801:LHG:HC82  | 25:4:503:BCR:HC22  | 1.89                     | 0.54              |
| 22:5:602:CLA:H141  | 22:5:607:CLA:H13   | 1.90                     | 0.54              |
| 26:B:5001:LHG:O3   | 26:B:5001:LHG:O1   | 2.26                     | 0.53              |
| 12:1:193:ALA:HB2   | 22:1:615:CLA:HED3  | 1.90                     | 0.53              |
| 2:B:8:LYS:HE2      | 22:B:1241:CLA:HAA1 | 1.90                     | 0.53              |
| 2:B:192:THR:HG21   | 2:B:279:LEU:HB2    | 1.89                     | 0.53              |
| 22:K:1401:CLA:HBB1 | 25:K:4002:BCR:H10C | 1.89                     | 0.53              |
| 17:5:172:PHE:HD2   | 39:5:501:LUT:H222  | 1.73                     | 0.53              |
| 16:4:260:ASP:OD1   | 16:4:263:ARG:NH2   | 2.40                     | 0.53              |
| 2:B:182:GLY:HA3    | 22:B:1210:CLA:HBB1 | 1.91                     | 0.53              |
| 32:9:802:DGA:HBN2  | 28:9:803:LMT:H101  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:572:ARG:NH1    | 26:A:5002:LHG:O10  | 2.42                     | 0.53              |
| 2:B:549:PRO:HB3    | 6:F:226:PRO:HG2    | 1.90                     | 0.53              |
| 14:7:195:ARG:NH2   | 22:7:604:CLA:O1D   | 2.41                     | 0.53              |
| 13:3:62:VAL:HG11   | 13:3:161:ALA:HB1   | 1.91                     | 0.52              |
| 25:5:503:BCR:H19C  | 22:5:613:CLA:H2    | 1.92                     | 0.52              |
| 39:4:501:LUT:H30   | 22:4:601:CLA:H52   | 1.91                     | 0.52              |
| 22:A:1105:CLA:H12  | 22:J:1901:CLA:HBC1 | 1.92                     | 0.52              |
| 13:3:40:LEU:HD22   | 39:3:502:LUT:H222  | 1.92                     | 0.52              |
| 14:7:129:GLY:O     | 14:7:133:THR:OG1   | 2.25                     | 0.52              |
| 16:4:60:SER:HB2    | 16:4:67:LEU:HD11   | 1.91                     | 0.52              |
| 39:4:502:LUT:H30   | 22:4:604:CLA:H72   | 1.90                     | 0.52              |
| 18:6:251:PHE:HB2   | 25:6:504:BCR:H282  | 1.91                     | 0.52              |
| 14:7:80:MET:SD     | 22:7:601:CLA:HAB   | 2.49                     | 0.52              |
| 20:9:78:MET:SD     | 22:9:601:CLA:HAB   | 2.49                     | 0.52              |
| 1:A:501:ASN:HB3    | 22:A:1115:CLA:HED2 | 1.91                     | 0.52              |
| 12:Z:79:ARG:NH1    | 22:Z:611:CLA:OBD   | 2.43                     | 0.52              |
| 19:2:198:ILE:HG21  | 22:2:603:CLA:H42   | 1.91                     | 0.52              |
| 2:B:423:LEU:HD13   | 2:B:533:LEU:HA     | 1.92                     | 0.52              |
| 1:A:77:HIS:ND1     | 22:A:1111:CLA:OBD  | 2.42                     | 0.51              |
| 1:A:274:ASP:N      | 1:A:274:ASP:OD1    | 2.41                     | 0.51              |
| 1:A:481:PRO:HG3    | 1:A:533:PHE:HB2    | 1.92                     | 0.51              |
| 22:A:1104:CLA:H8   | 26:A:5002:LHG:H351 | 1.91                     | 0.51              |
| 1:A:169:MET:HE2    | 32:A:5005:DGA:HAG1 | 1.92                     | 0.51              |
| 1:A:256:SER:OG     | 1:A:271:GLU:O      | 2.23                     | 0.51              |
| 2:B:361:PHE:HB3    | 2:B:364:ILE:HD11   | 1.92                     | 0.51              |
| 15:8:191:LYS:HD3   | 22:8:602:CLA:HBA2  | 1.92                     | 0.51              |
| 19:2:33:PRO:O      | 20:9:128:GLN:NE2   | 2.41                     | 0.51              |
| 19:2:78:MET:SD     | 22:2:601:CLA:HAB   | 2.49                     | 0.51              |
| 2:B:418:ALA:O      | 2:B:422:HIS:ND1    | 2.33                     | 0.51              |
| 22:A:1137:CLA:H143 | 25:A:4004:BCR:H371 | 1.92                     | 0.51              |
| 14:7:147:ASP:OD1   | 14:7:147:ASP:N     | 2.43                     | 0.51              |
| 13:3:42:LEU:HD13   | 22:3:604:CLA:H42   | 1.92                     | 0.51              |
| 1:A:734:GLY:O      | 1:A:738:THR:OG1    | 2.28                     | 0.51              |
| 22:K:1401:CLA:HBB1 | 25:K:4002:BCR:C11  | 2.41                     | 0.51              |
| 17:5:198:MET:HG3   | 22:5:605:CLA:HBB2  | 1.93                     | 0.51              |
| 25:5:503:BCR:HC42  | 26:6:801:LHG:H111  | 1.92                     | 0.51              |
| 19:2:162:ARG:HA    | 19:2:165:MET:HE3   | 1.93                     | 0.51              |
| 22:A:1121:CLA:H11  | 10:K:65:LEU:HD11   | 1.92                     | 0.51              |
| 22:A:1126:CLA:H92  | 22:A:1126:CLA:H41  | 1.92                     | 0.51              |
| 22:5:602:CLA:HHC   | 22:5:602:CLA:HBB1  | 1.93                     | 0.51              |
| 1:A:580:ARG:NH1    | 46:A:6042:HOH:O    | 2.43                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:5:131:TRP:HB2   | 22:6:609:CLA:H11   | 1.91                     | 0.51              |
| 19:2:117:VAL:HG12  | 19:2:121:LEU:HD13  | 1.93                     | 0.51              |
| 1:A:244:LEU:O      | 28:A:5006:LMT:O2'  | 2.29                     | 0.51              |
| 22:B:1212:CLA:H43  | 25:B:4003:BCR:H313 | 1.92                     | 0.51              |
| 22:B:1220:CLA:H171 | 22:B:1240:CLA:H51  | 1.93                     | 0.50              |
| 14:7:223:LEU:HD22  | 18:6:225:PRO:HB3   | 1.92                     | 0.50              |
| 20:9:149:MET:HE2   | 22:9:601:CLA:H42   | 1.92                     | 0.50              |
| 13:3:216:LEU:HB2   | 39:3:501:LUT:H22   | 1.93                     | 0.50              |
| 39:5:502:LUT:H371  | 22:5:604:CLA:H142  | 1.92                     | 0.50              |
| 2:B:588:ILE:HA     | 2:B:591:VAL:HG22   | 1.93                     | 0.50              |
| 22:B:1228:CLA:HBC2 | 22:B:1236:CLA:HMC2 | 1.93                     | 0.50              |
| 22:3:605:CLA:H101  | 22:3:612:CLA:H42   | 1.92                     | 0.50              |
| 22:3:613:CLA:H8    | 22:5:615:CLA:H42   | 1.92                     | 0.50              |
| 19:2:75:ARG:NE     | 19:2:157:GLU:OE2   | 2.38                     | 0.50              |
| 22:A:1012:CLA:HBC2 | 2:B:586:ASN:HB2    | 1.92                     | 0.50              |
| 22:A:1116:CLA:HAC1 | 22:A:1133:CLA:H42  | 1.92                     | 0.50              |
| 22:B:1222:CLA:H61  | 22:B:1240:CLA:H201 | 1.94                     | 0.50              |
| 39:8:501:LUT:H30   | 22:8:601:CLA:H72   | 1.93                     | 0.50              |
| 19:2:220:ILE:HD11  | 28:9:803:LMT:H81   | 1.93                     | 0.50              |
| 25:3:505:BCR:H343  | 22:3:603:CLA:HBC1  | 1.92                     | 0.50              |
| 17:5:90:VAL:HG11   | 22:5:606:CLA:HAC2  | 1.93                     | 0.50              |
| 22:B:1234:CLA:HMB1 | 22:B:1236:CLA:HED1 | 1.93                     | 0.50              |
| 22:7:616:CLA:H11   | 18:6:251:PHE:HA    | 1.94                     | 0.50              |
| 39:4:502:LUT:H32   | 22:4:604:CLA:HAB   | 1.94                     | 0.50              |
| 1:A:218:ILE:HA     | 1:A:222:LEU:HD12   | 1.94                     | 0.50              |
| 1:A:297:HIS:HB2    | 22:A:1116:CLA:C1B  | 2.42                     | 0.50              |
| 2:B:416:LYS:HA     | 2:B:419:LEU:HD12   | 1.94                     | 0.50              |
| 15:8:240:LEU:HD13  | 15:8:243:LEU:HD12  | 1.94                     | 0.50              |
| 22:6:609:CLA:HBB2  | 22:6:604:CLA:HHD   | 1.93                     | 0.50              |
| 22:B:1225:CLA:H8   | 25:B:4002:BCR:H21C | 1.93                     | 0.50              |
| 17:5:135:ARG:NH2   | 17:5:146:VAL:O     | 2.45                     | 0.50              |
| 12:1:72:GLU:HB3    | 12:1:148:VAL:HG22  | 1.93                     | 0.49              |
| 1:A:598:TRP:CH2    | 22:B:1022:CLA:HAB  | 2.48                     | 0.49              |
| 22:B:1216:CLA:H12  | 22:B:1221:CLA:HBB1 | 1.94                     | 0.49              |
| 22:A:1110:CLA:HHC  | 22:A:1110:CLA:HBB1 | 1.94                     | 0.49              |
| 2:B:185:GLY:HA3    | 2:B:286:ILE:HG13   | 1.94                     | 0.49              |
| 12:Z:46:PRO:HG2    | 12:Z:49:LEU:HB2    | 1.93                     | 0.49              |
| 22:7:601:CLA:H71   | 22:7:602:CLA:HMA2  | 1.95                     | 0.49              |
| 22:A:1109:CLA:H72  | 22:A:1101:CLA:HBB2 | 1.94                     | 0.49              |
| 22:A:1120:CLA:HED1 | 10:K:61:THR:H      | 1.76                     | 0.49              |
| 2:B:438:TYR:CD2    | 22:B:1021:CLA:H203 | 2.47                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:7:801:LHG:H101  | 26:7:801:LHG:H292  | 1.94                     | 0.49              |
| 12:1:106:ALA:HB1   | 12:1:123:LEU:HD22  | 1.94                     | 0.49              |
| 1:A:409:ALA:HB1    | 25:A:4003:BCR:H271 | 1.95                     | 0.49              |
| 22:F:1301:CLA:H93  | 22:1:615:CLA:HBB   | 1.94                     | 0.49              |
| 22:1:608:CLA:H11   | 40:Z:610:CHL:H203  | 1.94                     | 0.49              |
| 40:4:617:CHL:HHC   | 40:4:617:CHL:HBB1  | 1.95                     | 0.49              |
| 19:2:168:PHE:CZ    | 39:2:502:LUT:H30   | 2.48                     | 0.49              |
| 22:A:1138:CLA:H172 | 22:A:1140:CLA:H52  | 1.94                     | 0.49              |
| 2:B:224:THR:OG1    | 20:9:204:THR:O     | 2.31                     | 0.49              |
| 40:2:609:CHL:HHC   | 40:2:609:CHL:HBB1  | 1.95                     | 0.49              |
| 40:9:613:CHL:HHC   | 40:9:613:CHL:HBB1  | 1.95                     | 0.48              |
| 2:B:659:ALA:C      | 22:B:1023:CLA:HAB  | 2.39                     | 0.48              |
| 22:B:1224:CLA:HBA2 | 22:B:1224:CLA:H3A  | 1.59                     | 0.48              |
| 6:F:140:ALA:HA     | 6:F:145:HIS:HB2    | 1.94                     | 0.48              |
| 19:2:46:LEU:O      | 19:2:67:ARG:NH2    | 2.42                     | 0.48              |
| 22:A:1138:CLA:HED2 | 2:B:425:TRP:HB2    | 1.95                     | 0.48              |
| 2:B:457:GLU:OE1    | 6:F:132:HIS:ND1    | 2.41                     | 0.48              |
| 12:1:149:TYR:HB3   | 22:1:601:CLA:HED3  | 1.95                     | 0.48              |
| 22:3:606:CLA:H3A   | 22:3:606:CLA:HBA2  | 1.56                     | 0.48              |
| 18:6:192:MET:HE1   | 18:6:251:PHE:HB3   | 1.95                     | 0.48              |
| 40:6:617:CHL:HHC   | 40:6:617:CHL:HBB1  | 1.95                     | 0.48              |
| 5:E:44:LYS:HB2     | 5:E:96:ALA:HB3     | 1.94                     | 0.48              |
| 13:3:142:MET:HE1   | 14:7:35:PRO:HB2    | 1.96                     | 0.48              |
| 20:9:81:VAL:HG11   | 39:9:501:LUT:H12   | 1.96                     | 0.48              |
| 22:2:605:CLA:HBC1  | 40:2:610:CHL:HAB   | 1.95                     | 0.48              |
| 1:A:740:TRP:HB2    | 22:A:1126:CLA:HBB1 | 1.95                     | 0.48              |
| 13:3:27:LEU:HD21   | 13:3:43:LEU:HD12   | 1.95                     | 0.48              |
| 22:2:602:CLA:HBC1  | 22:2:607:CLA:HBC2  | 1.96                     | 0.48              |
| 1:A:598:TRP:HE1    | 22:B:1023:CLA:C1D  | 2.27                     | 0.48              |
| 22:A:1129:CLA:HAB  | 22:A:1137:CLA:HBB2 | 1.96                     | 0.48              |
| 13:3:162:TYR:HB3   | 22:3:601:CLA:HED3  | 1.96                     | 0.48              |
| 22:3:606:CLA:H2    | 22:3:613:CLA:CAD   | 2.44                     | 0.48              |
| 22:A:1114:CLA:H2   | 32:A:5005:DGA:HB22 | 1.96                     | 0.48              |
| 22:A:1122:CLA:HMD3 | 22:A:1123:CLA:HAB  | 1.94                     | 0.48              |
| 25:A:4001:BCR:H362 | 25:A:4002:BCR:H21C | 1.96                     | 0.48              |
| 38:7:804:SPH:H91   | 22:7:616:CLA:HAC2  | 1.95                     | 0.48              |
| 22:A:1116:CLA:H3A  | 22:A:1116:CLA:HBA2 | 1.59                     | 0.47              |
| 2:B:175:ARG:NH2    | 46:B:6051:HOH:O    | 2.47                     | 0.47              |
| 19:2:28:ARG:NH2    | 19:2:41:LEU:O      | 2.41                     | 0.47              |
| 1:A:679:TRP:CD2    | 21:A:1011:CL0:H5   | 2.50                     | 0.47              |
| 22:A:1116:CLA:O1A  | 22:A:1125:CLA:HBB2 | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:280:ALA:CB     | 22:B:1214:CLA:HAB  | 2.44                     | 0.47              |
| 22:B:1216:CLA:HBA2 | 22:B:1216:CLA:H3A  | 1.48                     | 0.47              |
| 22:4:605:CLA:HAC2  | 40:4:610:CHL:HBB2  | 1.96                     | 0.47              |
| 28:B:5005:LMT:H2'  | 28:1:803:LMT:H6'1  | 1.96                     | 0.47              |
| 38:K:5001:SPH:H72  | 13:3:229:LEU:HD22  | 1.96                     | 0.47              |
| 38:7:803:SPH:H142  | 22:8:607:CLA:H72   | 1.96                     | 0.47              |
| 19:2:165:MET:SD    | 22:2:604:CLA:HAB   | 2.54                     | 0.47              |
| 39:9:502:LUT:H32   | 22:9:604:CLA:CBB   | 2.44                     | 0.47              |
| 22:A:1138:CLA:H3A  | 22:A:1138:CLA:HBA2 | 1.67                     | 0.47              |
| 2:B:520:VAL:HG21   | 2:B:594:TYR:HB2    | 1.96                     | 0.47              |
| 22:3:618:CLA:HMA2  | 22:7:609:CLA:H93   | 1.97                     | 0.47              |
| 22:A:1114:CLA:C4C  | 22:3:610:CLA:HBB2  | 2.44                     | 0.47              |
| 22:B:1209:CLA:HHC  | 22:B:1209:CLA:HBB1 | 1.97                     | 0.47              |
| 22:B:1229:CLA:HBB2 | 25:B:4006:BCR:HC41 | 1.97                     | 0.47              |
| 22:1:608:CLA:H8    | 40:Z:610:CHL:H13   | 1.97                     | 0.47              |
| 2:B:181:SER:HB3    | 2:B:289:GLY:HA3    | 1.97                     | 0.47              |
| 22:B:1203:CLA:H111 | 22:B:1203:CLA:H71  | 1.57                     | 0.47              |
| 22:B:1236:CLA:H42  | 25:B:4005:BCR:H352 | 1.97                     | 0.47              |
| 8:I:95:LEU:O       | 8:I:99:ILE:HG12    | 2.15                     | 0.47              |
| 11:L:126:LEU:HD11  | 41:2:803:SQD:H312  | 1.96                     | 0.47              |
| 41:1:802:SQD:O9    | 15:8:142:ARG:NH2   | 2.41                     | 0.47              |
| 22:4:604:CLA:H3A   | 22:4:604:CLA:HBA2  | 1.62                     | 0.47              |
| 1:A:261:ILE:HD11   | 13:3:207:MET:HE1   | 1.95                     | 0.47              |
| 1:A:692:TYR:CE1    | 22:A:1013:CLA:HMD1 | 2.49                     | 0.47              |
| 22:B:1217:CLA:HBA2 | 22:B:1217:CLA:H3A  | 1.56                     | 0.47              |
| 22:B:1235:CLA:HBA2 | 22:B:1235:CLA:H3A  | 1.62                     | 0.47              |
| 12:1:91:VAL:HG23   | 12:1:96:TYR:HB2    | 1.96                     | 0.47              |
| 22:3:606:CLA:H102  | 22:5:615:CLA:H2    | 1.97                     | 0.47              |
| 22:7:607:CLA:H141  | 22:7:607:CLA:H161  | 1.80                     | 0.47              |
| 40:7:610:CHL:HHC   | 40:7:610:CHL:HBB1  | 1.96                     | 0.47              |
| 40:5:617:CHL:HHC   | 40:5:617:CHL:HBB1  | 1.96                     | 0.47              |
| 20:9:163:ARG:HA    | 20:9:166:MET:HE3   | 1.97                     | 0.47              |
| 22:A:1115:CLA:H93  | 10:K:101:VAL:HG12  | 1.97                     | 0.47              |
| 2:B:287:VAL:HG22   | 25:B:4001:BCR:H14C | 1.97                     | 0.47              |
| 12:Z:58:LEU:HD11   | 15:8:175:PRO:HB3   | 1.96                     | 0.47              |
| 16:4:157:PHE:HA    | 16:4:160:VAL:HG22  | 1.95                     | 0.47              |
| 22:4:612:CLA:H12   | 28:4:803:LMT:H92   | 1.96                     | 0.47              |
| 19:2:29:PRO:HG3    | 26:2:801:LHG:HC31  | 1.96                     | 0.47              |
| 22:A:1130:CLA:HBB1 | 22:A:1136:CLA:H193 | 1.97                     | 0.47              |
| 26:A:5001:LHG:H111 | 26:A:5001:LHG:H242 | 1.96                     | 0.47              |
| 6:F:196:ALA:HB1    | 22:F:1302:CLA:HED2 | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:7:610:CHL:CMC   | 22:7:613:CLA:HAB   | 2.45                     | 0.47              |
| 40:5:610:CHL:H142  | 22:6:619:CLA:H8    | 1.96                     | 0.47              |
| 40:2:610:CHL:HHC   | 40:2:610:CHL:HBB1  | 1.97                     | 0.47              |
| 15:8:36:ILE:HD12   | 15:8:53:GLY:HA3    | 1.97                     | 0.47              |
| 15:8:67:ARG:NH2    | 15:8:141:ILE:O     | 2.43                     | 0.47              |
| 22:B:1209:CLA:H43  | 28:B:6101:LMT:H41  | 1.97                     | 0.46              |
| 22:B:1240:CLA:H3A  | 22:B:1240:CLA:HBA2 | 1.47                     | 0.46              |
| 4:D:87:THR:HA      | 4:D:111:ASN:O      | 2.14                     | 0.46              |
| 7:G:58:ARG:NH2     | 7:G:94:GLY:O       | 2.47                     | 0.46              |
| 17:5:191:ARG:HA    | 17:5:194:MET:HE3   | 1.96                     | 0.46              |
| 22:5:601:CLA:H3A   | 22:5:601:CLA:HBA2  | 1.58                     | 0.46              |
| 19:2:117:VAL:C     | 19:2:121:LEU:HD13  | 2.38                     | 0.46              |
| 1:A:267:LEU:O      | 10:K:108:LYS:NZ    | 2.43                     | 0.46              |
| 22:A:1012:CLA:H112 | 22:B:1230:CLA:HBC1 | 1.97                     | 0.46              |
| 22:B:1222:CLA:H42  | 22:B:1235:CLA:HBA1 | 1.97                     | 0.46              |
| 1:A:418:ASP:O      | 1:A:422:ASN:ND2    | 2.47                     | 0.46              |
| 22:A:1111:CLA:H93  | 22:A:1111:CLA:H111 | 1.81                     | 0.46              |
| 22:B:1236:CLA:H193 | 22:B:1236:CLA:H102 | 1.97                     | 0.46              |
| 15:8:176:LEU:HD12  | 39:8:501:LUT:H222  | 1.98                     | 0.46              |
| 18:6:166:PRO:HD2   | 22:6:601:CLA:H11   | 1.97                     | 0.46              |
| 4:D:139:TYR:HD1    | 4:D:149:TYR:HA     | 1.79                     | 0.46              |
| 17:5:170:ASP:HA    | 39:5:501:LUT:H24   | 1.97                     | 0.46              |
| 18:6:208:HIS:CG    | 22:6:603:CLA:HAA2  | 2.51                     | 0.46              |
| 19:2:42:ASP:N      | 19:2:42:ASP:OD1    | 2.47                     | 0.46              |
| 2:B:352:HIS:HB3    | 22:B:1214:CLA:HED2 | 1.98                     | 0.46              |
| 12:Z:171:LEU:HD23  | 22:Z:607:CLA:HED3  | 1.96                     | 0.46              |
| 25:3:506:BCR:H271  | 22:3:604:CLA:HAC2  | 1.97                     | 0.46              |
| 1:A:213:TRP:NE1    | 22:A:1117:CLA:O1D  | 2.41                     | 0.46              |
| 2:B:277:HIS:HB2    | 22:B:1214:CLA:C1B  | 2.46                     | 0.46              |
| 22:B:1215:CLA:H3A  | 22:B:1215:CLA:HBA2 | 1.66                     | 0.46              |
| 6:F:97:ASP:OD1     | 6:F:97:ASP:N       | 2.48                     | 0.46              |
| 22:K:1402:CLA:H11  | 22:K:1402:CLA:H51  | 1.75                     | 0.46              |
| 12:Z:119:VAL:HG12  | 12:Z:121:PHE:H     | 1.80                     | 0.46              |
| 22:Z:611:CLA:H51   | 22:Z:611:CLA:H11   | 1.74                     | 0.46              |
| 13:3:153:ILE:HD13  | 17:5:58:LEU:HA     | 1.96                     | 0.46              |
| 22:8:607:CLA:HMA3  | 28:8:805:LMT:H5'   | 1.97                     | 0.46              |
| 19:2:41:LEU:HD11   | 19:2:52:ASP:HB2    | 1.98                     | 0.46              |
| 1:A:363:LEU:HD22   | 22:A:1127:CLA:HBC1 | 1.97                     | 0.46              |
| 1:A:677:PHE:CG     | 25:A:4005:BCR:H363 | 2.51                     | 0.46              |
| 2:B:524:ILE:HG12   | 2:B:591:VAL:HG12   | 1.97                     | 0.46              |
| 17:5:194:MET:SD    | 22:5:604:CLA:HBB1  | 2.56                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:5:618:CLA:H61   | 22:5:618:CLA:H41   | 1.72                     | 0.46              |
| 1:A:356:ASN:ND2    | 22:A:1103:CLA:OBD  | 2.38                     | 0.46              |
| 2:B:27:ALA:HB1     | 33:B:5003:DGD:HB21 | 1.97                     | 0.46              |
| 2:B:193:GLY:O      | 2:B:197:HIS:HB2    | 2.15                     | 0.46              |
| 2:B:374:THR:HG23   | 2:B:592:THR:HG21   | 1.98                     | 0.46              |
| 13:3:43:LEU:HD21   | 22:3:604:CLA:HMA2  | 1.97                     | 0.46              |
| 1:A:96:ALA:HB2     | 1:A:159:LEU:HB2    | 1.96                     | 0.46              |
| 22:A:1111:CLA:H61  | 22:A:1111:CLA:H41  | 1.58                     | 0.46              |
| 2:B:493:LEU:HD22   | 22:B:1213:CLA:HED2 | 1.98                     | 0.46              |
| 22:B:1205:CLA:H3A  | 22:B:1205:CLA:HBA2 | 1.67                     | 0.46              |
| 22:7:612:CLA:H3A   | 22:7:612:CLA:HBA2  | 1.54                     | 0.46              |
| 39:8:502:LUT:H35   | 39:8:502:LUT:H401  | 1.84                     | 0.46              |
| 22:8:612:CLA:HBA2  | 22:8:612:CLA:H3A   | 1.52                     | 0.46              |
| 22:6:607:CLA:H41   | 22:6:607:CLA:H62   | 1.75                     | 0.46              |
| 1:A:282:LEU:HD21   | 1:A:375:PRO:HD2    | 1.98                     | 0.46              |
| 2:B:16:ASP:HB3     | 2:B:21:ARG:HB2     | 1.98                     | 0.46              |
| 22:1:611:CLA:H51   | 22:1:611:CLA:H11   | 1.81                     | 0.46              |
| 40:3:611:CHL:HHC   | 40:3:611:CHL:HBB1  | 1.98                     | 0.46              |
| 14:7:164:TYR:HB3   | 22:7:601:CLA:HED3  | 1.98                     | 0.46              |
| 39:7:502:LUT:H35   | 39:7:502:LUT:H401  | 1.85                     | 0.46              |
| 22:A:1012:CLA:HAB  | 2:B:583:TRP:HH2    | 1.78                     | 0.45              |
| 22:A:1106:CLA:HBA2 | 22:A:1106:CLA:H3A  | 1.40                     | 0.45              |
| 2:B:438:TYR:CE1    | 2:B:519:LEU:HB3    | 2.51                     | 0.45              |
| 22:B:1206:CLA:HBA1 | 22:B:1206:CLA:H3A  | 1.52                     | 0.45              |
| 14:7:42:HIS:NE2    | 14:7:54:ASP:OD2    | 2.47                     | 0.45              |
| 19:2:75:ARG:HA     | 19:2:78:MET:HE3    | 1.98                     | 0.45              |
| 1:A:60:ASP:OD2     | 1:A:350:HIS:NE2    | 2.45                     | 0.45              |
| 22:A:1012:CLA:HMB2 | 22:B:1021:CLA:H191 | 1.98                     | 0.45              |
| 22:B:1227:CLA:HAB  | 22:B:1236:CLA:CBB  | 2.45                     | 0.45              |
| 12:Z:184:PHE:CD2   | 39:Z:502:LUT:H12   | 2.51                     | 0.45              |
| 1:A:161:THR:HG21   | 22:A:1114:CLA:HBA1 | 1.98                     | 0.45              |
| 1:A:680:ALA:HB3    | 22:A:1013:CLA:HBB2 | 1.98                     | 0.45              |
| 4:D:74:LEU:H       | 11:L:54:MET:HE1    | 1.81                     | 0.45              |
| 10:K:35:ASN:HD21   | 22:K:1401:CLA:HED2 | 1.81                     | 0.45              |
| 15:8:153:PHE:HD2   | 15:8:156:PHE:HB3   | 1.82                     | 0.45              |
| 17:5:248:PRO:HG2   | 40:5:610:CHL:H43   | 1.99                     | 0.45              |
| 19:2:156:LYS:HG3   | 22:2:607:CLA:HED2  | 1.99                     | 0.45              |
| 20:9:80:ALA:HA     | 22:9:606:CLA:HBB1  | 1.99                     | 0.45              |
| 22:9:603:CLA:HBA1  | 22:9:603:CLA:HBD   | 1.98                     | 0.45              |
| 22:B:1220:CLA:HBB1 | 22:B:1220:CLA:H162 | 1.97                     | 0.45              |
| 1:A:392:THR:HG23   | 1:A:607:ILE:HG21   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:A:1130:CLA:HBA2 | 22:A:1130:CLA:H3A  | 1.70                     | 0.45              |
| 2:B:438:TYR:HD2    | 22:B:1021:CLA:H203 | 1.81                     | 0.45              |
| 22:B:1207:CLA:HAB  | 8:I:84:GLY:HA3     | 1.98                     | 0.45              |
| 12:Z:83:LEU:HD13   | 22:Z:606:CLA:HBB2  | 1.99                     | 0.45              |
| 22:6:608:CLA:H62   | 22:6:609:CLA:H122  | 1.99                     | 0.45              |
| 22:A:1128:CLA:H191 | 22:A:1013:CLA:H191 | 1.98                     | 0.45              |
| 22:A:1136:CLA:H62  | 22:A:1136:CLA:H41  | 1.67                     | 0.45              |
| 2:B:59:PHE:HE2     | 25:B:4003:BCR:H373 | 1.82                     | 0.45              |
| 22:B:1214:CLA:H3A  | 22:B:1214:CLA:HBA2 | 1.45                     | 0.45              |
| 39:7:501:LUT:H35   | 39:7:501:LUT:H401  | 1.81                     | 0.45              |
| 22:8:609:CLA:HHC   | 22:8:609:CLA:HBB1  | 1.99                     | 0.45              |
| 39:5:501:LUT:H371  | 22:5:601:CLA:H52   | 1.98                     | 0.45              |
| 1:A:29:TRP:HE1     | 22:A:1109:CLA:CHB  | 2.29                     | 0.45              |
| 22:A:1124:CLA:H92  | 22:A:1124:CLA:H62  | 1.83                     | 0.45              |
| 22:B:1203:CLA:H51  | 33:B:5003:DGD:HB71 | 1.98                     | 0.45              |
| 22:B:1226:CLA:H41  | 22:B:1226:CLA:H62  | 1.57                     | 0.45              |
| 17:5:227:ILE:HB    | 22:5:603:CLA:H11   | 1.98                     | 0.45              |
| 22:5:609:CLA:H93   | 22:5:609:CLA:H111  | 1.86                     | 0.45              |
| 22:9:604:CLA:H141  | 22:9:604:CLA:H161  | 1.78                     | 0.45              |
| 2:B:378:TYR:CD2    | 22:B:1224:CLA:HAB  | 2.51                     | 0.45              |
| 39:1:501:LUT:H15   | 39:1:501:LUT:H201  | 1.87                     | 0.45              |
| 39:Z:503:LUT:H15   | 39:Z:503:LUT:H201  | 1.79                     | 0.45              |
| 22:Z:605:CLA:H2A   | 22:Z:605:CLA:H2    | 1.98                     | 0.45              |
| 22:8:606:CLA:H92   | 22:8:606:CLA:H61   | 1.83                     | 0.45              |
| 18:6:60:ASN:HB3    | 18:6:63:SER:HB2    | 1.98                     | 0.45              |
| 22:A:1129:CLA:CHA  | 26:A:5001:LHG:HC92 | 2.47                     | 0.45              |
| 2:B:375:HIS:HB2    | 22:B:1224:CLA:C1B  | 2.47                     | 0.45              |
| 22:6:615:CLA:HBA1  | 22:6:615:CLA:H3A   | 1.56                     | 0.45              |
| 20:9:75:ARG:HA     | 20:9:78:MET:HE3    | 1.99                     | 0.45              |
| 22:9:605:CLA:H92   | 22:9:605:CLA:H61   | 1.75                     | 0.45              |
| 1:A:17:VAL:HG11    | 1:A:184:ALA:HB1    | 1.99                     | 0.44              |
| 22:A:1103:CLA:H72  | 25:A:4002:BCR:HC8  | 1.98                     | 0.44              |
| 22:B:1023:CLA:H142 | 25:I:4001:BCR:H393 | 1.99                     | 0.44              |
| 22:B:1207:CLA:H142 | 22:B:1207:CLA:H111 | 1.76                     | 0.44              |
| 6:F:162:TYR:CE2    | 22:F:1302:CLA:HBD  | 2.52                     | 0.44              |
| 25:7:503:BCR:H10C  | 22:8:608:CLA:H41   | 1.99                     | 0.44              |
| 22:8:607:CLA:H3A   | 22:8:607:CLA:HBA2  | 1.45                     | 0.44              |
| 25:6:503:BCR:H393  | 22:6:606:CLA:H72   | 1.98                     | 0.44              |
| 20:9:32:LEU:HD12   | 20:9:32:LEU:HA     | 1.88                     | 0.44              |
| 3:C:26:LEU:HA      | 3:C:41:SER:O       | 2.17                     | 0.44              |
| 14:7:200:ALA:HA    | 22:7:603:CLA:HBB1  | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:8:81:MET:HG3    | 15:8:196:GLY:HA2   | 1.98                     | 0.44              |
| 22:5:607:CLA:H62   | 22:5:607:CLA:H102  | 1.67                     | 0.44              |
| 1:A:294:THR:O      | 1:A:298:HIS:ND1    | 2.51                     | 0.44              |
| 33:B:5003:DGD:HA51 | 33:B:5003:DGD:HA22 | 1.87                     | 0.44              |
| 14:7:115:ILE:HG12  | 25:7:504:BCR:H281  | 1.98                     | 0.44              |
| 22:7:606:CLA:HMA2  | 22:7:613:CLA:HAC2  | 1.99                     | 0.44              |
| 1:A:16:ALA:HB1     | 1:A:187:LYS:HD3    | 2.00                     | 0.44              |
| 2:B:663:MET:HB2    | 22:B:1023:CLA:C1C  | 2.48                     | 0.44              |
| 22:B:1208:CLA:H3A  | 22:B:1208:CLA:HBA2 | 1.52                     | 0.44              |
| 22:Z:607:CLA:H93   | 22:Z:607:CLA:H111  | 1.84                     | 0.44              |
| 18:6:127:ARG:NH2   | 18:6:138:VAL:O     | 2.50                     | 0.44              |
| 22:6:612:CLA:HBA2  | 22:6:612:CLA:H3A   | 1.58                     | 0.44              |
| 1:A:349:TRP:HB3    | 22:A:1103:CLA:HAC1 | 1.98                     | 0.44              |
| 1:A:740:TRP:NE1    | 22:A:1126:CLA:O1A  | 2.49                     | 0.44              |
| 21:A:1011:CL0:H15  | 22:A:1012:CLA:O1D  | 2.18                     | 0.44              |
| 2:B:578:TYR:HE1    | 2:B:711:LEU:HB2    | 1.82                     | 0.44              |
| 2:B:695:LYS:HB2    | 22:B:1238:CLA:HED3 | 2.00                     | 0.44              |
| 22:B:1209:CLA:H141 | 22:B:1209:CLA:H162 | 1.78                     | 0.44              |
| 22:B:1240:CLA:H91  | 22:B:1240:CLA:H112 | 1.87                     | 0.44              |
| 25:3:506:BCR:H351  | 25:3:506:BCR:H15C  | 1.68                     | 0.44              |
| 15:8:183:ASP:N     | 15:8:183:ASP:OD1   | 2.50                     | 0.44              |
| 16:4:83:PRO:HD2    | 39:4:502:LUT:H23   | 2.00                     | 0.44              |
| 21:A:1011:CL0:H8   | 21:A:1011:CL0:CGD  | 2.48                     | 0.44              |
| 22:A:1118:CLA:HAA2 | 10:K:87:VAL:HG13   | 2.00                     | 0.44              |
| 2:B:91:ALA:HA      | 2:B:114:VAL:HG12   | 1.99                     | 0.44              |
| 2:B:168:TRP:HB2    | 28:B:6101:LMT:H6'1 | 1.98                     | 0.44              |
| 22:B:1218:CLA:H2   | 25:B:4001:BCR:HC32 | 2.00                     | 0.44              |
| 22:B:1225:CLA:H3A  | 22:B:1225:CLA:HBA2 | 1.49                     | 0.44              |
| 22:1:604:CLA:H3A   | 22:1:604:CLA:HBA2  | 1.60                     | 0.44              |
| 25:7:503:BCR:H15C  | 25:7:503:BCR:H351  | 1.80                     | 0.44              |
| 22:8:606:CLA:HBA2  | 22:8:606:CLA:H3A   | 1.75                     | 0.44              |
| 1:A:655:SER:O      | 1:A:659:GLN:HG2    | 2.18                     | 0.44              |
| 22:A:1105:CLA:H3A  | 22:A:1105:CLA:HBA2 | 1.73                     | 0.44              |
| 22:B:1222:CLA:HBA2 | 22:B:1222:CLA:H3A  | 1.68                     | 0.44              |
| 22:3:607:CLA:H51   | 22:3:607:CLA:H11   | 1.75                     | 0.44              |
| 22:7:615:CLA:H3A   | 22:7:615:CLA:HBA2  | 1.61                     | 0.44              |
| 22:4:601:CLA:HBA2  | 22:4:601:CLA:H3A   | 1.63                     | 0.44              |
| 39:6:502:LUT:H15   | 39:6:502:LUT:H201  | 1.88                     | 0.44              |
| 22:A:1128:CLA:H41  | 22:A:1128:CLA:H62  | 1.64                     | 0.44              |
| 26:A:5002:LHG:H312 | 26:A:5002:LHG:H281 | 1.72                     | 0.44              |
| 2:B:423:LEU:HB3    | 2:B:533:LEU:HB2    | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:1216:CLA:HBC2 | 22:B:1221:CLA:H192 | 2.00                     | 0.44              |
| 12:1:140:GLN:HB3   | 22:1:611:CLA:HMC2  | 2.00                     | 0.44              |
| 22:1:606:CLA:HMA2  | 22:1:613:CLA:C3C   | 2.48                     | 0.44              |
| 22:8:605:CLA:H111  | 22:8:605:CLA:H71   | 1.74                     | 0.44              |
| 39:4:501:LUT:H35   | 39:4:501:LUT:H401  | 1.83                     | 0.44              |
| 22:B:1208:CLA:H52  | 22:B:1208:CLA:H8   | 1.82                     | 0.44              |
| 22:B:1210:CLA:H93  | 22:B:1210:CLA:H61  | 1.84                     | 0.44              |
| 12:1:162:ASP:OD1   | 12:1:162:ASP:N     | 2.49                     | 0.44              |
| 13:3:100:VAL:HG22  | 22:3:613:CLA:HMC2  | 2.00                     | 0.44              |
| 14:7:221:ASP:HB3   | 14:7:229:VAL:HG11  | 1.99                     | 0.44              |
| 22:8:601:CLA:H62   | 22:8:601:CLA:H41   | 1.75                     | 0.44              |
| 22:8:601:CLA:HBA2  | 22:8:601:CLA:H3A   | 1.63                     | 0.44              |
| 17:5:153:LYS:HA    | 17:5:153:LYS:HD3   | 1.88                     | 0.44              |
| 19:2:28:ARG:NH1    | 19:2:42:ASP:O      | 2.51                     | 0.44              |
| 19:2:30:MET:HB3    | 19:2:35:ALA:HB3    | 1.99                     | 0.44              |
| 39:2:502:LUT:H15   | 39:2:502:LUT:H201  | 1.82                     | 0.44              |
| 39:2:503:LUT:H15   | 39:2:503:LUT:H201  | 1.80                     | 0.44              |
| 22:A:1107:CLA:H122 | 25:J:4001:BCR:HC41 | 1.99                     | 0.43              |
| 22:A:1124:CLA:HAB  | 25:A:4004:BCR:C8   | 2.48                     | 0.43              |
| 2:B:708:LEU:HD23   | 33:B:5003:DGD:HA31 | 1.98                     | 0.43              |
| 22:B:1220:CLA:H3A  | 22:B:1220:CLA:HBA2 | 1.64                     | 0.43              |
| 22:B:1238:CLA:H193 | 25:I:4001:BCR:H16C | 2.00                     | 0.43              |
| 25:B:4004:BCR:H351 | 25:B:4004:BCR:H15C | 1.81                     | 0.43              |
| 22:K:1401:CLA:HBB1 | 25:K:4002:BCR:C10  | 2.47                     | 0.43              |
| 22:1:601:CLA:H3A   | 22:1:601:CLA:HBA2  | 1.59                     | 0.43              |
| 22:5:618:CLA:HED1  | 26:6:801:LHG:H301  | 1.99                     | 0.43              |
| 19:2:107:ASN:HA    | 19:2:110:LEU:HD12  | 1.99                     | 0.43              |
| 19:2:128:ILE:HD13  | 19:2:136:GLY:HA3   | 2.00                     | 0.43              |
| 40:9:610:CHL:HHC   | 40:9:610:CHL:HBB1  | 2.00                     | 0.43              |
| 1:A:278:PHE:HE1    | 1:A:296:HIS:HD2    | 1.65                     | 0.43              |
| 2:B:287:VAL:HG21   | 22:B:1213:CLA:H143 | 1.99                     | 0.43              |
| 22:B:1210:CLA:H143 | 22:B:1210:CLA:H112 | 1.76                     | 0.43              |
| 12:Z:105:TRP:CE2   | 12:Z:112:ALA:HB2   | 2.53                     | 0.43              |
| 22:A:1111:CLA:H143 | 22:A:1111:CLA:H161 | 1.80                     | 0.43              |
| 25:A:4002:BCR:H282 | 25:3:505:BCR:H10C  | 2.00                     | 0.43              |
| 2:B:578:TYR:CE1    | 2:B:711:LEU:HB2    | 2.53                     | 0.43              |
| 22:3:612:CLA:H3A   | 22:3:612:CLA:HBA2  | 1.49                     | 0.43              |
| 16:4:105:ARG:HA    | 16:4:108:MET:HE3   | 1.99                     | 0.43              |
| 22:4:608:CLA:H42   | 22:4:609:CLA:H41   | 2.00                     | 0.43              |
| 26:6:801:LHG:H311  | 22:6:603:CLA:H93   | 1.99                     | 0.43              |
| 39:2:502:LUT:H11   | 39:2:502:LUT:H191  | 1.81                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:566:LYS:NZ     | 2:B:674:GLU:OE2    | 2.42                     | 0.43              |
| 2:B:411:ARG:O      | 2:B:415:HIS:ND1    | 2.45                     | 0.43              |
| 12:1:48:ASP:OD1    | 12:1:48:ASP:N      | 2.50                     | 0.43              |
| 12:1:184:PHE:CD2   | 39:1:502:LUT:H12   | 2.52                     | 0.43              |
| 39:Z:503:LUT:H401  | 39:Z:503:LUT:H35   | 1.71                     | 0.43              |
| 22:4:602:CLA:H11   | 22:4:602:CLA:H52   | 1.77                     | 0.43              |
| 1:A:356:ASN:O      | 1:A:360:PHE:HB2    | 2.18                     | 0.43              |
| 22:A:1114:CLA:H2   | 32:A:5005:DGA:HB42 | 2.00                     | 0.43              |
| 22:B:1231:CLA:H91  | 22:B:1231:CLA:H111 | 1.86                     | 0.43              |
| 13:3:77:ALA:HB2    | 25:3:504:BCR:H383  | 2.00                     | 0.43              |
| 22:3:603:CLA:H2    | 22:3:608:CLA:OBD   | 2.19                     | 0.43              |
| 22:3:612:CLA:HHB   | 22:3:618:CLA:HBC2  | 2.01                     | 0.43              |
| 40:5:610:CHL:HHC   | 40:5:610:CHL:HBB1  | 2.00                     | 0.43              |
| 2:B:23:TRP:CG      | 2:B:705:GLN:HE22   | 2.36                     | 0.43              |
| 22:B:1215:CLA:HAB  | 22:B:1215:CLA:H8   | 2.00                     | 0.43              |
| 22:B:1216:CLA:H41  | 22:B:1216:CLA:H61  | 1.68                     | 0.43              |
| 22:B:1230:CLA:H61  | 22:B:1230:CLA:H41  | 1.82                     | 0.43              |
| 11:L:62:ALA:HB3    | 11:L:65:VAL:HG22   | 2.01                     | 0.43              |
| 40:1:609:CHL:HHC   | 40:1:609:CHL:HBB1  | 2.00                     | 0.43              |
| 39:Z:503:LUT:H7    | 40:Z:613:CHL:HAA1  | 2.00                     | 0.43              |
| 22:Z:604:CLA:H142  | 22:Z:604:CLA:H112  | 1.79                     | 0.43              |
| 22:A:1125:CLA:H2   | 22:A:1125:CLA:H61  | 1.80                     | 0.43              |
| 2:B:478:LEU:HD23   | 2:B:478:LEU:HA     | 1.86                     | 0.43              |
| 12:1:178:ARG:HA    | 12:1:181:MET:HE3   | 2.01                     | 0.43              |
| 22:1:608:CLA:HAA2  | 15:8:125:VAL:HG22  | 2.01                     | 0.43              |
| 22:7:603:CLA:HBA1  | 22:7:603:CLA:HBD   | 2.01                     | 0.43              |
| 1:A:605:ILE:HD12   | 21:A:1011:CL0:H53  | 2.01                     | 0.43              |
| 1:A:687:PHE:CD1    | 2:B:665:LEU:HB3    | 2.54                     | 0.43              |
| 23:A:2001:PQN:H302 | 23:A:2001:PQN:H262 | 1.79                     | 0.43              |
| 2:B:158:LEU:O      | 2:B:163:GLN:NE2    | 2.51                     | 0.43              |
| 22:B:1231:CLA:H193 | 22:B:1232:CLA:HBC3 | 2.01                     | 0.43              |
| 40:7:610:CHL:HMC   | 22:7:613:CLA:HAB   | 2.00                     | 0.43              |
| 16:4:89:ASP:HB3    | 16:4:92:LYS:HB2    | 2.00                     | 0.43              |
| 39:5:502:LUT:H15   | 39:5:502:LUT:H201  | 1.82                     | 0.43              |
| 18:6:188:VAL:HG11  | 22:6:604:CLA:H18   | 2.00                     | 0.43              |
| 22:6:609:CLA:HBA2  | 22:6:609:CLA:H3A   | 1.62                     | 0.43              |
| 19:2:198:ILE:HG12  | 19:2:207:THR:HG21  | 2.00                     | 0.43              |
| 39:9:501:LUT:H11   | 39:9:501:LUT:H191  | 1.94                     | 0.43              |
| 22:A:1107:CLA:H93  | 22:A:1107:CLA:H61  | 1.79                     | 0.43              |
| 22:A:1127:CLA:H102 | 22:A:1127:CLA:H62  | 1.73                     | 0.43              |
| 22:F:1301:CLA:H143 | 22:F:1301:CLA:H112 | 1.81                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:1:603:CLA:H8    | 26:1:801:LHG:H321  | 2.00                     | 0.43              |
| 22:1:615:CLA:H2    | 22:1:615:CLA:H61   | 1.59                     | 0.43              |
| 20:9:62:ARG:NH2    | 20:9:66:TYR:OH     | 2.50                     | 0.43              |
| 20:9:119:MET:HG3   | 22:9:612:CLA:HMC3  | 2.01                     | 0.43              |
| 2:B:671:TYR:OH     | 22:B:1023:CLA:OBD  | 2.33                     | 0.43              |
| 39:Z:502:LUT:H15   | 39:Z:502:LUT:H201  | 1.85                     | 0.43              |
| 39:Z:502:LUT:H35   | 39:Z:502:LUT:H401  | 1.87                     | 0.43              |
| 17:5:137:TRP:CG    | 22:5:618:CLA:HBC1  | 2.54                     | 0.43              |
| 22:6:605:CLA:H2    | 22:6:605:CLA:H61   | 1.89                     | 0.43              |
| 19:2:118:PHE:CZ    | 40:2:613:CHL:HAB   | 2.54                     | 0.43              |
| 20:9:170:ILE:HD11  | 22:9:605:CLA:HAB   | 2.00                     | 0.43              |
| 22:9:603:CLA:H93   | 22:9:603:CLA:H61   | 1.81                     | 0.43              |
| 10:K:72:ASN:OD1    | 10:K:72:ASN:N      | 2.52                     | 0.42              |
| 22:3:605:CLA:H111  | 22:3:605:CLA:H91   | 1.82                     | 0.42              |
| 40:8:613:CHL:HHC   | 40:8:613:CHL:HBB1  | 2.01                     | 0.42              |
| 39:9:501:LUT:H35   | 39:9:501:LUT:H401  | 1.83                     | 0.42              |
| 1:A:234:PRO:HA     | 1:A:237:ILE:HD12   | 2.01                     | 0.42              |
| 1:A:574:PRO:HB3    | 1:A:720:ILE:HB     | 2.02                     | 0.42              |
| 22:A:1122:CLA:H141 | 26:A:5001:LHG:H172 | 2.01                     | 0.42              |
| 22:B:1211:CLA:HMA2 | 25:B:4003:BCR:H272 | 2.00                     | 0.42              |
| 22:1:602:CLA:OBD   | 22:1:607:CLA:H2    | 2.19                     | 0.42              |
| 25:6:503:BCR:H351  | 25:6:503:BCR:H15C  | 1.74                     | 0.42              |
| 1:A:17:VAL:HG21    | 22:A:1108:CLA:HED3 | 2.00                     | 0.42              |
| 1:A:718:LEU:HB3    | 1:A:722:GLN:HG2    | 2.01                     | 0.42              |
| 22:A:1120:CLA:HMD1 | 25:K:4001:BCR:H24C | 2.00                     | 0.42              |
| 22:A:1139:CLA:H41  | 22:A:1139:CLA:H61  | 1.66                     | 0.42              |
| 2:B:453:GLN:HE21   | 6:F:130:LEU:HD13   | 1.84                     | 0.42              |
| 39:1:502:LUT:H15   | 39:1:502:LUT:H201  | 1.90                     | 0.42              |
| 40:Z:610:CHL:HAB   | 40:Z:613:CHL:HBB2  | 1.99                     | 0.42              |
| 22:3:606:CLA:H141  | 22:3:606:CLA:H161  | 1.84                     | 0.42              |
| 22:7:603:CLA:H203  | 22:7:603:CLA:H161  | 1.86                     | 0.42              |
| 16:4:111:VAL:HG11  | 39:4:501:LUT:H10   | 2.00                     | 0.42              |
| 22:2:603:CLA:HBA1  | 22:2:603:CLA:HBD   | 2.00                     | 0.42              |
| 22:A:1113:CLA:H141 | 22:A:1113:CLA:H161 | 1.74                     | 0.42              |
| 4:D:93:GLU:HA      | 4:D:106:MET:O      | 2.18                     | 0.42              |
| 12:1:79:ARG:NH1    | 22:1:611:CLA:OBD   | 2.47                     | 0.42              |
| 12:1:171:LEU:HD23  | 22:1:607:CLA:HED3  | 2.00                     | 0.42              |
| 39:3:501:LUT:H30   | 22:3:601:CLA:H72   | 2.01                     | 0.42              |
| 25:5:504:BCR:H383  | 40:5:610:CHL:H12   | 2.01                     | 0.42              |
| 22:5:618:CLA:H112  | 22:5:618:CLA:H91   | 1.79                     | 0.42              |
| 19:2:155:LEU:HD22  | 22:2:607:CLA:HED3  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:740:TRP:CG     | 25:A:4005:BCR:HC41 | 2.54                     | 0.42              |
| 22:A:1126:CLA:O1D  | 22:A:1127:CLA:HBB  | 2.19                     | 0.42              |
| 39:Z:501:LUT:H371  | 22:Z:601:CLA:H61   | 2.02                     | 0.42              |
| 14:7:156:GLU:OE2   | 14:7:168:ARG:NH1   | 2.52                     | 0.42              |
| 26:4:801:LHG:HC82  | 25:6:503:BCR:HC32  | 2.02                     | 0.42              |
| 22:2:603:CLA:H92   | 22:2:603:CLA:H61   | 1.77                     | 0.42              |
| 20:9:105:ASP:N     | 20:9:105:ASP:OD1   | 2.52                     | 0.42              |
| 31:A:5003:LMG:HC2  | 14:7:60:GLN:HE22   | 1.85                     | 0.42              |
| 2:B:338:ALA:HB1    | 22:B:1202:CLA:HED2 | 2.00                     | 0.42              |
| 22:B:1230:CLA:HBA2 | 22:B:1230:CLA:H3A  | 1.82                     | 0.42              |
| 25:3:503:BCR:H341  | 22:5:609:CLA:H172  | 2.01                     | 0.42              |
| 39:8:501:LUT:H32   | 22:8:601:CLA:CAB   | 2.50                     | 0.42              |
| 39:4:502:LUT:H32   | 22:4:604:CLA:CAB   | 2.49                     | 0.42              |
| 22:B:1212:CLA:H2A  | 22:B:1212:CLA:HED2 | 2.02                     | 0.42              |
| 22:B:1213:CLA:O1A  | 7:G:116:ALA:HB1    | 2.19                     | 0.42              |
| 3:C:66:ARG:HA      | 3:C:66:ARG:HD2     | 1.91                     | 0.42              |
| 39:3:502:LUT:H35   | 39:3:502:LUT:H401  | 1.89                     | 0.42              |
| 22:8:606:CLA:H111  | 45:8:803:LPX:H8    | 2.02                     | 0.42              |
| 17:5:202:LEU:HD23  | 17:5:202:LEU:HA    | 1.85                     | 0.42              |
| 19:2:71:LEU:HD23   | 19:2:71:LEU:HA     | 1.92                     | 0.42              |
| 22:A:1112:CLA:H91  | 22:A:1112:CLA:H111 | 1.89                     | 0.42              |
| 2:B:495:LEU:HD23   | 2:B:495:LEU:HA     | 1.85                     | 0.42              |
| 12:1:205:HIS:CG    | 22:1:603:CLA:HAA2  | 2.55                     | 0.42              |
| 39:3:502:LUT:H15   | 39:3:502:LUT:H201  | 1.85                     | 0.42              |
| 22:7:616:CLA:H93   | 22:7:616:CLA:H111  | 1.88                     | 0.42              |
| 39:8:502:LUT:H15   | 39:8:502:LUT:H201  | 1.90                     | 0.42              |
| 16:4:226:PHE:CZ    | 39:4:502:LUT:H10   | 2.55                     | 0.42              |
| 17:5:134:VAL:HG11  | 22:6:609:CLA:H2A   | 2.01                     | 0.42              |
| 19:2:96:TRP:CD1    | 19:2:97:THR:HG23   | 2.55                     | 0.42              |
| 1:A:396:TRP:HA     | 1:A:603:LEU:HD23   | 2.01                     | 0.42              |
| 22:B:1220:CLA:H142 | 22:B:1220:CLA:H111 | 1.84                     | 0.42              |
| 22:B:1222:CLA:HBD  | 22:B:1234:CLA:HMB2 | 2.02                     | 0.42              |
| 25:G:4001:BCR:H15C | 25:G:4001:BCR:H351 | 1.92                     | 0.42              |
| 22:1:608:CLA:H13   | 22:1:608:CLA:H102  | 1.86                     | 0.42              |
| 40:Z:610:CHL:HBB2  | 40:Z:613:CHL:HBB2  | 2.02                     | 0.42              |
| 43:7:802:3PH:H372  | 43:7:802:3PH:H3A1  | 1.66                     | 0.42              |
| 22:4:609:CLA:H92   | 22:4:609:CLA:H62   | 1.80                     | 0.42              |
| 17:5:197:TYR:CD2   | 39:5:502:LUT:H12   | 2.54                     | 0.42              |
| 18:6:125:GLU:HG3   | 22:6:612:CLA:C4B   | 2.50                     | 0.42              |
| 1:A:25:SER:O       | 22:A:1109:CLA:HBB  | 2.20                     | 0.42              |
| 1:A:81:LEU:HD12    | 22:A:1111:CLA:HED1 | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:605:ILE:HG13   | 21:A:1011:CL0:H66  | 2.02                     | 0.42              |
| 2:B:128:ILE:HG22   | 22:B:1215:CLA:HED2 | 2.02                     | 0.42              |
| 2:B:323:LEU:HA     | 2:B:326:THR:HG22   | 2.02                     | 0.42              |
| 22:B:1237:CLA:H142 | 22:B:1237:CLA:H111 | 1.87                     | 0.42              |
| 22:B:1208:CLA:H42  | 22:9:605:CLA:H71   | 2.02                     | 0.42              |
| 39:1:502:LUT:H11   | 39:1:502:LUT:H191  | 1.94                     | 0.42              |
| 16:4:240:PRO:O     | 39:4:501:LUT:O3    | 2.37                     | 0.42              |
| 18:6:192:MET:HG3   | 22:6:603:CLA:HAC2  | 2.02                     | 0.42              |
| 18:6:192:MET:HE3   | 22:6:615:CLA:H12   | 2.01                     | 0.42              |
| 22:A:1124:CLA:H193 | 22:A:1124:CLA:H162 | 1.88                     | 0.41              |
| 22:A:1133:CLA:H41  | 22:A:1133:CLA:H62  | 1.78                     | 0.41              |
| 22:A:1137:CLA:H143 | 22:A:1137:CLA:H111 | 1.84                     | 0.41              |
| 22:B:1204:CLA:H3A  | 22:B:1204:CLA:HBA2 | 1.74                     | 0.41              |
| 9:J:21:PHE:CD1     | 22:J:1901:CLA:HBB2 | 2.55                     | 0.41              |
| 9:J:28:GLU:OE1     | 9:J:31:ARG:NH2     | 2.49                     | 0.41              |
| 13:3:195:MET:SD    | 22:3:604:CLA:HAB   | 2.60                     | 0.41              |
| 15:8:160:LEU:HD22  | 22:8:611:CLA:HMC1  | 2.02                     | 0.41              |
| 22:8:603:CLA:HBD   | 22:8:603:CLA:HBA1  | 2.01                     | 0.41              |
| 22:4:609:CLA:H41   | 22:4:609:CLA:H61   | 1.80                     | 0.41              |
| 1:A:369:HIS:HA     | 1:A:372:TYR:CE1    | 2.56                     | 0.41              |
| 2:B:688:LEU:HB3    | 25:L:4002:BCR:HC31 | 2.02                     | 0.41              |
| 22:B:1021:CLA:H112 | 22:B:1021:CLA:H152 | 1.77                     | 0.41              |
| 13:3:66:ARG:HA     | 13:3:69:MET:HE3    | 2.02                     | 0.41              |
| 25:3:505:BCR:H17C  | 22:3:612:CLA:H142  | 2.01                     | 0.41              |
| 16:4:111:VAL:HG11  | 39:4:501:LUT:H12   | 2.02                     | 0.41              |
| 22:4:612:CLA:HBA2  | 22:4:612:CLA:H3A   | 1.49                     | 0.41              |
| 25:5:503:BCR:H15C  | 25:5:503:BCR:H351  | 1.86                     | 0.41              |
| 22:6:605:CLA:HBA1  | 22:6:605:CLA:H3A   | 1.82                     | 0.41              |
| 20:9:133:THR:HG23  | 20:9:135:THR:HG22  | 2.03                     | 0.41              |
| 22:A:1117:CLA:H2   | 22:A:1127:CLA:H92  | 2.02                     | 0.41              |
| 22:B:1237:CLA:HHD  | 25:B:4007:BCR:H383 | 2.01                     | 0.41              |
| 10:K:49:ALA:HB1    | 10:K:56:THR:HG22   | 2.02                     | 0.41              |
| 22:L:1502:CLA:H51  | 25:L:4002:BCR:HC21 | 2.02                     | 0.41              |
| 16:4:175:ASN:HB3   | 16:4:185:LEU:HB2   | 2.02                     | 0.41              |
| 22:9:604:CLA:HBB1  | 22:9:604:CLA:HHC   | 2.02                     | 0.41              |
| 1:A:296:HIS:CD2    | 22:A:1116:CLA:HMB1 | 2.55                     | 0.41              |
| 2:B:499:LEU:HA     | 2:B:502:ILE:HG22   | 2.02                     | 0.41              |
| 22:B:1205:CLA:H92  | 25:B:4007:BCR:HC7  | 2.01                     | 0.41              |
| 9:J:5:THR:HB       | 31:J:5001:LMG:HC92 | 2.03                     | 0.41              |
| 9:J:28:GLU:HG3     | 22:J:1901:CLA:C1B  | 2.50                     | 0.41              |
| 16:4:95:TRP:CZ2    | 22:4:612:CLA:HAA2  | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:4:502:LUT:H15   | 39:4:502:LUT:H201  | 1.91                     | 0.41              |
| 22:A:1126:CLA:H72  | 22:A:1126:CLA:H111 | 1.81                     | 0.41              |
| 2:B:320:HIS:HB3    | 2:B:323:LEU:HD12   | 2.02                     | 0.41              |
| 11:L:80:ALA:HB3    | 11:L:83:LEU:HD23   | 2.03                     | 0.41              |
| 12:1:210:TRP:HB3   | 15:8:117:ALA:HB2   | 2.03                     | 0.41              |
| 40:Z:610:CHL:CBB   | 40:Z:613:CHL:HBB2  | 2.50                     | 0.41              |
| 22:8:608:CLA:H62   | 22:8:608:CLA:H92   | 1.85                     | 0.41              |
| 18:6:165:ILE:HG12  | 22:6:601:CLA:HBA2  | 2.03                     | 0.41              |
| 40:6:610:CHL:HBB2  | 22:6:612:CLA:HBC1  | 2.02                     | 0.41              |
| 20:9:125:LYS:HA    | 20:9:125:LYS:HD2   | 1.90                     | 0.41              |
| 1:A:150:ALA:HB2    | 1:A:378:PRO:HD2    | 2.01                     | 0.41              |
| 22:A:1103:CLA:HBA1 | 22:A:1103:CLA:H3A  | 1.62                     | 0.41              |
| 32:A:5005:DGA:HA51 | 14:7:239:PRO:HB2   | 2.02                     | 0.41              |
| 2:B:277:HIS:CE1    | 2:B:281:ILE:HD13   | 2.56                     | 0.41              |
| 12:Z:83:LEU:HB3    | 22:Z:606:CLA:HAB   | 2.02                     | 0.41              |
| 22:Z:604:CLA:HHD   | 40:Z:609:CHL:HBB2  | 2.03                     | 0.41              |
| 22:Z:605:CLA:H112  | 22:Z:605:CLA:H151  | 1.84                     | 0.41              |
| 22:3:612:CLA:H91   | 22:3:612:CLA:H111  | 1.83                     | 0.41              |
| 25:7:503:BCR:H311  | 22:8:607:CLA:HAB   | 2.02                     | 0.41              |
| 22:8:605:CLA:H141  | 22:8:605:CLA:H162  | 1.85                     | 0.41              |
| 22:A:1115:CLA:H62  | 22:A:1115:CLA:H41  | 1.46                     | 0.41              |
| 22:A:1130:CLA:H111 | 22:A:1130:CLA:H143 | 1.80                     | 0.41              |
| 22:A:1133:CLA:H142 | 22:A:1133:CLA:H111 | 1.84                     | 0.41              |
| 22:A:1134:CLA:H52  | 22:A:1134:CLA:H11  | 1.86                     | 0.41              |
| 2:B:701:LEU:HB3    | 2:B:705:GLN:HG2    | 2.03                     | 0.41              |
| 22:B:1021:CLA:HBA2 | 22:B:1021:CLA:H3A  | 1.79                     | 0.41              |
| 14:7:195:ARG:HA    | 14:7:198:MET:HE3   | 2.03                     | 0.41              |
| 39:7:501:LUT:H30   | 22:7:601:CLA:H72   | 2.03                     | 0.41              |
| 18:6:181:ARG:HA    | 18:6:184:MET:HE3   | 2.01                     | 0.41              |
| 1:A:57:HIS:HB2     | 22:A:1128:CLA:HBA1 | 2.03                     | 0.41              |
| 22:A:1013:CLA:H161 | 22:A:1013:CLA:H121 | 1.81                     | 0.41              |
| 2:B:186:VAL:HG11   | 25:B:4002:BCR:H341 | 2.01                     | 0.41              |
| 22:B:1209:CLA:HBA2 | 22:B:1209:CLA:H3A  | 1.86                     | 0.41              |
| 4:D:117:LYS:HE3    | 4:D:119:GLU:HB3    | 2.01                     | 0.41              |
| 4:D:122:LEU:HD12   | 4:D:122:LEU:HA     | 1.84                     | 0.41              |
| 8:I:88:PRO:HG2     | 25:I:4001:BCR:H14C | 2.03                     | 0.41              |
| 12:1:157:LEU:HD12  | 39:1:501:LUT:H222  | 2.03                     | 0.41              |
| 22:3:618:CLA:HED1  | 26:7:801:LHG:H311  | 2.03                     | 0.41              |
| 25:8:503:BCR:H382  | 40:8:613:CHL:H111  | 2.03                     | 0.41              |
| 20:9:126:ARG:NH2   | 22:9:612:CLA:O1D   | 2.44                     | 0.41              |
| 1:A:318:ILE:HG13   | 22:A:1118:CLA:HED1 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:A:1117:CLA:H3A  | 22:A:1117:CLA:HBA2 | 1.74                     | 0.41              |
| 22:A:1126:CLA:H3A  | 22:A:1126:CLA:HBA2 | 1.72                     | 0.41              |
| 22:A:1133:CLA:H172 | 22:A:1137:CLA:H112 | 2.03                     | 0.41              |
| 22:A:1138:CLA:HED3 | 2:B:421:SER:HB3    | 2.03                     | 0.41              |
| 25:A:4005:BCR:H21C | 22:A:1013:CLA:H122 | 2.02                     | 0.41              |
| 2:B:462:GLN:HG2    | 2:B:473:TYR:CZ     | 2.56                     | 0.41              |
| 2:B:577:PHE:CE1    | 22:B:1226:CLA:HAC2 | 2.55                     | 0.41              |
| 22:B:1210:CLA:H203 | 25:B:4002:BCR:H271 | 2.03                     | 0.41              |
| 22:B:1213:CLA:H51  | 22:B:1213:CLA:NC   | 2.35                     | 0.41              |
| 7:G:59:ARG:NH2     | 28:1:803:LMT:O2B   | 2.52                     | 0.41              |
| 22:1:601:CLA:H41   | 22:1:601:CLA:H62   | 1.83                     | 0.41              |
| 40:1:610:CHL:HMC   | 22:1:613:CLA:HAB   | 2.03                     | 0.41              |
| 22:Z:605:CLA:H141  | 22:Z:605:CLA:H161  | 1.89                     | 0.41              |
| 39:8:501:LUT:H35   | 39:8:501:LUT:H401  | 1.88                     | 0.41              |
| 16:4:139:LYS:HE3   | 40:4:610:CHL:HED2  | 2.02                     | 0.41              |
| 16:4:204:SER:HB3   | 22:4:601:CLA:HAA2  | 2.02                     | 0.41              |
| 17:5:197:TYR:CZ    | 39:5:502:LUT:H10   | 2.56                     | 0.41              |
| 22:6:609:CLA:H143  | 22:6:609:CLA:H161  | 1.86                     | 0.41              |
| 19:2:53:PRO:HD2    | 39:2:502:LUT:H3    | 2.03                     | 0.41              |
| 19:2:225:LYS:HA    | 19:2:225:LYS:HD2   | 1.92                     | 0.41              |
| 28:9:803:LMT:H82   | 28:9:803:LMT:H51   | 1.94                     | 0.41              |
| 1:A:217:GLN:OE1    | 1:A:298:HIS:ND1    | 2.54                     | 0.41              |
| 22:A:1101:CLA:H62  | 22:A:1101:CLA:H101 | 1.73                     | 0.41              |
| 26:B:5006:LHG:H241 | 26:B:5006:LHG:H272 | 1.86                     | 0.41              |
| 40:Z:609:CHL:HED3  | 16:4:163:ARG:HD2   | 2.02                     | 0.41              |
| 15:8:45:ALA:O      | 15:8:51:ASN:ND2    | 2.53                     | 0.41              |
| 16:4:140:PHE:HB3   | 16:4:142:TYR:CE2   | 2.56                     | 0.41              |
| 20:9:140:ASN:OD1   | 20:9:140:ASN:N     | 2.53                     | 0.41              |
| 22:A:1124:CLA:H18  | 25:A:4003:BCR:H342 | 2.03                     | 0.40              |
| 2:B:257:THR:OG1    | 2:B:273:ASP:OD1    | 2.38                     | 0.40              |
| 22:B:1239:CLA:H203 | 22:B:1239:CLA:H161 | 1.81                     | 0.40              |
| 10:K:79:ASN:H      | 22:K:1404:CLA:HED1 | 1.87                     | 0.40              |
| 11:L:101:ILE:HG12  | 11:L:114:GLU:HA    | 2.03                     | 0.40              |
| 16:4:224:LEU:HD23  | 16:4:224:LEU:HA    | 1.93                     | 0.40              |
| 22:B:1202:CLA:HBD  | 22:B:1202:CLA:H122 | 2.03                     | 0.40              |
| 22:B:1229:CLA:H2   | 22:B:1229:CLA:H62  | 1.81                     | 0.40              |
| 12:Z:184:PHE:CE1   | 39:Z:502:LUT:H10   | 2.55                     | 0.40              |
| 22:Z:604:CLA:H3A   | 22:Z:604:CLA:H12   | 2.02                     | 0.40              |
| 13:3:228:ILE:HD12  | 22:3:603:CLA:H43   | 2.02                     | 0.40              |
| 22:8:602:CLA:HED3  | 22:4:605:CLA:H2    | 2.02                     | 0.40              |
| 16:4:109:LEU:HB3   | 22:4:606:CLA:HAB   | 2.02                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:4:252:TRP:HB3   | 18:6:109:GLY:H     | 1.87                     | 0.40              |
| 17:5:218:HIS:CG    | 22:5:603:CLA:HAA2  | 2.56                     | 0.40              |
| 18:6:257:PRO:HB2   | 22:6:619:CLA:CAB   | 2.50                     | 0.40              |
| 40:6:610:CHL:H8    | 40:6:610:CHL:H51   | 1.96                     | 0.40              |
| 22:A:1104:CLA:H12  | 22:A:1128:CLA:H2   | 2.02                     | 0.40              |
| 22:A:1108:CLA:HBC1 | 22:3:605:CLA:H121  | 2.02                     | 0.40              |
| 22:A:1125:CLA:H152 | 22:A:1125:CLA:H111 | 1.84                     | 0.40              |
| 22:B:1240:CLA:HED1 | 25:B:4004:BCR:H353 | 2.02                     | 0.40              |
| 22:8:606:CLA:HMA2  | 40:8:613:CHL:HAC2  | 2.04                     | 0.40              |
| 16:4:182:ASN:OD1   | 16:4:182:ASN:N     | 2.53                     | 0.40              |
| 22:5:607:CLA:H61   | 22:5:607:CLA:H41   | 1.81                     | 0.40              |
| 19:2:212:ALA:HB3   | 32:9:802:DGA:HBT1  | 2.02                     | 0.40              |
| 20:9:45:LEU:HD23   | 20:9:45:LEU:HA     | 1.93                     | 0.40              |
| 1:A:316:TRP:HB3    | 10:K:57:VAL:HG23   | 2.02                     | 0.40              |
| 1:A:746:ARG:O      | 1:A:750:VAL:HG22   | 2.22                     | 0.40              |
| 25:A:4003:BCR:H351 | 25:A:4003:BCR:H15C | 1.85                     | 0.40              |
| 2:B:346:THR:HB     | 2:B:380:ALA:HB2    | 2.04                     | 0.40              |
| 22:B:1214:CLA:H72  | 22:B:1214:CLA:H111 | 1.91                     | 0.40              |
| 22:B:1230:CLA:H2   | 25:B:4006:BCR:H333 | 2.03                     | 0.40              |
| 22:B:1240:CLA:H41  | 22:B:1240:CLA:H62  | 1.76                     | 0.40              |
| 4:D:128:LEU:HD22   | 4:D:134:LEU:HD12   | 2.03                     | 0.40              |
| 22:Z:604:CLA:H3A   | 22:Z:604:CLA:HBA2  | 1.63                     | 0.40              |
| 16:4:248:LEU:HD23  | 16:4:248:LEU:HA    | 1.96                     | 0.40              |
| 22:4:609:CLA:H11   | 18:6:123:TRP:HB2   | 2.03                     | 0.40              |
| 40:5:610:CHL:H202  | 22:5:618:CLA:HBB1  | 2.03                     | 0.40              |
| 19:2:117:VAL:CG1   | 19:2:121:LEU:HD13  | 2.51                     | 0.40              |
| 22:A:1131:CLA:HBB1 | 22:A:1132:CLA:H2   | 2.03                     | 0.40              |
| 10:K:60:ASN:N      | 10:K:68:VAL:O      | 2.47                     | 0.40              |
| 22:7:603:CLA:H51   | 22:7:603:CLA:NC    | 2.37                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 739/741 (100%)  | 720 (97%)  | 19 (3%)  | 0        | 100         | 100 |
| 2   | B     | 731/733 (100%)  | 707 (97%)  | 24 (3%)  | 0        | 100         | 100 |
| 3   | C     | 78/80 (98%)     | 75 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 4   | D     | 141/144 (98%)   | 135 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 5   | E     | 61/63 (97%)     | 57 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 6   | F     | 163/165 (99%)   | 158 (97%)  | 4 (2%)   | 1 (1%)   | 21          | 29  |
| 7   | G     | 70/91 (77%)     | 70 (100%)  | 0        | 0        | 100         | 100 |
| 8   | I     | 35/37 (95%)     | 34 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 9   | J     | 37/39 (95%)     | 36 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 10  | K     | 82/84 (98%)     | 81 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 11  | L     | 122/138 (88%)   | 119 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 12  | 1     | 192/194 (99%)   | 185 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 12  | Z     | 192/194 (99%)   | 188 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 13  | 3     | 217/219 (99%)   | 209 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 14  | 7     | 211/213 (99%)   | 203 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 15  | 8     | 215/217 (99%)   | 210 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 16  | 4     | 208/210 (99%)   | 199 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 17  | 5     | 225/227 (99%)   | 221 (98%)  | 3 (1%)   | 1 (0%)   | 30          | 39  |
| 18  | 6     | 227/229 (99%)   | 223 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 19  | 2     | 196/198 (99%)   | 187 (95%)  | 8 (4%)   | 1 (0%)   | 24          | 34  |
| 20  | 9     | 181/183 (99%)   | 170 (94%)  | 10 (6%)  | 1 (1%)   | 21          | 29  |
| All | All   | 4323/4399 (98%) | 4187 (97%) | 132 (3%) | 4 (0%)   | 49          | 61  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 150 | PHE  |
| 17  | 5     | 243 | GLN  |
| 19  | 2     | 180 | LYS  |
| 20  | 9     | 139 | ILE  |

### 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     | 601/601 (100%)  | 601 (100%)  | 0        | 100         | 100 |
| 2   | B     | 596/596 (100%)  | 596 (100%)  | 0        | 100         | 100 |
| 3   | C     | 69/69 (100%)    | 69 (100%)   | 0        | 100         | 100 |
| 4   | D     | 120/120 (100%)  | 120 (100%)  | 0        | 100         | 100 |
| 5   | E     | 54/54 (100%)    | 54 (100%)   | 0        | 100         | 100 |
| 6   | F     | 127/127 (100%)  | 127 (100%)  | 0        | 100         | 100 |
| 7   | G     | 54/68 (79%)     | 54 (100%)   | 0        | 100         | 100 |
| 8   | I     | 31/31 (100%)    | 31 (100%)   | 0        | 100         | 100 |
| 9   | J     | 35/35 (100%)    | 35 (100%)   | 0        | 100         | 100 |
| 10  | K     | 58/58 (100%)    | 58 (100%)   | 0        | 100         | 100 |
| 11  | L     | 92/102 (90%)    | 92 (100%)   | 0        | 100         | 100 |
| 12  | 1     | 137/137 (100%)  | 137 (100%)  | 0        | 100         | 100 |
| 12  | Z     | 137/137 (100%)  | 137 (100%)  | 0        | 100         | 100 |
| 13  | 3     | 167/167 (100%)  | 167 (100%)  | 0        | 100         | 100 |
| 14  | 7     | 164/164 (100%)  | 164 (100%)  | 0        | 100         | 100 |
| 15  | 8     | 163/163 (100%)  | 163 (100%)  | 0        | 100         | 100 |
| 16  | 4     | 164/165 (99%)   | 164 (100%)  | 0        | 100         | 100 |
| 17  | 5     | 184/184 (100%)  | 184 (100%)  | 0        | 100         | 100 |
| 18  | 6     | 183/183 (100%)  | 183 (100%)  | 0        | 100         | 100 |
| 19  | 2     | 154/156 (99%)   | 154 (100%)  | 0        | 100         | 100 |
| 20  | 9     | 141/141 (100%)  | 141 (100%)  | 0        | 100         | 100 |
| All | All   | 3431/3458 (99%) | 3431 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | ASN  |
| 1   | A     | 57  | HIS  |
| 1   | A     | 94  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 225 | ASN  |
| 1   | A     | 296 | HIS  |
| 1   | A     | 394 | HIS  |
| 1   | A     | 425 | ASN  |
| 1   | A     | 637 | GLN  |
| 2   | B     | 30  | HIS  |
| 2   | B     | 376 | HIS  |
| 2   | B     | 453 | GLN  |
| 2   | B     | 505 | ASN  |
| 2   | B     | 628 | ASN  |
| 4   | D     | 108 | GLN  |
| 6   | F     | 198 | GLN  |
| 10  | K     | 35  | ASN  |
| 12  | 1     | 52  | ASN  |
| 12  | 1     | 140 | GLN  |
| 12  | 1     | 191 | HIS  |
| 12  | Z     | 52  | ASN  |
| 12  | Z     | 176 | ASN  |
| 12  | Z     | 191 | HIS  |
| 13  | 3     | 47  | ASN  |
| 13  | 3     | 225 | ASN  |
| 13  | 3     | 226 | ASN  |
| 14  | 7     | 162 | ASN  |
| 14  | 7     | 193 | ASN  |
| 15  | 8     | 139 | GLN  |
| 15  | 8     | 230 | HIS  |
| 16  | 4     | 175 | ASN  |
| 18  | 6     | 206 | GLN  |
| 19  | 2     | 59  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | SNC  | D     | 137 | 4    | 4,7,8        | 1.06 | 0           | 2,7,9       | 2.27 | 1 (50%)     |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4   | SNC  | D     | 137 | 4    | -       | 0/0/6/8  | -     |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | D     | 137 | SNC  | CA-CB-SG | -3.15 | 105.28      | 112.49   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 1 is monoatomic - leaving 353 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | 5     | 608  | -    | 49,53,73     | 1.60 | 7 (14%)  | 58,89,113   | 2.08 | 16 (27%) |
| 22  | CLA  | B     | 1226 | -    | 69,73,73     | 1.43 | 8 (11%)  | 82,113,113  | 1.98 | 21 (25%) |
| 40  | CHL  | 9     | 610  | -    | 60,74,74     | 1.55 | 10 (16%) | 58,114,114  | 1.69 | 11 (18%) |
| 22  | CLA  | A     | 1141 | 26   | 56,60,73     | 1.51 | 7 (12%)  | 65,97,113   | 2.11 | 18 (27%) |
| 22  | CLA  | 3     | 605  | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.81 | 17 (20%) |
| 25  | BCR  | G     | 4001 | -    | 41,41,41     | 1.62 | 4 (9%)   | 56,56,56    | 4.37 | 13 (23%) |
| 22  | CLA  | 5     | 606  | -    | 54,58,73     | 1.54 | 6 (11%)  | 64,95,113   | 2.11 | 16 (25%) |
| 28  | LMT  | 9     | 803  | -    | 36,36,36     | 1.15 | 5 (13%)  | 47,47,47    | 1.05 | 4 (8%)   |
| 22  | CLA  | 2     | 612  | -    | 54,58,73     | 1.54 | 7 (12%)  | 64,95,113   | 2.07 | 18 (28%) |
| 22  | CLA  | 6     | 618  | -    | 50,54,73     | 1.59 | 7 (14%)  | 59,90,113   | 2.06 | 16 (27%) |
| 22  | CLA  | B     | 1222 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.86 | 23 (28%) |
| 22  | CLA  | 1     | 615  | 12   | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.79 | 15 (18%) |
| 22  | CLA  | B     | 1221 | -    | 69,73,73     | 1.38 | 8 (11%)  | 82,113,113  | 2.03 | 19 (23%) |
| 22  | CLA  | 7     | 608  | -    | 47,51,73     | 1.63 | 7 (14%)  | 55,86,113   | 2.09 | 16 (29%) |
| 22  | CLA  | 7     | 616  | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 2.00 | 19 (25%) |
| 22  | CLA  | B     | 1225 | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.74 | 12 (14%) |
| 22  | CLA  | A     | 1119 | -    | 69,73,73     | 1.37 | 6 (8%)   | 82,113,113  | 1.72 | 15 (18%) |
| 22  | CLA  | 8     | 607  | -    | 59,63,73     | 1.47 | 6 (10%)  | 70,101,113  | 1.94 | 16 (22%) |
| 22  | CLA  | A     | 1115 | -    | 64,68,73     | 1.41 | 6 (9%)   | 76,107,113  | 1.78 | 15 (19%) |
| 39  | LUT  | 2     | 502  | -    | 42,43,43     | 2.40 | 1 (2%)   | 51,60,60    | 1.82 | 14 (27%) |
| 22  | CLA  | 1     | 607  | -    | 64,68,73     | 1.42 | 7 (10%)  | 76,107,113  | 1.96 | 17 (22%) |
| 25  | BCR  | 3     | 504  | -    | 41,41,41     | 1.66 | 5 (12%)  | 56,56,56    | 4.49 | 14 (25%) |
| 22  | CLA  | 4     | 609  | 16   | 64,68,73     | 1.40 | 7 (10%)  | 76,107,113  | 1.93 | 19 (25%) |
| 22  | CLA  | Z     | 602  | -    | 50,54,73     | 1.60 | 6 (12%)  | 59,90,113   | 2.01 | 14 (23%) |
| 22  | CLA  | 9     | 606  | -    | 54,58,73     | 1.53 | 8 (14%)  | 64,95,113   | 2.06 | 18 (28%) |
| 22  | CLA  | 9     | 601  | -    | 64,68,73     | 1.42 | 6 (9%)   | 76,107,113  | 2.01 | 17 (22%) |
| 22  | CLA  | 3     | 601  | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.92 | 21 (25%) |
| 22  | CLA  | 5     | 622  | -    | 50,54,73     | 1.60 | 7 (14%)  | 59,90,113   | 2.09 | 14 (23%) |
| 22  | CLA  | A     | 1109 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.93 | 19 (23%) |
| 22  | CLA  | B     | 1229 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.93 | 22 (26%) |
| 27  | NKP  | A     | 5004 | -    | 28,28,28     | 1.55 | 3 (10%)  | 30,32,32    | 1.27 | 3 (10%)  |
| 25  | BCR  | B     | 4001 | -    | 41,41,41     | 1.64 | 5 (12%)  | 56,56,56    | 4.29 | 15 (26%) |
| 40  | CHL  | 4     | 611  | -    | 45,59,74     | 1.45 | 8 (17%)  | 40,96,114   | 2.08 | 13 (32%) |
| 25  | BCR  | B     | 4007 | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.32 | 13 (23%) |
| 40  | CHL  | 2     | 613  | -    | 45,59,74     | 1.64 | 8 (17%)  | 40,96,114   | 2.01 | 13 (32%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | L     | 1502 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.93 | 18 (21%) |
| 26  | LHG  | 4     | 801  | -    | 48,48,48     | 0.40 | 0        | 51,54,54    | 1.13 | 4 (7%)   |
| 22  | CLA  | 8     | 615  | 15   | 50,54,73     | 1.59 | 6 (12%)  | 59,90,113   | 2.11 | 17 (28%) |
| 40  | CHL  | 1     | 609  | 12   | 52,66,74     | 1.54 | 8 (15%)  | 48,104,114  | 1.95 | 13 (27%) |
| 22  | CLA  | 5     | 618  | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.90 | 18 (21%) |
| 22  | CLA  | B     | 1232 | -    | 49,53,73     | 1.60 | 7 (14%)  | 58,89,113   | 1.99 | 15 (25%) |
| 22  | CLA  | A     | 1120 | -    | 59,63,73     | 1.46 | 6 (10%)  | 70,101,113  | 2.09 | 21 (30%) |
| 22  | CLA  | A     | 1013 | -    | 69,73,73     | 1.38 | 6 (8%)   | 82,113,113  | 1.77 | 18 (21%) |
| 40  | CHL  | Z     | 613  | -    | 40,54,74     | 1.58 | 7 (17%)  | 34,90,114   | 2.16 | 11 (32%) |
| 43  | 3PH  | 5     | 802  | -    | 22,22,47     | 1.24 | 4 (18%)  | 25,27,52    | 1.31 | 2 (8%)   |
| 22  | CLA  | 2     | 604  | -    | 60,64,73     | 1.46 | 8 (13%)  | 71,102,113  | 2.10 | 18 (25%) |
| 26  | LHG  | B     | 5001 | -    | 22,22,48     | 0.55 | 0        | 25,28,54    | 1.31 | 1 (4%)   |
| 22  | CLA  | 8     | 612  | -    | 50,54,73     | 1.59 | 7 (14%)  | 59,90,113   | 2.00 | 13 (22%) |
| 26  | LHG  | 9     | 801  | -    | 32,32,48     | 0.46 | 0        | 35,38,54    | 1.13 | 2 (5%)   |
| 22  | CLA  | 5     | 607  | -    | 65,69,73     | 1.39 | 7 (10%)  | 77,108,113  | 1.90 | 17 (22%) |
| 39  | LUT  | Z     | 503  | -    | 42,43,43     | 2.45 | 1 (2%)   | 51,60,60    | 2.06 | 11 (21%) |
| 22  | CLA  | 4     | 615  | -    | 45,49,73     | 1.67 | 8 (17%)  | 54,84,113   | 2.14 | 15 (27%) |
| 22  | CLA  | B     | 1203 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.81 | 18 (21%) |
| 43  | 3PH  | 2     | 802  | -    | 26,26,47     | 1.15 | 4 (15%)  | 29,31,52    | 1.34 | 2 (6%)   |
| 22  | CLA  | 3     | 603  | -    | 69,73,73     | 1.36 | 8 (11%)  | 82,113,113  | 1.96 | 19 (23%) |
| 22  | CLA  | A     | 1106 | -    | 69,73,73     | 1.36 | 8 (11%)  | 82,113,113  | 1.94 | 18 (21%) |
| 22  | CLA  | A     | 1128 | -    | 69,73,73     | 1.40 | 6 (8%)   | 82,113,113  | 1.83 | 15 (18%) |
| 22  | CLA  | B     | 1213 | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.93 | 21 (25%) |
| 25  | BCR  | 7     | 503  | -    | 41,41,41     | 1.62 | 4 (9%)   | 56,56,56    | 4.48 | 15 (26%) |
| 22  | CLA  | G     | 1601 | -    | 54,58,73     | 1.53 | 6 (11%)  | 64,95,113   | 2.06 | 19 (29%) |
| 22  | CLA  | A     | 1123 | -    | 69,73,73     | 1.39 | 7 (10%)  | 82,113,113  | 1.91 | 17 (20%) |
| 25  | BCR  | 3     | 503  | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.34 | 16 (28%) |
| 25  | BCR  | 6     | 503  | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.44 | 12 (21%) |
| 22  | CLA  | A     | 1114 | -    | 65,69,73     | 1.41 | 7 (10%)  | 77,108,113  | 1.93 | 17 (22%) |
| 39  | LUT  | 2     | 501  | -    | 42,43,43     | 2.46 | 1 (2%)   | 51,60,60    | 2.85 | 15 (29%) |
| 22  | CLA  | 2     | 615  | -    | 50,54,73     | 1.58 | 6 (12%)  | 59,90,113   | 2.05 | 17 (28%) |
| 22  | CLA  | 8     | 603  | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 2.06 | 21 (25%) |
| 32  | DGA  | 9     | 802  | -    | 38,38,43     | 1.18 | 3 (7%)   | 40,40,45    | 1.62 | 3 (7%)   |
| 22  | CLA  | 6     | 612  | -    | 54,58,73     | 1.53 | 7 (12%)  | 64,95,113   | 2.10 | 18 (28%) |
| 22  | CLA  | Z     | 608  | -    | 60,64,73     | 1.45 | 7 (11%)  | 71,102,113  | 1.96 | 17 (23%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 1021 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.87 | 15 (18%) |
| 22  | CLA  | B     | 1220 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.83 | 18 (21%) |
| 22  | CLA  | 9     | 602  | -    | 49,53,73     | 1.63 | 6 (12%)  | 58,89,113   | 1.98 | 12 (20%) |
| 40  | CHL  | 1     | 610  | -    | 42,56,74     | 1.45 | 8 (19%)  | 36,92,114   | 2.11 | 12 (33%) |
| 22  | CLA  | 3     | 606  | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.94 | 16 (19%) |
| 40  | CHL  | 8     | 613  | -    | 60,74,74     | 1.51 | 10 (16%) | 58,114,114  | 1.72 | 13 (22%) |
| 25  | BCR  | A     | 4003 | -    | 41,41,41     | 1.58 | 4 (9%)   | 56,56,56    | 4.51 | 17 (30%) |
| 28  | LMT  | 1     | 803  | -    | 36,36,36     | 1.17 | 6 (16%)  | 47,47,47    | 0.99 | 2 (4%)   |
| 22  | CLA  | A     | 1139 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.91 | 19 (23%) |
| 22  | CLA  | B     | 1214 | -    | 63,67,73     | 1.42 | 7 (11%)  | 74,105,113  | 2.09 | 24 (32%) |
| 22  | CLA  | B     | 1205 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.96 | 18 (21%) |
| 22  | CLA  | 6     | 607  | -    | 59,63,73     | 1.47 | 7 (11%)  | 70,101,113  | 1.98 | 18 (25%) |
| 39  | LUT  | 1     | 502  | -    | 42,43,43     | 2.41 | 1 (2%)   | 51,60,60    | 1.75 | 13 (25%) |
| 45  | LPX  | 8     | 803  | -    | 29,29,29     | 1.02 | 2 (6%)   | 31,33,33    | 1.01 | 1 (3%)   |
| 22  | CLA  | 5     | 612  | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.86 | 16 (19%) |
| 22  | CLA  | L     | 1503 | -    | 54,58,73     | 1.54 | 6 (11%)  | 64,95,113   | 2.08 | 18 (28%) |
| 22  | CLA  | 6     | 605  | -    | 59,63,73     | 1.48 | 7 (11%)  | 70,101,113  | 1.99 | 20 (28%) |
| 22  | CLA  | Z     | 605  | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.91 | 20 (24%) |
| 24  | SF4  | C     | 3003 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 22  | CLA  | 7     | 612  | -    | 54,58,73     | 1.55 | 7 (12%)  | 64,95,113   | 2.06 | 16 (25%) |
| 22  | CLA  | 4     | 604  | -    | 64,68,73     | 1.42 | 7 (10%)  | 76,107,113  | 1.92 | 19 (25%) |
| 22  | CLA  | B     | 1236 | -    | 69,73,73     | 1.38 | 8 (11%)  | 82,113,113  | 1.88 | 20 (24%) |
| 22  | CLA  | A     | 1107 | 1    | 69,73,73     | 1.39 | 6 (8%)   | 82,113,113  | 1.83 | 14 (17%) |
| 22  | CLA  | A     | 1129 | -    | 54,58,73     | 1.55 | 8 (14%)  | 64,95,113   | 2.02 | 16 (25%) |
| 40  | CHL  | 5     | 617  | -    | 37,51,74     | 1.79 | 9 (24%)  | 30,86,114   | 2.31 | 10 (33%) |
| 41  | SQD  | 1     | 802  | -    | 46,48,54     | 0.82 | 1 (2%)   | 56,59,65    | 0.87 | 2 (3%)   |
| 22  | CLA  | B     | 1215 | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.93 | 17 (22%) |
| 27  | NKP  | 8     | 802  | -    | 28,28,28     | 1.52 | 3 (10%)  | 30,32,32    | 1.28 | 3 (10%)  |
| 22  | CLA  | 9     | 608  | -    | 49,53,73     | 1.61 | 7 (14%)  | 58,89,113   | 2.04 | 14 (24%) |
| 26  | LHG  | B     | 5002 | -    | 19,19,48     | 0.75 | 1 (5%)   | 20,24,54    | 1.39 | 1 (5%)   |
| 22  | CLA  | B     | 1235 | -    | 69,73,73     | 1.37 | 8 (11%)  | 82,113,113  | 1.89 | 16 (19%) |
| 22  | CLA  | A     | 1118 | -    | 64,68,73     | 1.40 | 7 (10%)  | 76,107,113  | 2.02 | 20 (26%) |
| 28  | LMT  | 8     | 805  | -    | 36,36,36     | 1.18 | 6 (16%)  | 47,47,47    | 1.16 | 3 (6%)   |
| 22  | CLA  | A     | 1103 | -    | 69,73,73     | 1.32 | 6 (8%)   | 82,113,113  | 1.90 | 17 (20%) |
| 22  | CLA  | 4     | 606  | -    | 54,58,73     | 1.53 | 7 (12%)  | 64,95,113   | 2.04 | 20 (31%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | 1     | 612  | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.87 | 20 (24%) |
| 26  | LHG  | A     | 5001 | 22   | 34,34,48     | 0.46 | 0        | 37,40,54    | 1.20 | 4 (10%)  |
| 22  | CLA  | 6     | 603  | -    | 69,73,73     | 1.37 | 6 (8%)   | 82,113,113  | 1.99 | 19 (23%) |
| 25  | BCR  | A     | 4001 | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.30 | 15 (26%) |
| 25  | BCR  | A     | 4002 | -    | 41,41,41     | 1.63 | 5 (12%)  | 56,56,56    | 4.35 | 14 (25%) |
| 26  | LHG  | 7     | 801  | -    | 36,36,48     | 0.46 | 0        | 39,42,54    | 1.19 | 3 (7%)   |
| 22  | CLA  | A     | 1116 | -    | 64,68,73     | 1.43 | 10 (15%) | 76,107,113  | 1.93 | 20 (26%) |
| 22  | CLA  | 1     | 605  | -    | 59,63,73     | 1.46 | 7 (11%)  | 70,101,113  | 2.05 | 19 (27%) |
| 26  | LHG  | 6     | 801  | -    | 48,48,48     | 0.40 | 0        | 51,54,54    | 1.10 | 4 (7%)   |
| 22  | CLA  | B     | 1201 | -    | 49,53,73     | 1.59 | 8 (16%)  | 58,89,113   | 2.02 | 16 (27%) |
| 25  | BCR  | A     | 4005 | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.39 | 12 (21%) |
| 25  | BCR  | A     | 4004 | -    | 41,41,41     | 1.62 | 5 (12%)  | 56,56,56    | 4.49 | 17 (30%) |
| 38  | SPH  | 7     | 803  | -    | 19,20,20     | 0.69 | 1 (5%)   | 18,21,21    | 0.96 | 0        |
| 40  | CHL  | 6     | 611  | -    | 45,59,74     | 1.40 | 8 (17%)  | 40,96,114   | 2.07 | 13 (32%) |
| 22  | CLA  | K     | 1401 | -    | 50,54,73     | 1.59 | 6 (12%)  | 59,90,113   | 2.00 | 14 (23%) |
| 25  | BCR  | L     | 4001 | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.40 | 14 (25%) |
| 22  | CLA  | A     | 1102 | -    | 59,63,73     | 1.48 | 7 (11%)  | 70,101,113  | 2.04 | 21 (30%) |
| 23  | PQN  | A     | 2001 | -    | 34,34,34     | 0.40 | 0        | 43,45,45    | 1.08 | 2 (4%)   |
| 22  | CLA  | A     | 1136 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.88 | 15 (18%) |
| 39  | LUT  | 4     | 502  | -    | 42,43,43     | 2.39 | 1 (2%)   | 51,60,60    | 1.70 | 13 (25%) |
| 22  | CLA  | 6     | 609  | 18   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.93 | 19 (23%) |
| 22  | CLA  | A     | 1124 | 46   | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.86 | 18 (21%) |
| 22  | CLA  | A     | 1134 | 1    | 59,63,73     | 1.47 | 6 (10%)  | 70,101,113  | 2.07 | 20 (28%) |
| 24  | SF4  | A     | 3001 | 1,2  | 0,12,12      | -    | -        | -           | -    | -        |
| 40  | CHL  | 2     | 609  | 19   | 45,59,74     | 2.00 | 10 (22%) | 40,96,114   | 1.87 | 11 (27%) |
| 26  | LHG  | 4     | 802  | -    | 31,31,48     | 0.48 | 0        | 34,37,54    | 1.14 | 3 (8%)   |
| 22  | CLA  | 2     | 601  | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.98 | 18 (23%) |
| 39  | LUT  | Z     | 501  | -    | 42,43,43     | 2.45 | 1 (2%)   | 51,60,60    | 1.71 | 13 (25%) |
| 22  | CLA  | 7     | 603  | 14   | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 2.03 | 21 (25%) |
| 26  | LHG  | 3     | 801  | -    | 19,19,48     | 0.82 | 1 (5%)   | 20,24,54    | 1.36 | 1 (5%)   |
| 22  | CLA  | 4     | 607  | -    | 59,63,73     | 1.47 | 8 (13%)  | 70,101,113  | 2.01 | 17 (24%) |
| 25  | BCR  | 4     | 503  | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.38 | 16 (28%) |
| 37  | C7Z  | 1     | 503  | -    | 43,43,43     | 5.48 | 26 (60%) | 56,60,60    | 2.34 | 18 (32%) |
| 22  | CLA  | 9     | 605  | -    | 59,63,73     | 1.48 | 7 (11%)  | 70,101,113  | 2.00 | 20 (28%) |
| 22  | CLA  | J     | 1901 | -    | 46,50,73     | 1.65 | 7 (15%)  | 53,85,113   | 2.11 | 17 (32%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | LUT  | 3     | 501  | -    | 42,43,43     | 2.42 | 1 (2%)   | 51,60,60    | 1.79 | 12 (23%) |
| 22  | CLA  | 2     | 603  | -    | 59,63,73     | 1.48 | 7 (11%)  | 70,101,113  | 2.16 | 22 (31%) |
| 35  | T7X  | B     | 5004 | -    | 49,49,61     | 0.94 | 5 (10%)  | 58,61,73    | 1.03 | 3 (5%)   |
| 22  | CLA  | 7     | 602  | -    | 54,58,73     | 1.53 | 6 (11%)  | 64,95,113   | 2.02 | 18 (28%) |
| 22  | CLA  | 6     | 604  | -    | 69,73,73     | 1.37 | 6 (8%)   | 82,113,113  | 1.91 | 21 (25%) |
| 22  | CLA  | B     | 1218 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.97 | 19 (23%) |
| 25  | BCR  | B     | 4006 | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.31 | 13 (23%) |
| 22  | CLA  | 6     | 602  | -    | 56,60,73     | 1.52 | 7 (12%)  | 65,97,113   | 2.06 | 19 (29%) |
| 32  | DGA  | A     | 5005 | -    | 43,43,43     | 1.18 | 3 (6%)   | 45,45,45    | 1.50 | 3 (6%)   |
| 22  | CLA  | B     | 1212 | -    | 61,65,73     | 1.46 | 7 (11%)  | 72,103,113  | 2.04 | 21 (29%) |
| 22  | CLA  | 7     | 601  | -    | 64,68,73     | 1.44 | 7 (10%)  | 76,107,113  | 1.99 | 20 (26%) |
| 40  | CHL  | 4     | 617  | -    | 37,51,74     | 1.78 | 9 (24%)  | 30,86,114   | 2.27 | 10 (33%) |
| 22  | CLA  | 9     | 607  | -    | 59,63,73     | 1.48 | 6 (10%)  | 70,101,113  | 2.01 | 18 (25%) |
| 22  | CLA  | B     | 1238 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.91 | 17 (20%) |
| 39  | LUT  | 2     | 503  | -    | 42,43,43     | 2.50 | 1 (2%)   | 51,60,60    | 2.67 | 23 (45%) |
| 25  | BCR  | I     | 4001 | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.41 | 14 (25%) |
| 22  | CLA  | B     | 1204 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.87 | 17 (20%) |
| 39  | LUT  | 9     | 501  | -    | 42,43,43     | 2.45 | 1 (2%)   | 51,60,60    | 1.80 | 15 (29%) |
| 39  | LUT  | Z     | 502  | -    | 42,43,43     | 2.33 | 1 (2%)   | 51,60,60    | 1.80 | 12 (23%) |
| 22  | CLA  | 8     | 605  | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.83 | 19 (23%) |
| 22  | CLA  | Z     | 604  | -    | 69,73,73     | 1.37 | 8 (11%)  | 82,113,113  | 1.90 | 21 (25%) |
| 25  | BCR  | B     | 4002 | -    | 41,41,41     | 1.62 | 4 (9%)   | 56,56,56    | 4.35 | 8 (14%)  |
| 22  | CLA  | 6     | 606  | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.90 | 19 (23%) |
| 22  | CLA  | 2     | 605  | -    | 54,58,73     | 1.56 | 8 (14%)  | 64,95,113   | 2.09 | 18 (28%) |
| 22  | CLA  | 1     | 602  | -    | 49,53,73     | 1.63 | 8 (16%)  | 58,89,113   | 1.99 | 16 (27%) |
| 37  | C7Z  | J     | 4002 | -    | 43,43,43     | 5.46 | 26 (60%) | 56,60,60    | 2.24 | 20 (35%) |
| 22  | CLA  | Z     | 601  | -    | 64,68,73     | 1.40 | 7 (10%)  | 76,107,113  | 1.96 | 19 (25%) |
| 22  | CLA  | B     | 1216 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.83 | 17 (20%) |
| 22  | CLA  | B     | 1202 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.97 | 20 (24%) |
| 40  | CHL  | 2     | 610  | -    | 42,56,74     | 1.57 | 9 (21%)  | 36,92,114   | 2.16 | 11 (30%) |
| 22  | CLA  | 3     | 604  | -    | 64,68,73     | 1.39 | 7 (10%)  | 76,107,113  | 2.02 | 19 (25%) |
| 42  | QTB  | Z     | 504  | -    | 19,19,19     | 2.51 | 4 (21%)  | 23,26,26    | 2.91 | 9 (39%)  |
| 22  | CLA  | 3     | 607  | -    | 64,68,73     | 1.42 | 8 (12%)  | 76,107,113  | 2.04 | 19 (25%) |
| 22  | CLA  | 2     | 602  | -    | 50,54,73     | 1.59 | 6 (12%)  | 59,90,113   | 2.08 | 17 (28%) |
| 22  | CLA  | 8     | 609  | 15   | 69,73,73     | 1.37 | 6 (8%)   | 82,113,113  | 1.92 | 18 (21%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | A     | 1125 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.93 | 22 (26%) |
| 25  | BCR  | 8     | 503  | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.42 | 13 (23%) |
| 22  | CLA  | 5     | 615  | 17   | 54,58,73     | 1.54 | 6 (11%)  | 64,95,113   | 2.13 | 20 (31%) |
| 22  | CLA  | 5     | 601  | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.96 | 19 (25%) |
| 22  | CLA  | A     | 1135 | -    | 55,59,73     | 1.55 | 8 (14%)  | 64,96,113   | 2.14 | 19 (29%) |
| 22  | CLA  | A     | 1012 | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.89 | 20 (24%) |
| 40  | CHL  | 7     | 610  | -    | 48,62,74     | 1.44 | 9 (18%)  | 43,99,114   | 1.99 | 13 (30%) |
| 26  | LHG  | Z     | 801  | -    | 42,42,48     | 0.41 | 0        | 45,48,54    | 1.18 | 4 (8%)   |
| 39  | LUT  | 6     | 501  | -    | 42,43,43     | 2.47 | 1 (2%)   | 51,60,60    | 1.77 | 14 (27%) |
| 25  | BCR  | 7     | 504  | -    | 41,41,41     | 1.59 | 4 (9%)   | 56,56,56    | 4.64 | 17 (30%) |
| 39  | LUT  | 7     | 501  | -    | 42,43,43     | 2.45 | 1 (2%)   | 51,60,60    | 1.74 | 12 (23%) |
| 22  | CLA  | 3     | 608  | -    | 49,53,73     | 1.60 | 7 (14%)  | 58,89,113   | 2.08 | 14 (24%) |
| 31  | LMG  | J     | 5001 | -    | 35,35,55     | 0.49 | 0        | 43,43,63    | 1.13 | 2 (4%)   |
| 25  | BCR  | 6     | 504  | -    | 41,41,41     | 1.66 | 4 (9%)   | 56,56,56    | 4.46 | 16 (28%) |
| 25  | BCR  | B     | 4003 | -    | 41,41,41     | 1.66 | 5 (12%)  | 56,56,56    | 4.41 | 18 (32%) |
| 22  | CLA  | 3     | 613  | 46   | 59,63,73     | 1.46 | 7 (11%)  | 70,101,113  | 1.97 | 15 (21%) |
| 39  | LUT  | 9     | 502  | -    | 42,43,43     | 2.32 | 1 (2%)   | 51,60,60    | 1.79 | 13 (25%) |
| 22  | CLA  | A     | 1127 | -    | 69,73,73     | 1.38 | 6 (8%)   | 82,113,113  | 1.78 | 16 (19%) |
| 22  | CLA  | 8     | 604  | -    | 66,70,73     | 1.40 | 7 (10%)  | 78,109,113  | 1.97 | 23 (29%) |
| 22  | CLA  | Z     | 611  | -    | 59,63,73     | 1.46 | 7 (11%)  | 70,101,113  | 2.03 | 20 (28%) |
| 22  | CLA  | 8     | 601  | -    | 64,68,73     | 1.42 | 8 (12%)  | 76,107,113  | 1.96 | 19 (25%) |
| 40  | CHL  | 4     | 613  | -    | 50,64,74     | 1.36 | 8 (16%)  | 46,102,114  | 1.95 | 11 (23%) |
| 22  | CLA  | 1     | 601  | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.89 | 21 (25%) |
| 22  | CLA  | 9     | 609  | 20   | 50,54,73     | 1.61 | 7 (14%)  | 59,90,113   | 2.06 | 16 (27%) |
| 22  | CLA  | B     | 1239 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.94 | 18 (21%) |
| 22  | CLA  | 5     | 605  | -    | 59,63,73     | 1.49 | 8 (13%)  | 70,101,113  | 2.07 | 23 (32%) |
| 22  | CLA  | 1     | 611  | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.92 | 19 (23%) |
| 36  | RRX  | F     | 4001 | -    | 42,42,42     | 4.95 | 24 (57%) | 56,58,58    | 2.53 | 23 (41%) |
| 39  | LUT  | 5     | 502  | -    | 42,43,43     | 2.34 | 1 (2%)   | 51,60,60    | 1.71 | 10 (19%) |
| 40  | CHL  | 9     | 613  | -    | 36,50,74     | 2.18 | 10 (27%) | 29,85,114   | 2.17 | 10 (34%) |
| 22  | CLA  | F     | 1302 | -    | 49,53,73     | 1.59 | 7 (14%)  | 58,89,113   | 2.00 | 16 (27%) |
| 22  | CLA  | 3     | 618  | -    | 50,54,73     | 1.60 | 8 (16%)  | 59,90,113   | 2.01 | 15 (25%) |
| 40  | CHL  | 3     | 611  | -    | 60,74,74     | 1.45 | 8 (13%)  | 58,114,114  | 1.72 | 14 (24%) |
| 22  | CLA  | 1     | 603  | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.95 | 20 (24%) |
| 22  | CLA  | Z     | 615  | 12   | 50,54,73     | 1.58 | 6 (12%)  | 59,90,113   | 2.06 | 17 (28%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 1240 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.88 | 22 (26%) |
| 22  | CLA  | 4     | 603  | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.98 | 21 (25%) |
| 22  | CLA  | B     | 1207 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.86 | 19 (23%) |
| 22  | CLA  | 5     | 609  | 17   | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.85 | 20 (24%) |
| 39  | LUT  | 8     | 501  | -    | 42,43,43     | 2.39 | 1 (2%)   | 51,60,60    | 1.77 | 13 (25%) |
| 28  | LMT  | F     | 5001 | -    | 36,36,36     | 1.16 | 5 (13%)  | 47,47,47    | 0.98 | 2 (4%)   |
| 22  | CLA  | 9     | 604  | -    | 69,73,73     | 1.38 | 8 (11%)  | 82,113,113  | 1.93 | 22 (26%) |
| 40  | CHL  | 4     | 610  | -    | 45,59,74     | 1.29 | 7 (15%)  | 40,96,114   | 2.02 | 13 (32%) |
| 22  | CLA  | 9     | 612  | -    | 54,58,73     | 1.56 | 8 (14%)  | 64,95,113   | 2.08 | 17 (26%) |
| 28  | LMT  | A     | 5006 | -    | 36,36,36     | 1.18 | 6 (16%)  | 47,47,47    | 1.05 | 1 (2%)   |
| 22  | CLA  | B     | 1241 | -    | 69,73,73     | 1.35 | 8 (11%)  | 82,113,113  | 2.01 | 22 (26%) |
| 22  | CLA  | 4     | 608  | -    | 59,63,73     | 1.47 | 6 (10%)  | 70,101,113  | 2.00 | 18 (25%) |
| 22  | CLA  | 5     | 603  | -    | 60,64,73     | 1.44 | 6 (10%)  | 71,102,113  | 2.14 | 20 (28%) |
| 22  | CLA  | Z     | 607  | -    | 61,65,73     | 1.44 | 7 (11%)  | 72,103,113  | 1.96 | 18 (25%) |
| 22  | CLA  | 7     | 607  | -    | 69,73,73     | 1.36 | 8 (11%)  | 82,113,113  | 1.85 | 18 (21%) |
| 40  | CHL  | 5     | 611  | -    | 45,59,74     | 1.41 | 8 (17%)  | 40,96,114   | 2.12 | 13 (32%) |
| 22  | CLA  | B     | 1228 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.85 | 19 (23%) |
| 22  | CLA  | 5     | 604  | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.89 | 22 (26%) |
| 22  | CLA  | B     | 1234 | -    | 64,68,73     | 1.43 | 7 (10%)  | 76,107,113  | 1.93 | 21 (27%) |
| 22  | CLA  | 5     | 613  | -    | 59,63,73     | 1.47 | 8 (13%)  | 70,101,113  | 1.94 | 18 (25%) |
| 22  | CLA  | B     | 1219 | -    | 63,67,73     | 1.44 | 7 (11%)  | 74,105,113  | 2.02 | 17 (22%) |
| 22  | CLA  | A     | 1132 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.95 | 19 (23%) |
| 22  | CLA  | Z     | 606  | -    | 61,65,73     | 1.43 | 6 (9%)   | 72,103,113  | 2.05 | 18 (25%) |
| 22  | CLA  | 6     | 619  | 18   | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.92 | 18 (21%) |
| 22  | CLA  | B     | 1223 | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.87 | 19 (23%) |
| 22  | CLA  | 8     | 602  | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.84 | 17 (20%) |
| 22  | CLA  | B     | 1023 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.95 | 18 (21%) |
| 22  | CLA  | 7     | 606  | -    | 60,64,73     | 1.46 | 8 (13%)  | 71,102,113  | 2.00 | 16 (22%) |
| 22  | CLA  | A     | 1113 | -    | 69,73,73     | 1.37 | 6 (8%)   | 82,113,113  | 1.88 | 17 (20%) |
| 26  | LHG  | 2     | 801  | -    | 33,33,48     | 0.46 | 0        | 36,39,54    | 1.24 | 3 (8%)   |
| 22  | CLA  | B     | 1217 | -    | 60,64,73     | 1.46 | 7 (11%)  | 71,102,113  | 1.98 | 20 (28%) |
| 22  | CLA  | A     | 1108 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.89 | 20 (24%) |
| 25  | BCR  | 5     | 503  | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.42 | 15 (26%) |
| 37  | C7Z  | 5     | 505  | -    | 43,43,43     | 5.51 | 26 (60%) | 56,60,60    | 2.28 | 16 (28%) |
| 26  | LHG  | B     | 5006 | -    | 32,32,48     | 0.45 | 0        | 35,38,54    | 1.22 | 4 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | 7     | 611  | -    | 54,58,73     | 1.51 | 7 (12%)  | 64,95,113   | 2.13 | 21 (32%) |
| 22  | CLA  | 2     | 606  | -    | 50,54,73     | 1.60 | 7 (14%)  | 59,90,113   | 2.09 | 13 (22%) |
| 25  | BCR  | B     | 4004 | -    | 41,41,41     | 1.62 | 4 (9%)   | 56,56,56    | 4.40 | 14 (25%) |
| 22  | CLA  | A     | 1121 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.94 | 19 (23%) |
| 39  | LUT  | 5     | 501  | -    | 42,43,43     | 2.54 | 2 (4%)   | 51,60,60    | 1.77 | 12 (23%) |
| 38  | SPH  | K     | 5001 | -    | 19,20,20     | 0.63 | 0        | 18,21,21    | 1.12 | 2 (11%)  |
| 40  | CHL  | 6     | 613  | -    | 50,64,74     | 1.45 | 8 (16%)  | 46,102,114  | 1.92 | 12 (26%) |
| 22  | CLA  | B     | 1227 | -    | 54,58,73     | 1.54 | 8 (14%)  | 64,95,113   | 1.96 | 18 (28%) |
| 40  | CHL  | Z     | 609  | 12   | 60,74,74     | 1.54 | 8 (13%)  | 58,114,114  | 1.72 | 13 (22%) |
| 28  | LMT  | B     | 5005 | -    | 36,36,36     | 1.19 | 5 (13%)  | 47,47,47    | 1.12 | 3 (6%)   |
| 22  | CLA  | 7     | 605  | -    | 65,69,73     | 1.39 | 6 (9%)   | 77,108,113  | 1.94 | 21 (27%) |
| 22  | CLA  | B     | 1206 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.89 | 14 (17%) |
| 25  | BCR  | 3     | 506  | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.56 | 13 (23%) |
| 23  | PQN  | B     | 2002 | -    | 34,34,34     | 0.42 | 0        | 43,45,45    | 1.06 | 2 (4%)   |
| 22  | CLA  | B     | 1022 | 46   | 69,73,73     | 1.38 | 6 (8%)   | 82,113,113  | 1.83 | 21 (25%) |
| 22  | CLA  | A     | 1131 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.88 | 18 (21%) |
| 27  | NKP  | 3     | 802  | -    | 15,15,28     | 2.10 | 3 (20%)  | 17,19,32    | 1.58 | 2 (11%)  |
| 22  | CLA  | 7     | 615  | 14   | 62,66,73     | 1.44 | 7 (11%)  | 73,104,113  | 1.98 | 20 (27%) |
| 33  | DGD  | B     | 5003 | -    | 67,67,67     | 1.30 | 7 (10%)  | 81,81,81    | 1.03 | 4 (4%)   |
| 26  | LHG  | 8     | 801  | -    | 37,37,48     | 0.44 | 0        | 40,43,54    | 1.09 | 2 (5%)   |
| 22  | CLA  | 4     | 601  | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 2.00 | 21 (27%) |
| 26  | LHG  | A     | 5002 | -    | 48,48,48     | 0.40 | 0        | 51,54,54    | 0.99 | 2 (3%)   |
| 39  | LUT  | 1     | 501  | -    | 42,43,43     | 2.44 | 1 (2%)   | 51,60,60    | 1.68 | 13 (25%) |
| 22  | CLA  | 1     | 606  | -    | 65,69,73     | 1.39 | 8 (12%)  | 77,108,113  | 1.92 | 16 (20%) |
| 22  | CLA  | A     | 1104 | 1    | 69,73,73     | 1.36 | 8 (11%)  | 82,113,113  | 1.88 | 20 (24%) |
| 22  | CLA  | F     | 1301 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.92 | 22 (26%) |
| 22  | CLA  | 3     | 612  | -    | 64,68,73     | 1.40 | 8 (12%)  | 76,107,113  | 1.92 | 16 (21%) |
| 30  | DAO  | A     | 5007 | -    | 13,13,13     | 0.80 | 1 (7%)   | 13,13,13    | 0.97 | 0        |
| 22  | CLA  | 8     | 611  | -    | 54,58,73     | 1.52 | 7 (12%)  | 64,95,113   | 2.12 | 18 (28%) |
| 22  | CLA  | A     | 1126 | -    | 69,73,73     | 1.37 | 8 (11%)  | 82,113,113  | 1.90 | 19 (23%) |
| 22  | CLA  | 5     | 602  | -    | 65,69,73     | 1.40 | 8 (12%)  | 77,108,113  | 1.85 | 18 (23%) |
| 25  | BCR  | K     | 4001 | -    | 41,41,41     | 1.58 | 4 (9%)   | 56,56,56    | 4.52 | 13 (23%) |
| 39  | LUT  | 7     | 502  | -    | 42,43,43     | 2.40 | 1 (2%)   | 51,60,60    | 1.85 | 12 (23%) |
| 22  | CLA  | A     | 1117 | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 1.88 | 16 (19%) |
| 28  | LMT  | B     | 6101 | -    | 36,36,36     | 1.16 | 5 (13%)  | 47,47,47    | 1.09 | 3 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 1208 | -    | 60,64,73     | 1.46 | 8 (13%)  | 71,102,113  | 2.00 | 18 (25%) |
| 22  | CLA  | A     | 1122 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.89 | 19 (23%) |
| 39  | LUT  | 3     | 502  | -    | 42,43,43     | 2.48 | 1 (2%)   | 51,60,60    | 1.83 | 14 (27%) |
| 43  | 3PH  | 8     | 806  | -    | 29,29,47     | 1.09 | 4 (13%)  | 32,34,52    | 1.14 | 2 (6%)   |
| 39  | LUT  | 6     | 502  | -    | 42,43,43     | 2.41 | 1 (2%)   | 51,60,60    | 1.76 | 14 (27%) |
| 22  | CLA  | A     | 1112 | -    | 64,68,73     | 1.42 | 7 (10%)  | 76,107,113  | 1.96 | 17 (22%) |
| 22  | CLA  | Z     | 603  | -    | 54,58,73     | 1.52 | 7 (12%)  | 64,95,113   | 2.14 | 20 (31%) |
| 22  | CLA  | 6     | 601  | -    | 64,68,73     | 1.42 | 6 (9%)   | 76,107,113  | 1.96 | 18 (23%) |
| 22  | CLA  | K     | 1402 | -    | 59,63,73     | 1.47 | 7 (11%)  | 70,101,113  | 2.06 | 20 (28%) |
| 22  | CLA  | G     | 1602 | -    | 50,54,73     | 1.60 | 7 (14%)  | 59,90,113   | 2.05 | 14 (23%) |
| 22  | CLA  | 7     | 609  | 14   | 69,73,73     | 1.34 | 7 (10%)  | 82,113,113  | 1.92 | 19 (23%) |
| 40  | CHL  | Z     | 610  | -    | 60,74,74     | 1.21 | 7 (11%)  | 58,114,114  | 1.69 | 13 (22%) |
| 22  | CLA  | 2     | 608  | -    | 49,53,73     | 1.61 | 7 (14%)  | 58,89,113   | 2.11 | 16 (27%) |
| 21  | CL0  | A     | 1011 | -    | 58,73,73     | 3.22 | 17 (29%) | 60,113,113  | 2.88 | 17 (28%) |
| 25  | BCR  | J     | 4001 | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.39 | 16 (28%) |
| 44  | PLM  | 7     | 805  | -    | 17,17,17     | 0.57 | 0        | 17,17,17    | 1.10 | 0        |
| 22  | CLA  | K     | 1403 | 10   | 53,57,73     | 1.56 | 6 (11%)  | 61,93,113   | 2.11 | 15 (24%) |
| 25  | BCR  | 3     | 505  | -    | 41,41,41     | 1.60 | 4 (9%)   | 56,56,56    | 4.48 | 11 (19%) |
| 29  | OCA  | A     | 5008 | -    | 9,9,9        | 0.72 | 0        | 9,9,9       | 1.36 | 1 (11%)  |
| 26  | LHG  | 5     | 801  | -    | 36,36,48     | 0.43 | 0        | 39,42,54    | 1.19 | 4 (10%)  |
| 39  | LUT  | 8     | 502  | -    | 42,43,43     | 2.36 | 1 (2%)   | 51,60,60    | 1.78 | 13 (25%) |
| 22  | CLA  | A     | 1111 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.92 | 20 (24%) |
| 40  | CHL  | 8     | 610  | -    | 50,64,74     | 1.33 | 8 (16%)  | 46,102,114  | 1.85 | 11 (23%) |
| 22  | CLA  | B     | 1231 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.85 | 16 (19%) |
| 40  | CHL  | 6     | 610  | -    | 50,64,74     | 1.34 | 7 (14%)  | 46,102,114  | 1.89 | 13 (28%) |
| 43  | 3PH  | 7     | 802  | -    | 38,38,47     | 0.95 | 4 (10%)  | 41,43,52    | 1.15 | 2 (4%)   |
| 22  | CLA  | 4     | 612  | -    | 54,58,73     | 1.51 | 6 (11%)  | 64,95,113   | 2.16 | 19 (29%) |
| 22  | CLA  | 4     | 605  | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.86 | 17 (20%) |
| 43  | 3PH  | 6     | 802  | -    | 28,28,47     | 1.12 | 4 (14%)  | 31,33,52    | 1.29 | 2 (6%)   |
| 22  | CLA  | B     | 1224 | -    | 69,73,73     | 1.39 | 7 (10%)  | 82,113,113  | 1.90 | 18 (21%) |
| 22  | CLA  | A     | 1137 | -    | 69,73,73     | 1.37 | 6 (8%)   | 82,113,113  | 1.92 | 19 (23%) |
| 40  | CHL  | 6     | 617  | -    | 37,51,74     | 1.80 | 9 (24%)  | 30,86,114   | 2.25 | 10 (33%) |
| 22  | CLA  | 7     | 613  | -    | 46,50,73     | 1.66 | 7 (15%)  | 53,85,113   | 2.07 | 16 (30%) |
| 22  | CLA  | 8     | 606  | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.89 | 19 (25%) |
| 22  | CLA  | 6     | 615  | -    | 65,69,73     | 1.40 | 6 (9%)   | 77,108,113  | 1.99 | 21 (27%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | BCR  | B     | 4005 | -    | 41,41,41     | 1.63 | 4 (9%)   | 56,56,56    | 4.65 | 16 (28%) |
| 31  | LMG  | A     | 5003 | -    | 29,29,55     | 0.58 | 0        | 37,37,63    | 1.22 | 4 (10%)  |
| 22  | CLA  | 1     | 604  | -    | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.94 | 18 (23%) |
| 38  | SPH  | 7     | 804  | -    | 19,20,20     | 0.66 | 0        | 18,21,21    | 1.13 | 1 (5%)   |
| 22  | CLA  | 8     | 608  | -    | 59,63,73     | 1.46 | 6 (10%)  | 70,101,113  | 1.94 | 18 (25%) |
| 22  | CLA  | Z     | 612  | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.86 | 17 (20%) |
| 28  | LMT  | 4     | 803  | -    | 36,36,36     | 1.14 | 5 (13%)  | 47,47,47    | 1.02 | 1 (2%)   |
| 22  | CLA  | A     | 1133 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.83 | 15 (18%) |
| 22  | CLA  | 2     | 607  | -    | 50,54,73     | 1.61 | 7 (14%)  | 59,90,113   | 2.07 | 15 (25%) |
| 25  | BCR  | 5     | 504  | -    | 41,41,41     | 1.63 | 5 (12%)  | 56,56,56    | 4.63 | 21 (37%) |
| 22  | CLA  | B     | 1209 | -    | 69,73,73     | 1.38 | 6 (8%)   | 82,113,113  | 1.89 | 17 (20%) |
| 22  | CLA  | A     | 1140 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.85 | 19 (23%) |
| 22  | CLA  | B     | 1230 | -    | 62,66,73     | 1.41 | 6 (9%)   | 73,104,113  | 2.03 | 20 (27%) |
| 22  | CLA  | A     | 1101 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.92 | 21 (25%) |
| 22  | CLA  | 3     | 616  | -    | 60,64,73     | 1.45 | 7 (11%)  | 71,102,113  | 2.05 | 20 (28%) |
| 22  | CLA  | A     | 1138 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.91 | 16 (19%) |
| 25  | BCR  | K     | 4002 | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.41 | 16 (28%) |
| 26  | LHG  | 1     | 801  | -    | 42,42,48     | 0.45 | 0        | 45,48,54    | 1.19 | 4 (8%)   |
| 22  | CLA  | A     | 1130 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.83 | 16 (19%) |
| 41  | SQD  | 2     | 803  | -    | 41,43,54     | 0.86 | 1 (2%)   | 51,54,65    | 0.91 | 2 (3%)   |
| 39  | LUT  | 4     | 501  | -    | 42,43,43     | 2.46 | 1 (2%)   | 51,60,60    | 1.69 | 11 (21%) |
| 22  | CLA  | 3     | 602  | -    | 50,54,73     | 1.58 | 6 (12%)  | 59,90,113   | 1.98 | 14 (23%) |
| 22  | CLA  | 3     | 610  | 13   | 64,68,73     | 1.42 | 7 (10%)  | 76,107,113  | 1.95 | 19 (25%) |
| 22  | CLA  | A     | 1105 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.87 | 19 (23%) |
| 25  | BCR  | L     | 4002 | -    | 41,41,41     | 1.61 | 4 (9%)   | 56,56,56    | 4.38 | 15 (26%) |
| 22  | CLA  | K     | 1404 | -    | 59,63,73     | 1.48 | 7 (11%)  | 70,101,113  | 2.06 | 17 (24%) |
| 22  | CLA  | 6     | 608  | -    | 59,63,73     | 1.48 | 7 (11%)  | 70,101,113  | 2.03 | 16 (22%) |
| 22  | CLA  | B     | 1210 | -    | 69,73,73     | 1.38 | 7 (10%)  | 82,113,113  | 2.01 | 21 (25%) |
| 22  | CLA  | 7     | 604  | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.94 | 23 (28%) |
| 24  | SF4  | C     | 3002 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 22  | CLA  | B     | 1237 | -    | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.87 | 16 (19%) |
| 22  | CLA  | 1     | 608  | -    | 64,68,73     | 1.38 | 7 (10%)  | 76,107,113  | 1.96 | 16 (21%) |
| 40  | CHL  | 5     | 610  | -    | 60,74,74     | 1.38 | 9 (15%)  | 58,114,114  | 1.68 | 11 (18%) |
| 22  | CLA  | A     | 1110 | -    | 69,73,73     | 1.37 | 7 (10%)  | 82,113,113  | 1.90 | 18 (21%) |
| 22  | CLA  | 9     | 603  | -    | 64,68,73     | 1.43 | 6 (9%)   | 76,107,113  | 2.09 | 18 (23%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | B     | 1211 | -    | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 2.05 | 19 (25%) |
| 22  | CLA  | 1     | 613  | -    | 50,54,73     | 1.61 | 8 (16%)  | 59,90,113   | 2.02 | 15 (25%) |
| 22  | CLA  | 4     | 602  | -    | 56,60,73     | 1.51 | 7 (12%)  | 65,97,113   | 2.05 | 18 (27%) |

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

| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | 5     | 608  | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 22  | CLA  | B     | 1226 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 40  | CHL  | 9     | 610  | -    | 4/4/20/26 | 5/39/137/137  | -       |
| 22  | CLA  | A     | 1141 | 26   | 1/1/12/20 | 8/24/100/115  | -       |
| 22  | CLA  | 3     | 605  | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 25  | BCR  | G     | 4001 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 5     | 606  | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 28  | LMT  | 9     | 803  | -    | -         | 9/21/61/61    | 0/2/2/2 |
| 22  | CLA  | 2     | 612  | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 22  | CLA  | 6     | 618  | -    | 1/1/11/20 | 8/17/93/115   | -       |
| 22  | CLA  | B     | 1222 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | 1     | 615  | 12   | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | B     | 1221 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 7     | 608  | -    | 1/1/10/20 | 5/13/89/115   | -       |
| 22  | CLA  | 7     | 616  | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 22  | CLA  | B     | 1225 | -    | 1/1/15/20 | 4/39/115/115  | -       |
| 22  | CLA  | A     | 1119 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 8     | 607  | -    | 1/1/13/20 | 13/27/103/115 | -       |
| 22  | CLA  | A     | 1115 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 39  | LUT  | 2     | 502  | -    | -         | 5/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 1     | 607  | -    | 1/1/14/20 | 14/33/109/115 | -       |
| 25  | BCR  | 3     | 504  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 4     | 609  | 16   | 1/1/14/20 | 12/33/109/115 | -       |
| 22  | CLA  | Z     | 602  | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 22  | CLA  | 9     | 606  | -    | 1/1/12/20 | 11/21/97/115  | -       |
| 22  | CLA  | 9     | 601  | -    | 1/1/14/20 | 14/33/109/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | 3     | 601  | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | 5     | 622  | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 22  | CLA  | A     | 1109 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | B     | 1229 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 27  | NKP  | A     | 5004 | -    | -         | 12/28/28/28   | -       |
| 25  | BCR  | B     | 4001 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 40  | CHL  | 4     | 611  | -    | 3/3/17/26 | 4/21/119/137  | -       |
| 25  | BCR  | B     | 4007 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 40  | CHL  | 2     | 613  | -    | 3/3/17/26 | 3/21/119/137  | -       |
| 22  | CLA  | L     | 1502 | -    | 1/1/15/20 | 22/39/115/115 | -       |
| 26  | LHG  | 4     | 801  | -    | -         | 28/53/53/53   | -       |
| 22  | CLA  | 8     | 615  | 15   | 1/1/11/20 | 7/17/93/115   | -       |
| 40  | CHL  | 1     | 609  | 12   | 4/4/18/26 | 1/30/128/137  | -       |
| 22  | CLA  | 5     | 618  | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | B     | 1232 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 22  | CLA  | A     | 1120 | -    | 1/1/13/20 | 11/27/103/115 | -       |
| 22  | CLA  | A     | 1013 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 40  | CHL  | Z     | 613  | -    | 3/3/16/26 | 5/15/113/137  | -       |
| 43  | 3PH  | 5     | 802  | -    | -         | 7/24/24/49    | -       |
| 22  | CLA  | 2     | 604  | -    | 1/1/13/20 | 11/29/105/115 | -       |
| 26  | LHG  | B     | 5001 | -    | -         | 13/26/26/53   | -       |
| 22  | CLA  | 8     | 612  | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 26  | LHG  | 9     | 801  | -    | -         | 18/37/37/53   | -       |
| 22  | CLA  | 5     | 607  | -    | 1/1/14/20 | 14/35/111/115 | -       |
| 39  | LUT  | Z     | 503  | -    | -         | 10/29/67/67   | 0/2/2/2 |
| 22  | CLA  | 4     | 615  | -    | 1/1/10/20 | 4/10/86/115   | -       |
| 22  | CLA  | B     | 1203 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 43  | 3PH  | 2     | 802  | -    | -         | 8/28/28/49    | -       |
| 22  | CLA  | 3     | 603  | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 1106 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 1128 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | B     | 1213 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | BCR  | 7     | 503  | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 22  | CLA  | G     | 1601 | -    | 1/1/12/20 | 9/21/97/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | A     | 1123 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | BCR  | 3     | 503  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 25  | BCR  | 6     | 503  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 1114 | -    | 1/1/14/20 | 9/35/111/115  | -       |
| 39  | LUT  | 2     | 501  | -    | 1/1/12/27 | 7/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 2     | 615  | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 22  | CLA  | 8     | 603  | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 32  | DGA  | 9     | 802  | -    | -         | 21/40/40/45   | -       |
| 22  | CLA  | 6     | 612  | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | Z     | 608  | -    | 1/1/13/20 | 13/29/105/115 | -       |
| 22  | CLA  | B     | 1021 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 22  | CLA  | B     | 1220 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | 9     | 602  | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 40  | CHL  | 1     | 610  | -    | 3/3/16/26 | 6/18/116/137  | -       |
| 22  | CLA  | 3     | 606  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 40  | CHL  | 8     | 613  | -    | 5/5/20/26 | 12/39/137/137 | -       |
| 25  | BCR  | A     | 4003 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 28  | LMT  | 1     | 803  | -    | -         | 4/21/61/61    | 0/2/2/2 |
| 22  | CLA  | A     | 1139 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | B     | 1214 | -    | 1/1/13/20 | 13/32/108/115 | -       |
| 22  | CLA  | B     | 1205 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | 6     | 607  | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 39  | LUT  | 1     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 45  | LPX  | 8     | 803  | -    | -         | 10/31/31/31   | -       |
| 22  | CLA  | 5     | 612  | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | L     | 1503 | -    | 1/1/12/20 | 9/21/97/115   | -       |
| 22  | CLA  | 6     | 605  | -    | 1/1/13/20 | 14/27/103/115 | -       |
| 22  | CLA  | Z     | 605  | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 24  | SF4  | C     | 3003 | 3    | -         | -             | 0/6/5/5 |
| 22  | CLA  | 7     | 612  | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | 4     | 604  | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 22  | CLA  | B     | 1236 | -    | 1/1/15/20 | 21/39/115/115 | -       |
| 22  | CLA  | A     | 1107 | 1    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | A     | 1129 | -    | 1/1/12/20 | 9/21/97/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 40  | CHL  | 5     | 617  | -    | 3/3/15/26 | 2/12/110/137  | -       |
| 41  | SQD  | 1     | 802  | -    | -         | 17/43/63/69   | 0/1/1/1 |
| 22  | CLA  | B     | 1215 | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 27  | NKP  | 8     | 802  | -    | -         | 12/28/28/28   | -       |
| 22  | CLA  | 9     | 608  | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 26  | LHG  | B     | 5002 | -    | -         | 12/22/22/53   | -       |
| 22  | CLA  | B     | 1235 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | A     | 1118 | -    | 1/1/14/20 | 9/33/109/115  | -       |
| 28  | LMT  | 8     | 805  | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 22  | CLA  | A     | 1103 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | 4     | 606  | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 22  | CLA  | 1     | 612  | -    | 1/1/15/20 | 24/39/115/115 | -       |
| 26  | LHG  | A     | 5001 | 22   | -         | 15/39/39/53   | -       |
| 22  | CLA  | 6     | 603  | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 25  | BCR  | A     | 4001 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 25  | BCR  | A     | 4002 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 26  | LHG  | 7     | 801  | -    | -         | 20/41/41/53   | -       |
| 22  | CLA  | A     | 1116 | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 22  | CLA  | 1     | 605  | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 26  | LHG  | 6     | 801  | -    | -         | 35/53/53/53   | -       |
| 22  | CLA  | B     | 1201 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 25  | BCR  | A     | 4005 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 25  | BCR  | A     | 4004 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 38  | SPH  | 7     | 803  | -    | -         | 11/21/21/21   | -       |
| 40  | CHL  | 6     | 611  | -    | 3/3/17/26 | 6/21/119/137  | -       |
| 22  | CLA  | K     | 1401 | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 25  | BCR  | L     | 4001 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 1102 | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 23  | PQN  | A     | 2001 | -    | -         | 3/23/43/43    | 0/2/2/2 |
| 22  | CLA  | A     | 1136 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 39  | LUT  | 4     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 6     | 609  | 18   | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | A     | 1124 | 46   | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | A     | 1134 | 1    | 1/1/13/20 | 13/27/103/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 40  | CHL  | 2     | 609  | 19   | 3/3/17/26 | 2/21/119/137  | -       |
| 24  | SF4  | A     | 3001 | 1,2  | -         | -             | 0/6/5/5 |
| 26  | LHG  | 4     | 802  | -    | -         | 25/36/36/53   | -       |
| 22  | CLA  | 2     | 601  | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 39  | LUT  | Z     | 501  | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 7     | 603  | 14   | 1/1/15/20 | 13/39/115/115 | -       |
| 26  | LHG  | 3     | 801  | -    | -         | 11/22/22/53   | -       |
| 22  | CLA  | 4     | 607  | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 25  | BCR  | 4     | 503  | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 37  | C7Z  | 1     | 503  | -    | 1/1/12/26 | 8/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 9     | 605  | -    | -         | 7/27/103/115  | -       |
| 22  | CLA  | J     | 1901 | -    | 1/1/10/20 | 6/12/88/115   | -       |
| 39  | LUT  | 3     | 501  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 2     | 603  | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 35  | T7X  | B     | 5004 | -    | -         | 13/44/68/80   | 0/1/1/1 |
| 22  | CLA  | 7     | 602  | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | 6     | 604  | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | B     | 1218 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | BCR  | B     | 4006 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 6     | 602  | -    | 1/1/12/20 | 8/24/100/115  | -       |
| 32  | DGA  | A     | 5005 | -    | -         | 24/45/45/45   | -       |
| 22  | CLA  | B     | 1212 | -    | 1/1/13/20 | 14/30/106/115 | -       |
| 22  | CLA  | 7     | 601  | -    | 1/1/14/20 | 9/33/109/115  | -       |
| 40  | CHL  | 4     | 617  | -    | 3/3/15/26 | 0/12/110/137  | -       |
| 22  | CLA  | 9     | 607  | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 22  | CLA  | B     | 1238 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 39  | LUT  | 2     | 503  | -    | 1/1/12/27 | 9/29/67/67    | 0/2/2/2 |
| 25  | BCR  | I     | 4001 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 1204 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 39  | LUT  | 9     | 501  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 39  | LUT  | Z     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 8     | 605  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | Z     | 604  | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 25  | BCR  | B     | 4002 | -    | -         | 11/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | 6     | 606  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 2     | 605  | -    | 1/1/12/20 | 10/21/97/115  | -       |
| 22  | CLA  | 1     | 602  | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 37  | C7Z  | J     | 4002 | -    | 1/1/12/26 | 13/29/67/67   | 0/2/2/2 |
| 22  | CLA  | Z     | 601  | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 22  | CLA  | B     | 1216 | -    | 1/1/15/20 | 26/39/115/115 | -       |
| 22  | CLA  | B     | 1202 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 40  | CHL  | 2     | 610  | -    | 4/4/16/26 | 2/18/116/137  | -       |
| 22  | CLA  | 3     | 604  | -    | 1/1/14/20 | 4/33/109/115  | -       |
| 42  | QTB  | Z     | 504  | -    | 1/1/5/10  | 7/11/28/28    | 0/1/1/1 |
| 22  | CLA  | 3     | 607  | -    | 1/1/14/20 | 18/33/109/115 | -       |
| 22  | CLA  | 2     | 602  | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 22  | CLA  | 8     | 609  | 15   | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | A     | 1125 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | BCR  | 8     | 503  | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 5     | 615  | 17   | 1/1/12/20 | 10/21/97/115  | -       |
| 22  | CLA  | 5     | 601  | -    | 1/1/14/20 | 14/33/109/115 | -       |
| 22  | CLA  | A     | 1135 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 22  | CLA  | A     | 1012 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 40  | CHL  | 7     | 610  | -    | 3/3/17/26 | 4/25/123/137  | -       |
| 26  | LHG  | Z     | 801  | -    | -         | 27/47/47/53   | -       |
| 39  | LUT  | 6     | 501  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 25  | BCR  | 7     | 504  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 39  | LUT  | 7     | 501  | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 3     | 608  | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 31  | LMG  | J     | 5001 | -    | -         | 14/30/50/70   | 0/1/1/1 |
| 25  | BCR  | 6     | 504  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 25  | BCR  | B     | 4003 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | CLA  | 3     | 613  | 46   | 1/1/13/20 | 8/27/103/115  | -       |
| 39  | LUT  | 9     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 22  | CLA  | A     | 1127 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | 8     | 604  | -    | 1/1/14/20 | 8/36/112/115  | -       |
| 22  | CLA  | Z     | 611  | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 22  | CLA  | 8     | 601  | -    | 1/1/14/20 | 11/33/109/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 40  | CHL  | 4     | 613  | -    | 4/4/18/26 | 4/27/125/137  | -       |
| 22  | CLA  | 1     | 601  | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | 9     | 609  | 20   | 1/1/11/20 | 7/17/93/115   | -       |
| 22  | CLA  | B     | 1239 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 5     | 605  | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 22  | CLA  | 1     | 611  | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 36  | RRX  | F     | 4001 | -    | 1/1/11/25 | 9/29/65/65    | 0/2/2/2 |
| 39  | LUT  | 5     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 40  | CHL  | 9     | 613  | -    | 3/3/15/26 | 0/10/108/137  | -       |
| 22  | CLA  | F     | 1302 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 22  | CLA  | 3     | 618  | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 40  | CHL  | 3     | 611  | -    | 4/4/20/26 | 3/39/137/137  | -       |
| 22  | CLA  | 1     | 603  | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | Z     | 615  | 12   | 1/1/11/20 | 7/17/93/115   | -       |
| 22  | CLA  | B     | 1240 | -    | 1/1/15/20 | 21/39/115/115 | -       |
| 22  | CLA  | 4     | 603  | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | B     | 1207 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 5     | 609  | 17   | 1/1/15/20 | 19/39/115/115 | -       |
| 39  | LUT  | 8     | 501  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 28  | LMT  | F     | 5001 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 22  | CLA  | 9     | 604  | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 40  | CHL  | 4     | 610  | -    | 4/4/17/26 | 1/21/119/137  | -       |
| 22  | CLA  | 9     | 612  | -    | 1/1/12/20 | 2/21/97/115   | -       |
| 28  | LMT  | A     | 5006 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 22  | CLA  | B     | 1241 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | 4     | 608  | -    | 1/1/13/20 | 15/27/103/115 | -       |
| 22  | CLA  | 5     | 603  | -    | 1/1/13/20 | 8/29/105/115  | -       |
| 22  | CLA  | Z     | 607  | -    | 1/1/13/20 | 14/30/106/115 | -       |
| 22  | CLA  | 7     | 607  | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 40  | CHL  | 5     | 611  | -    | 3/3/17/26 | 5/21/119/137  | -       |
| 22  | CLA  | B     | 1228 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | 5     | 604  | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 22  | CLA  | B     | 1234 | -    | 1/1/14/20 | 14/33/109/115 | -       |
| 22  | CLA  | 5     | 613  | -    | 1/1/13/20 | 10/27/103/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22  | CLA  | B     | 1219 | -    | 1/1/13/20 | 17/32/108/115 | -       |
| 22  | CLA  | A     | 1132 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | Z     | 606  | -    | 1/1/13/20 | 12/30/106/115 | -       |
| 22  | CLA  | 6     | 619  | 18   | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | B     | 1223 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | 8     | 602  | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | B     | 1023 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | 7     | 606  | -    | 1/1/13/20 | 15/29/105/115 | -       |
| 22  | CLA  | A     | 1113 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 26  | LHG  | 2     | 801  | -    | -         | 14/38/38/53   | -       |
| 22  | CLA  | B     | 1217 | -    | 1/1/13/20 | 13/29/105/115 | -       |
| 22  | CLA  | A     | 1108 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | BCR  | 5     | 503  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 37  | C7Z  | 5     | 505  | -    | 1/1/12/26 | 10/29/67/67   | 0/2/2/2 |
| 26  | LHG  | B     | 5006 | -    | -         | 16/37/37/53   | -       |
| 22  | CLA  | 7     | 611  | -    | 1/1/12/20 | 3/21/97/115   | -       |
| 22  | CLA  | 2     | 606  | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 25  | BCR  | B     | 4004 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 22  | CLA  | A     | 1121 | -    | 1/1/15/20 | 23/39/115/115 | -       |
| 39  | LUT  | 5     | 501  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 38  | SPH  | K     | 5001 | -    | -         | 12/21/21/21   | -       |
| 40  | CHL  | 6     | 613  | -    | 4/4/18/26 | 4/27/125/137  | -       |
| 22  | CLA  | B     | 1227 | -    | 1/1/12/20 | 9/21/97/115   | -       |
| 40  | CHL  | Z     | 609  | 12   | 4/4/20/26 | 10/39/137/137 | -       |
| 28  | LMT  | B     | 5005 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 22  | CLA  | 7     | 605  | -    | 1/1/14/20 | 10/35/111/115 | -       |
| 22  | CLA  | B     | 1206 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 25  | BCR  | 3     | 506  | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 23  | PQN  | B     | 2002 | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 22  | CLA  | B     | 1022 | 46   | 1/1/15/20 | 8/39/115/115  | -       |
| 22  | CLA  | A     | 1131 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | NKP  | 3     | 802  | -    | -         | 5/15/15/28    | -       |
| 22  | CLA  | 7     | 615  | 14   | 1/1/13/20 | 12/31/107/115 | -       |
| 33  | DGD  | B     | 5003 | -    | -         | 15/55/95/95   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 26  | LHG  | 8     | 801  | -    | -         | 22/42/42/53   | -       |
| 22  | CLA  | 4     | 601  | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 26  | LHG  | A     | 5002 | -    | -         | 29/53/53/53   | -       |
| 39  | LUT  | 1     | 501  | -    | -         | 1/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 1     | 606  | -    | 1/1/14/20 | 13/35/111/115 | -       |
| 22  | CLA  | A     | 1104 | 1    | 1/1/15/20 | 22/39/115/115 | -       |
| 22  | CLA  | F     | 1301 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | 3     | 612  | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 30  | DAO  | A     | 5007 | -    | -         | 3/11/11/11    | -       |
| 22  | CLA  | 8     | 611  | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 22  | CLA  | A     | 1126 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 22  | CLA  | 5     | 602  | -    | 1/1/14/20 | 13/35/111/115 | -       |
| 25  | BCR  | K     | 4001 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 39  | LUT  | 7     | 502  | -    | -         | 3/29/67/67    | 0/2/2/2 |
| 22  | CLA  | A     | 1117 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 28  | LMT  | B     | 6101 | -    | -         | 10/21/61/61   | 0/2/2/2 |
| 22  | CLA  | B     | 1208 | -    | 1/1/13/20 | 10/29/105/115 | -       |
| 22  | CLA  | A     | 1122 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 39  | LUT  | 3     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 43  | 3PH  | 8     | 806  | -    | -         | 18/31/31/49   | -       |
| 39  | LUT  | 6     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 22  | CLA  | A     | 1112 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 22  | CLA  | Z     | 603  | -    | 1/1/12/20 | 9/21/97/115   | -       |
| 22  | CLA  | 6     | 601  | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | K     | 1402 | -    | 1/1/13/20 | 14/27/103/115 | -       |
| 22  | CLA  | G     | 1602 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 22  | CLA  | 7     | 609  | 14   | 1/1/15/20 | 19/39/115/115 | -       |
| 40  | CHL  | Z     | 610  | -    | 4/4/20/26 | 9/39/137/137  | -       |
| 22  | CLA  | 2     | 608  | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 21  | CL0  | A     | 1011 | -    | 3/3/20/25 | 13/37/135/135 | -       |
| 25  | BCR  | J     | 4001 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 44  | PLM  | 7     | 805  | -    | -         | 3/15/15/15    | -       |
| 22  | CLA  | K     | 1403 | 10   | 1/1/11/20 | 8/20/96/115   | -       |
| 25  | BCR  | 3     | 505  | -    | -         | 11/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 29  | OCA  | A     | 5008 | -    | -         | 0/7/7/7       | -       |
| 26  | LHG  | 5     | 801  | -    | -         | 26/41/41/53   | -       |
| 39  | LUT  | 8     | 502  | -    | -         | 2/29/67/67    | 0/2/2/2 |
| 22  | CLA  | A     | 1111 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 40  | CHL  | 8     | 610  | -    | 4/4/18/26 | 5/27/125/137  | -       |
| 22  | CLA  | B     | 1231 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 40  | CHL  | 6     | 610  | -    | 4/4/18/26 | 1/27/125/137  | -       |
| 43  | 3PH  | 7     | 802  | -    | -         | 19/40/40/49   | -       |
| 22  | CLA  | 4     | 612  | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 22  | CLA  | 4     | 605  | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 43  | 3PH  | 6     | 802  | -    | -         | 12/30/30/49   | -       |
| 22  | CLA  | B     | 1224 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 1137 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 40  | CHL  | 6     | 617  | -    | 3/3/15/26 | 0/12/110/137  | -       |
| 22  | CLA  | 7     | 613  | -    | 1/1/10/20 | 4/12/88/115   | -       |
| 22  | CLA  | 8     | 606  | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | 6     | 615  | -    | 1/1/14/20 | 15/35/111/115 | -       |
| 25  | BCR  | B     | 4005 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 31  | LMG  | A     | 5003 | -    | -         | 8/24/44/70    | 0/1/1/1 |
| 22  | CLA  | 1     | 604  | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 38  | SPH  | 7     | 804  | -    | -         | 7/21/21/21    | -       |
| 22  | CLA  | 8     | 608  | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 22  | CLA  | Z     | 612  | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 28  | LMT  | 4     | 803  | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 22  | CLA  | A     | 1133 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | 2     | 607  | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 25  | BCR  | 5     | 504  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 1209 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | A     | 1140 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 22  | CLA  | B     | 1230 | -    | 1/1/13/20 | 16/31/107/115 | -       |
| 22  | CLA  | A     | 1101 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | 3     | 616  | -    | 1/1/13/20 | 13/29/105/115 | -       |
| 22  | CLA  | A     | 1138 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | BCR  | K     | 4002 | -    | -         | 11/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 26  | LHG  | 1     | 801  | -    | -         | 23/47/47/53   | -       |
| 22  | CLA  | A     | 1130 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 41  | SQD  | 2     | 803  | -    | -         | 18/38/58/69   | 0/1/1/1 |
| 39  | LUT  | 4     | 501  | -    | -         | 1/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 3     | 602  | -    | 1/1/11/20 | 6/17/93/115   | -       |
| 22  | CLA  | 3     | 610  | 13   | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | A     | 1105 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 25  | BCR  | L     | 4002 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 22  | CLA  | K     | 1404 | -    | 1/1/13/20 | 13/27/103/115 | -       |
| 22  | CLA  | 6     | 608  | -    | 1/1/13/20 | 12/27/103/115 | -       |
| 22  | CLA  | B     | 1210 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 7     | 604  | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 24  | SF4  | C     | 3002 | 3    | -         | -             | 0/6/5/5 |
| 22  | CLA  | B     | 1237 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | 1     | 608  | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 40  | CHL  | 5     | 610  | -    | 4/4/20/26 | 9/39/137/137  | -       |
| 22  | CLA  | A     | 1110 | -    | 1/1/15/20 | 18/39/115/115 | -       |
| 22  | CLA  | 9     | 603  | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | B     | 1211 | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 22  | CLA  | 1     | 613  | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 22  | CLA  | 4     | 602  | -    | 1/1/12/20 | 9/24/100/115  | -       |

All (2076) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 37  | 1     | 503  | C7Z  | C25-C26 | 16.41 | 1.62        | 1.34     |
| 37  | 5     | 505  | C7Z  | C25-C26 | 16.38 | 1.62        | 1.34     |
| 37  | J     | 4002 | C7Z  | C25-C26 | 16.22 | 1.61        | 1.34     |
| 37  | 5     | 505  | C7Z  | C5-C6   | 15.88 | 1.61        | 1.34     |
| 37  | 1     | 503  | C7Z  | C5-C6   | 15.84 | 1.61        | 1.34     |
| 36  | F     | 4001 | RRX  | C26-C25 | 15.64 | 1.60        | 1.34     |
| 39  | 5     | 501  | LUT  | C24-C25 | 15.60 | 1.51        | 1.33     |
| 37  | J     | 4002 | C7Z  | C5-C6   | 15.59 | 1.60        | 1.34     |
| 39  | 2     | 503  | LUT  | C24-C25 | 15.46 | 1.51        | 1.33     |
| 39  | 3     | 502  | LUT  | C24-C25 | 15.35 | 1.51        | 1.33     |
| 39  | 6     | 501  | LUT  | C24-C25 | 15.30 | 1.51        | 1.33     |
| 39  | 4     | 501  | LUT  | C24-C25 | 15.25 | 1.51        | 1.33     |
| 39  | 7     | 501  | LUT  | C24-C25 | 15.20 | 1.51        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 39  | 2     | 501  | LUT  | C24-C25 | 15.19  | 1.51        | 1.33     |
| 39  | Z     | 501  | LUT  | C24-C25 | 15.15  | 1.51        | 1.33     |
| 39  | Z     | 503  | LUT  | C24-C25 | 15.14  | 1.51        | 1.33     |
| 39  | 9     | 501  | LUT  | C24-C25 | 15.14  | 1.51        | 1.33     |
| 39  | 1     | 501  | LUT  | C24-C25 | 15.10  | 1.51        | 1.33     |
| 39  | 3     | 501  | LUT  | C24-C25 | 14.99  | 1.51        | 1.33     |
| 39  | 6     | 502  | LUT  | C24-C25 | 14.88  | 1.50        | 1.33     |
| 39  | 1     | 502  | LUT  | C24-C25 | 14.88  | 1.50        | 1.33     |
| 39  | 2     | 502  | LUT  | C24-C25 | 14.86  | 1.50        | 1.33     |
| 39  | 7     | 502  | LUT  | C24-C25 | 14.83  | 1.50        | 1.33     |
| 39  | 8     | 501  | LUT  | C24-C25 | 14.77  | 1.50        | 1.33     |
| 36  | F     | 4001 | RRX  | C5-C6   | 14.71  | 1.59        | 1.34     |
| 39  | 4     | 502  | LUT  | C24-C25 | 14.65  | 1.50        | 1.33     |
| 39  | 8     | 502  | LUT  | C24-C25 | 14.62  | 1.50        | 1.33     |
| 39  | 5     | 502  | LUT  | C24-C25 | 14.45  | 1.50        | 1.33     |
| 39  | Z     | 502  | LUT  | C24-C25 | 14.39  | 1.50        | 1.33     |
| 39  | 9     | 502  | LUT  | C24-C25 | 14.25  | 1.50        | 1.33     |
| 37  | 5     | 505  | C7Z  | C24-C23 | 11.69  | 1.72        | 1.52     |
| 37  | 1     | 503  | C7Z  | C24-C23 | 11.66  | 1.72        | 1.52     |
| 37  | J     | 4002 | C7Z  | C24-C23 | 11.53  | 1.72        | 1.52     |
| 37  | 1     | 503  | C7Z  | C2-C3   | -10.76 | 1.37        | 1.52     |
| 37  | 5     | 505  | C7Z  | C22-C23 | -10.74 | 1.37        | 1.52     |
| 37  | 5     | 505  | C7Z  | C2-C3   | -10.71 | 1.37        | 1.52     |
| 37  | J     | 4002 | C7Z  | C22-C23 | -10.69 | 1.37        | 1.52     |
| 37  | J     | 4002 | C7Z  | C2-C3   | -10.64 | 1.37        | 1.52     |
| 37  | 1     | 503  | C7Z  | C22-C23 | -10.64 | 1.37        | 1.52     |
| 36  | F     | 4001 | RRX  | C29-C28 | -9.83  | 1.38        | 1.52     |
| 21  | A     | 1011 | CL0  | C1A-CHA | 9.77   | 1.51        | 1.40     |
| 21  | A     | 1011 | CL0  | C1B-C2B | 9.03   | 1.49        | 1.39     |
| 37  | J     | 4002 | C7Z  | C4-C3   | 8.50   | 1.67        | 1.52     |
| 37  | 5     | 505  | C7Z  | C4-C3   | 8.45   | 1.67        | 1.52     |
| 21  | A     | 1011 | CL0  | C1D-C2D | 8.37   | 1.49        | 1.39     |
| 37  | 1     | 503  | C7Z  | C4-C3   | 8.34   | 1.66        | 1.52     |
| 36  | F     | 4001 | RRX  | C27-C28 | 8.25   | 1.66        | 1.52     |
| 42  | Z     | 504  | QTB  | C11-C12 | -8.07  | 1.36        | 1.54     |
| 40  | 9     | 613  | CHL  | C2A-C3A | -7.91  | 1.48        | 1.54     |
| 40  | 2     | 609  | CHL  | C3A-C2A | -7.87  | 1.47        | 1.54     |
| 40  | Z     | 609  | CHL  | C3A-C2A | -7.61  | 1.48        | 1.54     |
| 27  | 3     | 802  | NKP  | PAC-OAF | 7.07   | 1.82        | 1.60     |
| 27  | A     | 5004 | NKP  | PAC-OAF | 7.02   | 1.82        | 1.60     |
| 36  | F     | 4001 | RRX  | C1-C6   | -6.99  | 1.44        | 1.53     |
| 21  | A     | 1011 | CL0  | C3B-C4B | 6.99   | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 9     | 610  | CHL  | C3A-C2A | -6.96 | 1.48        | 1.54     |
| 27  | 8     | 802  | NKP  | PAC-OAF | 6.87  | 1.82        | 1.60     |
| 22  | A     | 1110 | CLA  | MG-NA   | 6.52  | 2.21        | 2.06     |
| 22  | 3     | 618  | CLA  | MG-NA   | 6.50  | 2.21        | 2.06     |
| 22  | B     | 1240 | CLA  | MG-NA   | 6.48  | 2.21        | 2.06     |
| 22  | 2     | 605  | CLA  | MG-NA   | 6.48  | 2.21        | 2.06     |
| 22  | 5     | 604  | CLA  | MG-NA   | 6.48  | 2.21        | 2.06     |
| 22  | A     | 1116 | CLA  | MG-NA   | 6.48  | 2.21        | 2.06     |
| 22  | A     | 1123 | CLA  | MG-NA   | 6.47  | 2.21        | 2.06     |
| 22  | B     | 1209 | CLA  | MG-NA   | 6.47  | 2.21        | 2.06     |
| 22  | 1     | 613  | CLA  | MG-NA   | 6.47  | 2.21        | 2.06     |
| 22  | 1     | 615  | CLA  | MG-NA   | 6.46  | 2.21        | 2.06     |
| 22  | K     | 1401 | CLA  | MG-NA   | 6.46  | 2.21        | 2.06     |
| 22  | 7     | 615  | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 22  | 3     | 605  | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 22  | 6     | 605  | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 22  | A     | 1135 | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 22  | 8     | 605  | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 22  | 3     | 603  | CLA  | MG-NA   | 6.45  | 2.21        | 2.06     |
| 22  | A     | 1130 | CLA  | MG-NA   | 6.44  | 2.21        | 2.06     |
| 22  | 1     | 607  | CLA  | MG-NA   | 6.44  | 2.21        | 2.06     |
| 22  | 3     | 607  | CLA  | MG-NA   | 6.44  | 2.21        | 2.06     |
| 22  | 9     | 604  | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 22  | 9     | 609  | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 22  | A     | 1107 | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 22  | 3     | 602  | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 22  | 7     | 605  | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 22  | 8     | 609  | CLA  | MG-NA   | 6.43  | 2.21        | 2.06     |
| 22  | 4     | 605  | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | 7     | 604  | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | B     | 1213 | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | 3     | 608  | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | 2     | 606  | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | B     | 1236 | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | 6     | 604  | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 22  | 9     | 605  | CLA  | MG-NA   | 6.41  | 2.21        | 2.06     |
| 22  | 4     | 607  | CLA  | MG-NA   | 6.41  | 2.21        | 2.06     |
| 22  | A     | 1129 | CLA  | MG-NA   | 6.41  | 2.21        | 2.06     |
| 22  | 5     | 602  | CLA  | MG-NA   | 6.41  | 2.21        | 2.06     |
| 22  | 5     | 609  | CLA  | MG-NA   | 6.41  | 2.21        | 2.06     |
| 22  | B     | 1221 | CLA  | MG-NA   | 6.40  | 2.21        | 2.06     |
| 22  | Z     | 602  | CLA  | MG-NA   | 6.40  | 2.21        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | B     | 1232 | CLA  | MG-NA | 6.40  | 2.21        | 2.06     |
| 22  | 5     | 622  | CLA  | MG-NA | 6.40  | 2.21        | 2.06     |
| 22  | 4     | 604  | CLA  | MG-NA | 6.40  | 2.21        | 2.06     |
| 22  | 4     | 603  | CLA  | MG-NA | 6.40  | 2.21        | 2.06     |
| 22  | 2     | 607  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | K     | 1403 | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | Z     | 604  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 5     | 613  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 4     | 602  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | A     | 1140 | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 9     | 603  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 7     | 613  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 6     | 602  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 1     | 612  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 5     | 607  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | 9     | 602  | CLA  | MG-NA | 6.39  | 2.21        | 2.06     |
| 22  | K     | 1402 | CLA  | MG-NA | 6.38  | 2.21        | 2.06     |
| 22  | 3     | 616  | CLA  | MG-NA | 6.38  | 2.21        | 2.06     |
| 22  | 7     | 603  | CLA  | MG-NA | 6.38  | 2.21        | 2.06     |
| 22  | A     | 1127 | CLA  | MG-NA | 6.38  | 2.21        | 2.06     |
| 22  | K     | 1404 | CLA  | MG-NA | 6.38  | 2.21        | 2.06     |
| 22  | A     | 1114 | CLA  | MG-NA | 6.38  | 2.21        | 2.06     |
| 22  | B     | 1207 | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 36  | F     | 4001 | RRX  | C2-C3 | -6.37 | 1.37        | 1.52     |
| 22  | A     | 1139 | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | 4     | 608  | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | 7     | 616  | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | 8     | 604  | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | 1     | 602  | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | 6     | 608  | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | B     | 1234 | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | B     | 1229 | CLA  | MG-NA | 6.37  | 2.21        | 2.06     |
| 22  | 6     | 603  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | A     | 1112 | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | Z     | 607  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | 5     | 615  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | 1     | 605  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | A     | 1101 | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | 4     | 615  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | 6     | 607  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | 6     | 615  | CLA  | MG-NA | 6.36  | 2.21        | 2.06     |
| 22  | B     | 1224 | CLA  | MG-NA | 6.35  | 2.21        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 22  | B     | 1227 | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | A     | 1113 | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | 7     | 602  | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | A     | 1105 | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | 8     | 603  | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | 1     | 604  | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | Z     | 612  | CLA  | MG-NA | 6.35 | 2.21        | 2.06     |
| 22  | A     | 1134 | CLA  | MG-NA | 6.34 | 2.21        | 2.06     |
| 22  | B     | 1219 | CLA  | MG-NA | 6.34 | 2.21        | 2.06     |
| 22  | A     | 1141 | CLA  | MG-NA | 6.34 | 2.21        | 2.06     |
| 22  | 5     | 618  | CLA  | MG-NA | 6.34 | 2.21        | 2.06     |
| 22  | G     | 1602 | CLA  | MG-NA | 6.34 | 2.21        | 2.06     |
| 22  | A     | 1121 | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | A     | 1104 | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 2     | 603  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 2     | 602  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 8     | 615  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 6     | 601  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | Z     | 605  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | B     | 1206 | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 5     | 608  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 6     | 606  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 5     | 603  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | 9     | 607  | CLA  | MG-NA | 6.33 | 2.21        | 2.06     |
| 22  | B     | 1239 | CLA  | MG-NA | 6.32 | 2.21        | 2.06     |
| 22  | 6     | 618  | CLA  | MG-NA | 6.32 | 2.21        | 2.06     |
| 22  | B     | 1226 | CLA  | MG-NA | 6.32 | 2.21        | 2.06     |
| 22  | B     | 1238 | CLA  | MG-NA | 6.32 | 2.21        | 2.06     |
| 22  | 7     | 607  | CLA  | MG-NA | 6.31 | 2.21        | 2.06     |
| 22  | B     | 1228 | CLA  | MG-NA | 6.31 | 2.21        | 2.06     |
| 22  | 8     | 602  | CLA  | MG-NA | 6.31 | 2.21        | 2.06     |
| 22  | 2     | 608  | CLA  | MG-NA | 6.31 | 2.21        | 2.06     |
| 22  | L     | 1503 | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | Z     | 615  | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | A     | 1137 | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | 5     | 606  | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | B     | 1223 | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | A     | 1117 | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | J     | 1901 | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | A     | 1128 | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | 1     | 603  | CLA  | MG-NA | 6.30 | 2.21        | 2.06     |
| 22  | Z     | 611  | CLA  | MG-NA | 6.29 | 2.21        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | A     | 1120 | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | 8     | 611  | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | A     | 1122 | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | 2     | 612  | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | 8     | 607  | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | 9     | 608  | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | F     | 1302 | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | L     | 1502 | CLA  | MG-NA | 6.29  | 2.21        | 2.06     |
| 22  | A     | 1115 | CLA  | MG-NA | 6.28  | 2.21        | 2.06     |
| 22  | 7     | 608  | CLA  | MG-NA | 6.28  | 2.21        | 2.06     |
| 22  | 6     | 612  | CLA  | MG-NA | 6.28  | 2.21        | 2.06     |
| 22  | G     | 1601 | CLA  | MG-NA | 6.27  | 2.21        | 2.06     |
| 22  | A     | 1136 | CLA  | MG-NA | 6.27  | 2.21        | 2.06     |
| 22  | B     | 1214 | CLA  | MG-NA | 6.27  | 2.21        | 2.06     |
| 22  | B     | 1235 | CLA  | MG-NA | 6.26  | 2.21        | 2.06     |
| 22  | 7     | 601  | CLA  | MG-NA | 6.26  | 2.21        | 2.06     |
| 22  | Z     | 603  | CLA  | MG-NA | 6.26  | 2.21        | 2.06     |
| 22  | B     | 1225 | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 22  | 3     | 610  | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 22  | 1     | 611  | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 22  | 4     | 601  | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 22  | B     | 1237 | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 22  | 4     | 606  | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 22  | 3     | 601  | CLA  | MG-NA | 6.25  | 2.21        | 2.06     |
| 37  | J     | 4002 | C7Z  | C1-C6 | -6.24 | 1.45        | 1.53     |
| 22  | B     | 1215 | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | Z     | 606  | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | 8     | 608  | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | 5     | 605  | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | 4     | 609  | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | 6     | 609  | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | B     | 1022 | CLA  | MG-NA | 6.24  | 2.21        | 2.06     |
| 22  | A     | 1108 | CLA  | MG-NA | 6.23  | 2.21        | 2.06     |
| 22  | 8     | 606  | CLA  | MG-NA | 6.23  | 2.21        | 2.06     |
| 22  | 9     | 606  | CLA  | MG-NA | 6.23  | 2.21        | 2.06     |
| 22  | B     | 1217 | CLA  | MG-NA | 6.23  | 2.21        | 2.06     |
| 22  | 3     | 612  | CLA  | MG-NA | 6.23  | 2.21        | 2.06     |
| 22  | A     | 1126 | CLA  | MG-NA | 6.22  | 2.21        | 2.06     |
| 22  | F     | 1301 | CLA  | MG-NA | 6.22  | 2.21        | 2.06     |
| 22  | B     | 1212 | CLA  | MG-NA | 6.22  | 2.21        | 2.06     |
| 22  | 9     | 601  | CLA  | MG-NA | 6.22  | 2.21        | 2.06     |
| 22  | A     | 1131 | CLA  | MG-NA | 6.21  | 2.21        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 22  | 8     | 601  | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | 2     | 601  | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | A     | 1012 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | B     | 1204 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | A     | 1102 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | B     | 1203 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | 6     | 619  | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | 9     | 612  | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | 3     | 613  | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | B     | 1218 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | A     | 1106 | CLA  | MG-NA | 6.19 | 2.21        | 2.06     |
| 22  | A     | 1118 | CLA  | MG-NA | 6.18 | 2.21        | 2.06     |
| 22  | Z     | 608  | CLA  | MG-NA | 6.18 | 2.21        | 2.06     |
| 22  | 5     | 601  | CLA  | MG-NA | 6.18 | 2.21        | 2.06     |
| 22  | 7     | 611  | CLA  | MG-NA | 6.18 | 2.21        | 2.06     |
| 22  | A     | 1111 | CLA  | MG-NA | 6.18 | 2.21        | 2.06     |
| 22  | A     | 1125 | CLA  | MG-NA | 6.18 | 2.21        | 2.06     |
| 22  | 4     | 612  | CLA  | MG-NA | 6.17 | 2.20        | 2.06     |
| 22  | A     | 1124 | CLA  | MG-NA | 6.17 | 2.20        | 2.06     |
| 22  | 2     | 615  | CLA  | MG-NA | 6.17 | 2.20        | 2.06     |
| 22  | A     | 1132 | CLA  | MG-NA | 6.17 | 2.20        | 2.06     |
| 22  | 7     | 606  | CLA  | MG-NA | 6.17 | 2.20        | 2.06     |
| 22  | 1     | 601  | CLA  | MG-NA | 6.17 | 2.20        | 2.06     |
| 22  | B     | 1210 | CLA  | MG-NA | 6.16 | 2.20        | 2.06     |
| 22  | 2     | 604  | CLA  | MG-NA | 6.16 | 2.20        | 2.06     |
| 22  | A     | 1109 | CLA  | MG-NA | 6.16 | 2.20        | 2.06     |
| 22  | B     | 1231 | CLA  | MG-NA | 6.14 | 2.20        | 2.06     |
| 22  | B     | 1208 | CLA  | MG-NA | 6.13 | 2.20        | 2.06     |
| 22  | B     | 1230 | CLA  | MG-NA | 6.13 | 2.20        | 2.06     |
| 22  | B     | 1216 | CLA  | MG-NA | 6.13 | 2.20        | 2.06     |
| 22  | 1     | 606  | CLA  | MG-NA | 6.13 | 2.20        | 2.06     |
| 22  | A     | 1119 | CLA  | MG-NA | 6.11 | 2.20        | 2.06     |
| 22  | Z     | 601  | CLA  | MG-NA | 6.11 | 2.20        | 2.06     |
| 22  | A     | 1133 | CLA  | MG-NA | 6.11 | 2.20        | 2.06     |
| 22  | B     | 1220 | CLA  | MG-NA | 6.11 | 2.20        | 2.06     |
| 22  | 8     | 612  | CLA  | MG-NA | 6.10 | 2.20        | 2.06     |
| 22  | A     | 1138 | CLA  | MG-NA | 6.08 | 2.20        | 2.06     |
| 22  | 1     | 608  | CLA  | MG-NA | 6.07 | 2.20        | 2.06     |
| 22  | 7     | 612  | CLA  | MG-NA | 6.06 | 2.20        | 2.06     |
| 22  | B     | 1241 | CLA  | MG-NA | 6.06 | 2.20        | 2.06     |
| 22  | 3     | 606  | CLA  | MG-NA | 6.06 | 2.20        | 2.06     |
| 22  | 7     | 609  | CLA  | MG-NA | 6.06 | 2.20        | 2.06     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1205 | CLA  | MG-NA   | 6.05  | 2.20        | 2.06     |
| 22  | B     | 1222 | CLA  | MG-NA   | 6.04  | 2.20        | 2.06     |
| 36  | F     | 4001 | RRX  | C30-C25 | -6.04 | 1.46        | 1.53     |
| 22  | 5     | 612  | CLA  | MG-NA   | 6.02  | 2.20        | 2.06     |
| 40  | 1     | 609  | CHL  | C3B-C4B | 6.01  | 1.47        | 1.41     |
| 22  | B     | 1202 | CLA  | MG-NA   | 6.00  | 2.20        | 2.06     |
| 22  | B     | 1021 | CLA  | MG-NA   | 5.97  | 2.20        | 2.06     |
| 22  | A     | 1013 | CLA  | MG-NA   | 5.97  | 2.20        | 2.06     |
| 25  | 3     | 506  | BCR  | C24-C23 | 5.96  | 1.50        | 1.33     |
| 25  | 6     | 504  | BCR  | C24-C23 | 5.93  | 1.50        | 1.33     |
| 40  | 2     | 609  | CHL  | C3B-C4B | 5.91  | 1.47        | 1.41     |
| 22  | B     | 1201 | CLA  | MG-NA   | 5.90  | 2.20        | 2.06     |
| 40  | 3     | 611  | CHL  | C3A-C2A | -5.89 | 1.49        | 1.54     |
| 25  | 5     | 504  | BCR  | C24-C23 | 5.89  | 1.50        | 1.33     |
| 25  | B     | 4003 | BCR  | C24-C23 | 5.88  | 1.50        | 1.33     |
| 22  | B     | 1023 | CLA  | MG-NA   | 5.87  | 2.20        | 2.06     |
| 22  | A     | 1103 | CLA  | MG-NA   | 5.86  | 2.20        | 2.06     |
| 25  | 3     | 504  | BCR  | C24-C23 | 5.86  | 1.50        | 1.33     |
| 25  | G     | 4001 | BCR  | C24-C23 | 5.85  | 1.50        | 1.33     |
| 37  | 5     | 505  | C7Z  | C1-C6   | -5.84 | 1.46        | 1.53     |
| 25  | K     | 4002 | BCR  | C24-C23 | 5.83  | 1.50        | 1.33     |
| 37  | 1     | 503  | C7Z  | C1-C6   | -5.82 | 1.46        | 1.53     |
| 25  | B     | 4004 | BCR  | C24-C23 | 5.81  | 1.50        | 1.33     |
| 22  | 3     | 604  | CLA  | MG-NA   | 5.81  | 2.20        | 2.06     |
| 25  | 4     | 503  | BCR  | C24-C23 | 5.81  | 1.50        | 1.33     |
| 37  | 5     | 505  | C7Z  | C12-C13 | 5.80  | 1.58        | 1.46     |
| 25  | 7     | 503  | BCR  | C24-C23 | 5.78  | 1.50        | 1.33     |
| 25  | J     | 4001 | BCR  | C24-C23 | 5.77  | 1.50        | 1.33     |
| 25  | 3     | 505  | BCR  | C24-C23 | 5.76  | 1.50        | 1.33     |
| 25  | 5     | 503  | BCR  | C24-C23 | 5.74  | 1.50        | 1.33     |
| 25  | B     | 4005 | BCR  | C24-C23 | 5.74  | 1.50        | 1.33     |
| 25  | A     | 4001 | BCR  | C24-C23 | 5.73  | 1.50        | 1.33     |
| 25  | B     | 4007 | BCR  | C24-C23 | 5.71  | 1.50        | 1.33     |
| 25  | 7     | 504  | BCR  | C24-C23 | 5.71  | 1.50        | 1.33     |
| 25  | 6     | 503  | BCR  | C24-C23 | 5.70  | 1.50        | 1.33     |
| 25  | L     | 4002 | BCR  | C24-C23 | 5.70  | 1.50        | 1.33     |
| 25  | 8     | 503  | BCR  | C24-C23 | 5.69  | 1.50        | 1.33     |
| 22  | B     | 1211 | CLA  | MG-NA   | 5.69  | 2.19        | 2.06     |
| 25  | K     | 4001 | BCR  | C24-C23 | 5.68  | 1.50        | 1.33     |
| 25  | A     | 4002 | BCR  | C24-C23 | 5.68  | 1.50        | 1.33     |
| 25  | L     | 4001 | BCR  | C24-C23 | 5.68  | 1.50        | 1.33     |
| 25  | A     | 4004 | BCR  | C24-C23 | 5.68  | 1.50        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | 3     | 503  | BCR  | C24-C23 | 5.67  | 1.50        | 1.33     |
| 25  | B     | 4006 | BCR  | C24-C23 | 5.67  | 1.50        | 1.33     |
| 25  | B     | 4001 | BCR  | C24-C23 | 5.66  | 1.50        | 1.33     |
| 25  | A     | 4003 | BCR  | C24-C23 | 5.63  | 1.49        | 1.33     |
| 25  | B     | 4002 | BCR  | C24-C23 | 5.62  | 1.49        | 1.33     |
| 25  | A     | 4005 | BCR  | C24-C23 | 5.57  | 1.49        | 1.33     |
| 25  | I     | 4001 | BCR  | C24-C23 | 5.57  | 1.49        | 1.33     |
| 37  | 1     | 503  | C7Z  | C12-C13 | 5.56  | 1.57        | 1.46     |
| 21  | A     | 1011 | CL0  | O2A-C1  | 5.53  | 1.61        | 1.46     |
| 25  | B     | 4001 | BCR  | C11-C12 | -5.53 | 1.20        | 1.34     |
| 40  | 2     | 610  | CHL  | C3B-C4B | 5.50  | 1.46        | 1.41     |
| 40  | 8     | 613  | CHL  | C3B-C4B | 5.49  | 1.46        | 1.41     |
| 37  | J     | 4002 | C7Z  | C12-C13 | 5.49  | 1.57        | 1.46     |
| 25  | 3     | 504  | BCR  | C11-C12 | -5.48 | 1.20        | 1.34     |
| 25  | B     | 4003 | BCR  | C11-C12 | -5.45 | 1.20        | 1.34     |
| 25  | A     | 4002 | BCR  | C11-C12 | -5.45 | 1.20        | 1.34     |
| 40  | 1     | 609  | CHL  | C3A-C2A | -5.42 | 1.50        | 1.54     |
| 25  | A     | 4004 | BCR  | C11-C12 | -5.42 | 1.20        | 1.34     |
| 40  | 2     | 613  | CHL  | C3B-C4B | 5.41  | 1.46        | 1.41     |
| 40  | Z     | 613  | CHL  | C3A-C2A | -5.40 | 1.50        | 1.54     |
| 40  | 9     | 613  | CHL  | C3B-C4B | 5.39  | 1.46        | 1.41     |
| 25  | 6     | 504  | BCR  | C11-C12 | -5.37 | 1.20        | 1.34     |
| 21  | A     | 1011 | CL0  | CHB-C1B | 5.37  | 1.48        | 1.39     |
| 25  | B     | 4002 | BCR  | C11-C12 | -5.36 | 1.20        | 1.34     |
| 25  | 7     | 503  | BCR  | C11-C12 | -5.36 | 1.20        | 1.34     |
| 25  | 3     | 503  | BCR  | C11-C12 | -5.34 | 1.20        | 1.34     |
| 25  | G     | 4001 | BCR  | C11-C12 | -5.31 | 1.20        | 1.34     |
| 25  | J     | 4001 | BCR  | C11-C12 | -5.31 | 1.20        | 1.34     |
| 40  | 7     | 610  | CHL  | C3B-C4B | 5.30  | 1.46        | 1.41     |
| 36  | F     | 4001 | RRX  | C2-C1   | 5.29  | 1.66        | 1.54     |
| 25  | I     | 4001 | BCR  | C11-C12 | -5.29 | 1.20        | 1.34     |
| 25  | L     | 4002 | BCR  | C11-C12 | -5.28 | 1.20        | 1.34     |
| 25  | L     | 4001 | BCR  | C11-C12 | -5.28 | 1.20        | 1.34     |
| 25  | B     | 4005 | BCR  | C11-C12 | -5.26 | 1.20        | 1.34     |
| 25  | B     | 4007 | BCR  | C11-C12 | -5.26 | 1.20        | 1.34     |
| 25  | B     | 4006 | BCR  | C11-C12 | -5.25 | 1.21        | 1.34     |
| 25  | K     | 4002 | BCR  | C11-C12 | -5.25 | 1.21        | 1.34     |
| 25  | B     | 4004 | BCR  | C11-C12 | -5.22 | 1.21        | 1.34     |
| 25  | A     | 4001 | BCR  | C11-C12 | -5.22 | 1.21        | 1.34     |
| 25  | A     | 4005 | BCR  | C11-C12 | -5.22 | 1.21        | 1.34     |
| 25  | 5     | 503  | BCR  | C11-C12 | -5.21 | 1.21        | 1.34     |
| 40  | Z     | 609  | CHL  | C3B-C4B | 5.21  | 1.46        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 6     | 617  | CHL  | C3B-C4B | 5.21  | 1.46        | 1.41     |
| 25  | 8     | 503  | BCR  | C11-C12 | -5.20 | 1.21        | 1.34     |
| 40  | 4     | 617  | CHL  | C3B-C4B | 5.18  | 1.46        | 1.41     |
| 25  | 3     | 505  | BCR  | C11-C12 | -5.17 | 1.21        | 1.34     |
| 25  | 6     | 503  | BCR  | C11-C12 | -5.16 | 1.21        | 1.34     |
| 25  | 5     | 504  | BCR  | C11-C12 | -5.14 | 1.21        | 1.34     |
| 21  | A     | 1011 | CL0  | C3A-C2A | -5.14 | 1.50        | 1.54     |
| 25  | K     | 4001 | BCR  | C11-C12 | -5.14 | 1.21        | 1.34     |
| 25  | A     | 4003 | BCR  | C11-C12 | -5.12 | 1.21        | 1.34     |
| 40  | 8     | 613  | CHL  | C3A-C2A | -5.11 | 1.50        | 1.54     |
| 21  | A     | 1011 | CL0  | CHC-C4B | 5.11  | 1.47        | 1.39     |
| 25  | 4     | 503  | BCR  | C11-C12 | -5.11 | 1.21        | 1.34     |
| 40  | 5     | 617  | CHL  | C3B-C4B | 5.10  | 1.46        | 1.41     |
| 37  | 1     | 503  | C7Z  | C28-C29 | 5.10  | 1.56        | 1.46     |
| 40  | 6     | 610  | CHL  | C3A-C2A | -5.09 | 1.50        | 1.54     |
| 37  | 5     | 505  | C7Z  | C28-C29 | 5.08  | 1.56        | 1.46     |
| 25  | 7     | 504  | BCR  | C11-C12 | -5.03 | 1.21        | 1.34     |
| 36  | F     | 4001 | RRX  | C19-C18 | 5.03  | 1.56        | 1.46     |
| 40  | 5     | 610  | CHL  | C3B-C4B | 5.03  | 1.46        | 1.41     |
| 25  | 3     | 506  | BCR  | C11-C12 | -5.01 | 1.21        | 1.34     |
| 40  | 3     | 611  | CHL  | C3B-C2B | -4.99 | 1.33        | 1.40     |
| 40  | Z     | 610  | CHL  | C3A-C2A | -4.97 | 1.50        | 1.54     |
| 21  | A     | 1011 | CL0  | O2D-CGD | 4.96  | 1.45        | 1.33     |
| 37  | J     | 4002 | C7Z  | C28-C29 | 4.90  | 1.56        | 1.46     |
| 21  | A     | 1011 | CL0  | OBD-CAD | 4.89  | 1.28        | 1.22     |
| 40  | 6     | 617  | CHL  | C3A-C2A | -4.81 | 1.50        | 1.54     |
| 37  | 5     | 505  | C7Z  | C32-C33 | 4.79  | 1.56        | 1.46     |
| 37  | 1     | 503  | C7Z  | C32-C33 | 4.77  | 1.56        | 1.46     |
| 37  | J     | 4002 | C7Z  | C32-C33 | 4.76  | 1.56        | 1.46     |
| 37  | J     | 4002 | C7Z  | C24-C25 | -4.76 | 1.43        | 1.51     |
| 40  | 8     | 613  | CHL  | C2C-C3C | 4.76  | 1.41        | 1.36     |
| 40  | 5     | 617  | CHL  | C3A-C2A | -4.76 | 1.50        | 1.54     |
| 21  | A     | 1011 | CL0  | C3D-C4D | -4.74 | 1.34        | 1.41     |
| 37  | 5     | 505  | C7Z  | C24-C25 | -4.69 | 1.43        | 1.51     |
| 37  | 1     | 503  | C7Z  | C24-C25 | -4.69 | 1.43        | 1.51     |
| 36  | F     | 4001 | RRX  | C8-C9   | 4.68  | 1.56        | 1.46     |
| 40  | 2     | 613  | CHL  | C3A-C2A | -4.66 | 1.50        | 1.54     |
| 42  | Z     | 504  | QTB  | C17-C11 | -4.65 | 1.51        | 1.55     |
| 40  | 9     | 610  | CHL  | C3B-C4B | 4.62  | 1.45        | 1.41     |
| 21  | A     | 1011 | CL0  | CHD-C1D | 4.57  | 1.47        | 1.39     |
| 37  | 5     | 505  | C7Z  | C31-C30 | 4.50  | 1.57        | 1.43     |
| 21  | A     | 1011 | CL0  | CHD-C4C | 4.48  | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | L     | 1503 | CLA  | CBB-CAB | 4.46  | 1.51        | 1.30     |
| 22  | B     | 1201 | CLA  | CBB-CAB | 4.46  | 1.51        | 1.30     |
| 22  | 2     | 612  | CLA  | CBB-CAB | 4.46  | 1.51        | 1.30     |
| 37  | 1     | 503  | C7Z  | C31-C30 | 4.45  | 1.57        | 1.43     |
| 40  | 6     | 613  | CHL  | C2C-C3C | 4.45  | 1.40        | 1.36     |
| 40  | 2     | 609  | CHL  | C2C-C3C | 4.45  | 1.40        | 1.36     |
| 22  | B     | 1226 | CLA  | CBB-CAB | 4.44  | 1.51        | 1.30     |
| 22  | A     | 1128 | CLA  | CBB-CAB | 4.44  | 1.51        | 1.30     |
| 22  | A     | 1102 | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 21  | A     | 1011 | CL0  | CHC-C1C | 4.43  | 1.47        | 1.39     |
| 22  | 9     | 602  | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 22  | 4     | 605  | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 22  | K     | 1404 | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 22  | 6     | 605  | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 22  | Z     | 608  | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 22  | 8     | 615  | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 22  | 8     | 606  | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 22  | 5     | 606  | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 37  | J     | 4002 | C7Z  | C31-C30 | 4.42  | 1.56        | 1.43     |
| 22  | 7     | 612  | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 22  | 5     | 615  | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 37  | 5     | 505  | C7Z  | C8-C9   | 4.42  | 1.55        | 1.46     |
| 22  | 5     | 602  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 8     | 612  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 2     | 608  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | A     | 1103 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 6     | 608  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 5     | 601  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 2     | 603  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | A     | 1138 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 6     | 619  | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 5     | 622  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | A     | 1129 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | K     | 1403 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 21  | A     | 1011 | CL0  | C3D-C2D | 4.40  | 1.47        | 1.39     |
| 22  | Z     | 602  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 6     | 606  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 4     | 612  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | B     | 1207 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | A     | 1128 | CLA  | MG-ND   | -4.40 | 1.97        | 2.05     |
| 22  | 5     | 605  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 4     | 606  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 2     | 615  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 2     | 606  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 8     | 607  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 6     | 601  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 9     | 608  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 3     | 607  | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | B     | 1221 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | A     | 1123 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | 7     | 613  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 4     | 609  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | A     | 1117 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1228 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 7     | 606  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 5     | 607  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 8     | 609  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 1     | 602  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1223 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 2     | 605  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1202 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | Z     | 607  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | Z     | 605  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1213 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1236 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 4     | 615  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 1     | 606  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 6     | 607  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 7     | 611  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 8     | 611  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1222 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | A     | 1110 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 8     | 608  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | A     | 1121 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | B     | 1239 | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 3     | 606  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 25  | B     | 4005 | BCR  | C16-C17 | -4.39 | 1.29        | 1.43     |
| 22  | 3     | 608  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 4     | 602  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 5     | 612  | CLA  | CBB-CAB | 4.39  | 1.51        | 1.30     |
| 22  | 9     | 603  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 1023 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 4     | 604  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 1118 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | B     | 4001 | BCR  | C16-C17 | -4.38 | 1.29        | 1.43     |
| 22  | A     | 1108 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 1114 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 1235 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | Z     | 615  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | Z     | 606  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 3     | 601  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 8     | 604  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 25  | 3     | 503  | BCR  | C16-C17 | -4.38 | 1.29        | 1.43     |
| 22  | A     | 1122 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 608  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 6     | 612  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 9     | 607  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 6     | 602  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 607  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 4     | 601  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 6     | 609  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 1111 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 8     | 605  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 1206 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 611  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 612  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 7     | 615  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 613  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 9     | 605  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 7     | 608  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 2     | 601  | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 5     | 603  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 3     | 603  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 4     | 607  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 25  | A     | 4004 | BCR  | C16-C17 | -4.37 | 1.29        | 1.43     |
| 22  | A     | 1119 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | B     | 1230 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | K     | 1402 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 4     | 608  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | Z     | 604  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | G     | 1601 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 1     | 605  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | B     | 1234 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 3     | 618  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 5     | 618  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 9     | 601  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1215 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 6     | 604  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 1132 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | Z     | 601  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 3     | 613  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 5     | 608  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | B     | 1209 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 1012 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 1     | 604  | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 1120 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 1105 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | Z     | 611  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 1013 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 6     | 615  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 2     | 607  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | L     | 1502 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | Z     | 603  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 7     | 607  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 5     | 609  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 9     | 609  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | B     | 1220 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 3     | 612  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 2     | 602  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 25  | B     | 4004 | BCR  | C16-C17 | -4.36 | 1.29        | 1.43     |
| 22  | B     | 1219 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 1113 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 1109 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 8     | 601  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 5     | 613  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 21  | A     | 1011 | CL0  | C3B-C2B | 4.36  | 1.46        | 1.40     |
| 22  | B     | 1224 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 6     | 618  | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 1137 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 1141 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 25  | B     | 4003 | BCR  | C16-C17 | -4.35 | 1.29        | 1.43     |
| 22  | 7     | 602  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | B     | 1231 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 7     | 609  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 1     | 615  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 25  | 8     | 503  | BCR  | C16-C17 | -4.35 | 1.29        | 1.43     |
| 22  | B     | 1237 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | A     | 1131 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | G     | 1602 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | A     | 1115 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 7     | 616  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | A     | 1124 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | B     | 1226 | CLA  | MG-ND   | -4.35 | 1.97        | 2.05     |
| 22  | 7     | 601  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | B     | 1240 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 3     | 602  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 6     | 603  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 36  | F     | 4001 | RRX  | C27-C26 | -4.35 | 1.44        | 1.51     |
| 22  | A     | 1140 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 25  | I     | 4001 | BCR  | C16-C17 | -4.35 | 1.29        | 1.43     |
| 40  | 9     | 613  | CHL  | C2C-C3C | 4.35  | 1.40        | 1.36     |
| 22  | K     | 1401 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 8     | 602  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | A     | 1101 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 8     | 603  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 1     | 603  | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | A     | 1107 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | B     | 1210 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | A     | 1139 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | 4     | 603  | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | B     | 1241 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 25  | 5     | 504  | BCR  | C16-C17 | -4.34 | 1.29        | 1.43     |
| 22  | A     | 1126 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | A     | 1106 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | B     | 1214 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | B     | 1216 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | 2     | 604  | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | B     | 1217 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | B     | 1225 | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 22  | A     | 1134 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | B     | 1204 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | B     | 1211 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | B     | 1232 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | F     | 1302 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | A     | 1127 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 36  | F     | 4001 | RRX  | C12-C13 | 4.33  | 1.55        | 1.46     |
| 22  | 9     | 612  | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | A     | 1133 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | B     | 1218 | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | 3     | 616  | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 1     | 601  | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 22  | 7     | 604  | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 40  | Z     | 613  | CHL  | C3B-C4B | 4.33  | 1.45        | 1.41     |
| 22  | B     | 1208 | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | 3     | 604  | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | B     | 1203 | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 25  | 6     | 504  | BCR  | C16-C17 | -4.32 | 1.29        | 1.43     |
| 22  | 7     | 605  | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | A     | 1104 | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | 3     | 605  | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | B     | 1212 | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | 3     | 610  | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | Z     | 612  | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 22  | B     | 1229 | CLA  | CBB-CAB | 4.31  | 1.51        | 1.30     |
| 22  | B     | 1205 | CLA  | CBB-CAB | 4.31  | 1.51        | 1.30     |
| 36  | F     | 4001 | RRX  | C3-C4   | 4.31  | 1.66        | 1.52     |
| 22  | A     | 1112 | CLA  | CBB-CAB | 4.30  | 1.51        | 1.30     |
| 22  | J     | 1901 | CLA  | CBB-CAB | 4.30  | 1.51        | 1.30     |
| 22  | A     | 1125 | CLA  | CBB-CAB | 4.30  | 1.51        | 1.30     |
| 25  | K     | 4002 | BCR  | C16-C17 | -4.30 | 1.29        | 1.43     |
| 25  | A     | 4002 | BCR  | C16-C17 | -4.30 | 1.29        | 1.43     |
| 22  | A     | 1130 | CLA  | CBB-CAB | 4.29  | 1.51        | 1.30     |
| 22  | F     | 1301 | CLA  | CBB-CAB | 4.29  | 1.51        | 1.30     |
| 37  | 5     | 505  | C7Z  | C11-C10 | 4.29  | 1.56        | 1.43     |
| 25  | B     | 4007 | BCR  | C16-C17 | -4.29 | 1.29        | 1.43     |
| 25  | 7     | 504  | BCR  | C10-C9  | 4.29  | 1.45        | 1.35     |
| 22  | B     | 1238 | CLA  | CBB-CAB | 4.29  | 1.51        | 1.30     |
| 22  | B     | 1021 | CLA  | CBB-CAB | 4.29  | 1.51        | 1.30     |
| 25  | 7     | 503  | BCR  | C16-C17 | -4.28 | 1.29        | 1.43     |
| 22  | 7     | 603  | CLA  | CBB-CAB | 4.28  | 1.50        | 1.30     |
| 25  | A     | 4005 | BCR  | C16-C17 | -4.27 | 1.29        | 1.43     |
| 25  | L     | 4001 | BCR  | C16-C17 | -4.27 | 1.29        | 1.43     |
| 22  | B     | 1227 | CLA  | CBB-CAB | 4.26  | 1.50        | 1.30     |
| 37  | J     | 4002 | C7Z  | C8-C9   | 4.26  | 1.55        | 1.46     |
| 22  | B     | 1022 | CLA  | CBB-CAB | 4.26  | 1.50        | 1.30     |
| 42  | Z     | 504  | QTB  | C11-C10 | -4.26 | 1.44        | 1.50     |
| 25  | 6     | 503  | BCR  | C16-C17 | -4.26 | 1.30        | 1.43     |
| 25  | 5     | 503  | BCR  | C16-C17 | -4.26 | 1.30        | 1.43     |
| 25  | 4     | 503  | BCR  | C16-C17 | -4.25 | 1.30        | 1.43     |
| 40  | 4     | 613  | CHL  | C3A-C2A | -4.25 | 1.51        | 1.54     |
| 33  | B     | 5003 | DGD  | O1G-C1A | 4.25  | 1.45        | 1.33     |
| 22  | A     | 1136 | CLA  | CBB-CAB | 4.25  | 1.50        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 25  | L     | 4002 | BCR  | C16-C17 | -4.24 | 1.30        | 1.43     |
| 25  | 3     | 504  | BCR  | C16-C17 | -4.24 | 1.30        | 1.43     |
| 25  | B     | 4002 | BCR  | C16-C17 | -4.23 | 1.30        | 1.43     |
| 25  | A     | 4001 | BCR  | C16-C17 | -4.23 | 1.30        | 1.43     |
| 37  | 1     | 503  | C7Z  | C8-C9   | 4.23  | 1.55        | 1.46     |
| 22  | A     | 1116 | CLA  | CBB-CAB | 4.23  | 1.50        | 1.30     |
| 25  | A     | 4003 | BCR  | C16-C17 | -4.22 | 1.30        | 1.43     |
| 22  | 5     | 604  | CLA  | CBB-CAB | 4.21  | 1.50        | 1.30     |
| 25  | J     | 4001 | BCR  | C16-C17 | -4.21 | 1.30        | 1.43     |
| 25  | B     | 4006 | BCR  | C16-C17 | -4.21 | 1.30        | 1.43     |
| 25  | G     | 4001 | BCR  | C16-C17 | -4.20 | 1.30        | 1.43     |
| 25  | 3     | 506  | BCR  | C10-C9  | 4.20  | 1.45        | 1.35     |
| 37  | J     | 4002 | C7Z  | C4-C5   | -4.20 | 1.44        | 1.51     |
| 40  | 4     | 617  | CHL  | C2C-C3C | 4.20  | 1.40        | 1.36     |
| 25  | K     | 4001 | BCR  | C16-C17 | -4.20 | 1.30        | 1.43     |
| 22  | 9     | 604  | CLA  | CBB-CAB | 4.19  | 1.50        | 1.30     |
| 22  | A     | 1127 | CLA  | MG-ND   | -4.18 | 1.97        | 2.05     |
| 25  | 3     | 505  | BCR  | C16-C17 | -4.17 | 1.30        | 1.43     |
| 40  | 3     | 611  | CHL  | C3B-C4B | 4.15  | 1.45        | 1.41     |
| 40  | 6     | 613  | CHL  | C3B-C4B | 4.15  | 1.45        | 1.41     |
| 40  | 4     | 617  | CHL  | C3A-C2A | -4.15 | 1.51        | 1.54     |
| 22  | A     | 1012 | CLA  | MG-ND   | -4.13 | 1.97        | 2.05     |
| 22  | A     | 1013 | CLA  | MG-ND   | -4.12 | 1.97        | 2.05     |
| 22  | B     | 1022 | CLA  | MG-ND   | -4.12 | 1.97        | 2.05     |
| 37  | 1     | 503  | C7Z  | C11-C10 | 4.11  | 1.55        | 1.43     |
| 22  | A     | 1135 | CLA  | CBB-CAB | 4.10  | 1.50        | 1.30     |
| 22  | 9     | 612  | CLA  | MG-ND   | -4.10 | 1.97        | 2.05     |
| 25  | 3     | 506  | BCR  | C16-C17 | -4.09 | 1.30        | 1.43     |
| 37  | 1     | 503  | C7Z  | C4-C5   | -4.09 | 1.44        | 1.51     |
| 22  | B     | 1224 | CLA  | MG-ND   | -4.09 | 1.97        | 2.05     |
| 25  | K     | 4001 | BCR  | C10-C9  | 4.08  | 1.45        | 1.35     |
| 22  | 9     | 606  | CLA  | CBB-CAB | 4.07  | 1.50        | 1.30     |
| 25  | 6     | 504  | BCR  | C10-C9  | 4.07  | 1.45        | 1.35     |
| 25  | 4     | 503  | BCR  | C10-C9  | 4.07  | 1.45        | 1.35     |
| 37  | 5     | 505  | C7Z  | C22-C21 | 4.06  | 1.67        | 1.54     |
| 36  | F     | 4001 | RRX  | C20-C21 | 4.05  | 1.55        | 1.43     |
| 37  | J     | 4002 | C7Z  | C11-C10 | 4.05  | 1.55        | 1.43     |
| 37  | 1     | 503  | C7Z  | C22-C21 | 4.04  | 1.66        | 1.54     |
| 22  | B     | 1023 | CLA  | MG-ND   | -4.02 | 1.97        | 2.05     |
| 25  | 3     | 505  | BCR  | C10-C9  | 4.02  | 1.45        | 1.35     |
| 37  | J     | 4002 | C7Z  | C22-C21 | 4.02  | 1.66        | 1.54     |
| 25  | 7     | 504  | BCR  | C16-C17 | -4.01 | 1.30        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1126 | CLA  | MG-ND   | -4.01 | 1.97        | 2.05     |
| 25  | A     | 4003 | BCR  | C10-C9  | 4.01  | 1.45        | 1.35     |
| 25  | 6     | 503  | BCR  | C10-C9  | 4.01  | 1.45        | 1.35     |
| 22  | B     | 1021 | CLA  | MG-ND   | -4.01 | 1.97        | 2.05     |
| 25  | 5     | 503  | BCR  | C10-C9  | 4.01  | 1.45        | 1.35     |
| 22  | B     | 1215 | CLA  | MG-ND   | -4.00 | 1.97        | 2.05     |
| 22  | A     | 1123 | CLA  | MG-ND   | -4.00 | 1.97        | 2.05     |
| 22  | B     | 1223 | CLA  | MG-ND   | -4.00 | 1.97        | 2.05     |
| 25  | 8     | 503  | BCR  | C10-C9  | 3.99  | 1.45        | 1.35     |
| 36  | F     | 4001 | RRX  | C23-C22 | 3.99  | 1.54        | 1.46     |
| 40  | 6     | 613  | CHL  | C3A-C2A | -3.99 | 1.51        | 1.54     |
| 22  | B     | 1219 | CLA  | MG-ND   | -3.98 | 1.97        | 2.05     |
| 25  | A     | 4005 | BCR  | C10-C9  | 3.97  | 1.45        | 1.35     |
| 22  | K     | 1404 | CLA  | MG-ND   | -3.97 | 1.97        | 2.05     |
| 25  | B     | 4007 | BCR  | C10-C9  | 3.97  | 1.45        | 1.35     |
| 25  | B     | 4005 | BCR  | C10-C9  | 3.96  | 1.45        | 1.35     |
| 22  | 2     | 606  | CLA  | MG-ND   | -3.96 | 1.97        | 2.05     |
| 22  | B     | 1225 | CLA  | MG-ND   | -3.96 | 1.97        | 2.05     |
| 22  | A     | 1116 | CLA  | MG-ND   | -3.96 | 1.97        | 2.05     |
| 22  | 1     | 607  | CLA  | MG-ND   | -3.95 | 1.98        | 2.05     |
| 40  | 4     | 611  | CHL  | C3A-C2A | -3.95 | 1.51        | 1.54     |
| 22  | A     | 1107 | CLA  | MG-ND   | -3.95 | 1.98        | 2.05     |
| 22  | A     | 1125 | CLA  | MG-ND   | -3.94 | 1.98        | 2.05     |
| 25  | B     | 4004 | BCR  | C10-C9  | 3.94  | 1.44        | 1.35     |
| 37  | 5     | 505  | C7Z  | C4-C5   | -3.94 | 1.44        | 1.51     |
| 22  | 9     | 605  | CLA  | MG-ND   | -3.94 | 1.98        | 2.05     |
| 22  | 7     | 601  | CLA  | MG-ND   | -3.94 | 1.98        | 2.05     |
| 22  | B     | 1221 | CLA  | MG-ND   | -3.93 | 1.98        | 2.05     |
| 37  | 5     | 505  | C7Z  | C15-C14 | 3.93  | 1.55        | 1.43     |
| 22  | A     | 1131 | CLA  | MG-ND   | -3.93 | 1.98        | 2.05     |
| 22  | B     | 1205 | CLA  | MG-ND   | -3.92 | 1.98        | 2.05     |
| 25  | G     | 4001 | BCR  | C10-C9  | 3.92  | 1.44        | 1.35     |
| 22  | A     | 1117 | CLA  | MG-ND   | -3.92 | 1.98        | 2.05     |
| 22  | 8     | 605  | CLA  | MG-ND   | -3.92 | 1.98        | 2.05     |
| 22  | B     | 1235 | CLA  | MG-ND   | -3.91 | 1.98        | 2.05     |
| 25  | L     | 4002 | BCR  | C10-C9  | 3.90  | 1.44        | 1.35     |
| 40  | 5     | 617  | CHL  | C2C-C3C | 3.90  | 1.40        | 1.36     |
| 22  | B     | 1227 | CLA  | MG-ND   | -3.90 | 1.98        | 2.05     |
| 22  | A     | 1135 | CLA  | MG-ND   | -3.90 | 1.98        | 2.05     |
| 40  | 6     | 617  | CHL  | C2C-C3C | 3.90  | 1.40        | 1.36     |
| 40  | 9     | 610  | CHL  | C2C-C3C | 3.90  | 1.40        | 1.36     |
| 22  | A     | 1139 | CLA  | MG-ND   | -3.90 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1134 | CLA  | MG-ND   | -3.90 | 1.98        | 2.05     |
| 22  | B     | 1237 | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 22  | 9     | 608  | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 25  | A     | 4001 | BCR  | C10-C9  | 3.89  | 1.44        | 1.35     |
| 22  | B     | 1208 | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 22  | 2     | 605  | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 25  | K     | 4002 | BCR  | C10-C9  | 3.89  | 1.44        | 1.35     |
| 22  | 1     | 613  | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 22  | 2     | 615  | CLA  | MG-ND   | -3.89 | 1.98        | 2.05     |
| 22  | L     | 1502 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 22  | B     | 1241 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 22  | 3     | 618  | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 25  | 3     | 504  | BCR  | C10-C9  | 3.88  | 1.44        | 1.35     |
| 22  | B     | 1203 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 22  | A     | 1130 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 25  | I     | 4001 | BCR  | C10-C9  | 3.87  | 1.44        | 1.35     |
| 22  | A     | 1132 | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 22  | 9     | 607  | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 22  | A     | 1124 | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 22  | 9     | 602  | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 37  | 5     | 505  | C7Z  | C27-C26 | 3.87  | 1.58        | 1.45     |
| 22  | A     | 1133 | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 22  | A     | 1136 | CLA  | MG-ND   | -3.87 | 1.98        | 2.05     |
| 22  | B     | 1206 | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 25  | L     | 4001 | BCR  | C10-C9  | 3.86  | 1.44        | 1.35     |
| 22  | G     | 1602 | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 22  | 7     | 613  | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 22  | 2     | 612  | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 22  | 9     | 609  | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 22  | 7     | 612  | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 22  | 8     | 601  | CLA  | MG-ND   | -3.86 | 1.98        | 2.05     |
| 25  | 7     | 503  | BCR  | C10-C9  | 3.86  | 1.44        | 1.35     |
| 40  | 1     | 610  | CHL  | C2C-C3C | 3.85  | 1.40        | 1.36     |
| 22  | B     | 1213 | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 22  | B     | 1217 | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 22  | A     | 1115 | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 22  | 9     | 603  | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 22  | B     | 1214 | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 22  | 2     | 603  | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 22  | K     | 1403 | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 37  | J     | 4002 | C7Z  | C27-C26 | 3.85  | 1.58        | 1.45     |
| 22  | B     | 1210 | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 8     | 612  | CLA  | MG-ND   | -3.84 | 1.98        | 2.05     |
| 22  | 6     | 619  | CLA  | MG-ND   | -3.84 | 1.98        | 2.05     |
| 22  | 9     | 601  | CLA  | MG-ND   | -3.84 | 1.98        | 2.05     |
| 22  | Z     | 604  | CLA  | MG-ND   | -3.84 | 1.98        | 2.05     |
| 22  | B     | 1209 | CLA  | MG-ND   | -3.84 | 1.98        | 2.05     |
| 22  | 3     | 608  | CLA  | MG-ND   | -3.84 | 1.98        | 2.05     |
| 25  | B     | 4002 | BCR  | C10-C9  | 3.83  | 1.44        | 1.35     |
| 25  | J     | 4001 | BCR  | C10-C9  | 3.83  | 1.44        | 1.35     |
| 22  | 1     | 602  | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |
| 22  | 6     | 602  | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |
| 22  | 5     | 613  | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |
| 22  | 6     | 618  | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |
| 22  | 2     | 608  | CLA  | MG-ND   | -3.83 | 1.98        | 2.05     |
| 22  | 4     | 608  | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | A     | 1114 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | A     | 1102 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | 8     | 611  | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | 7     | 608  | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | 7     | 615  | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | A     | 1137 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | A     | 1112 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | B     | 1218 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 40  | 2     | 613  | CHL  | C2C-C3C | 3.82  | 1.40        | 1.36     |
| 22  | A     | 1118 | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | 3     | 607  | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | 4     | 607  | CLA  | MG-ND   | -3.82 | 1.98        | 2.05     |
| 22  | 6     | 607  | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | 5     | 618  | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | A     | 1119 | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | A     | 1141 | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | B     | 1234 | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | 1     | 615  | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 25  | B     | 4006 | BCR  | C10-C9  | 3.81  | 1.44        | 1.35     |
| 25  | 3     | 503  | BCR  | C10-C9  | 3.81  | 1.44        | 1.35     |
| 40  | 4     | 610  | CHL  | C2C-C3C | 3.81  | 1.40        | 1.36     |
| 22  | 5     | 622  | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | 6     | 608  | CLA  | MG-ND   | -3.81 | 1.98        | 2.05     |
| 22  | A     | 1111 | CLA  | MG-ND   | -3.80 | 1.98        | 2.05     |
| 22  | A     | 1113 | CLA  | MG-ND   | -3.80 | 1.98        | 2.05     |
| 22  | 5     | 615  | CLA  | MG-ND   | -3.80 | 1.98        | 2.05     |
| 37  | 1     | 503  | C7Z  | C27-C26 | 3.80  | 1.58        | 1.45     |
| 40  | 8     | 610  | CHL  | C2C-C3C | 3.80  | 1.40        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1138 | CLA  | MG-ND   | -3.80 | 1.98        | 2.05     |
| 22  | J     | 1901 | CLA  | MG-ND   | -3.80 | 1.98        | 2.05     |
| 22  | F     | 1302 | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 22  | 2     | 601  | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 22  | 5     | 606  | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 22  | 6     | 615  | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 22  | B     | 1204 | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 22  | 8     | 609  | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 37  | 1     | 503  | C7Z  | C15-C14 | 3.79  | 1.54        | 1.43     |
| 36  | F     | 4001 | RRX  | C15-C14 | 3.79  | 1.54        | 1.43     |
| 22  | 8     | 607  | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 25  | 5     | 504  | BCR  | C10-C9  | 3.79  | 1.44        | 1.35     |
| 22  | Z     | 602  | CLA  | MG-ND   | -3.79 | 1.98        | 2.05     |
| 22  | 5     | 601  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | B     | 1212 | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | B     | 1236 | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 9     | 606  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | L     | 1503 | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | K     | 1401 | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 3     | 601  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 4     | 603  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | B     | 1228 | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 8     | 615  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 3     | 610  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | Z     | 612  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 6     | 605  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 40  | 5     | 610  | CHL  | C2C-C3C | 3.78  | 1.40        | 1.36     |
| 22  | 1     | 612  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | 3     | 613  | CLA  | MG-ND   | -3.78 | 1.98        | 2.05     |
| 22  | Z     | 615  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | B     | 1211 | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | 2     | 602  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | 7     | 602  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | B     | 1220 | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | 2     | 604  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | 8     | 602  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | 1     | 604  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 40  | 1     | 610  | CHL  | C3A-C2A | -3.77 | 1.51        | 1.54     |
| 22  | 3     | 606  | CLA  | MG-ND   | -3.77 | 1.98        | 2.05     |
| 22  | 4     | 615  | CLA  | MG-ND   | -3.76 | 1.98        | 2.05     |
| 22  | Z     | 611  | CLA  | MG-ND   | -3.76 | 1.98        | 2.05     |
| 22  | K     | 1402 | CLA  | MG-ND   | -3.76 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 6     | 612  | CLA  | MG-ND   | -3.76 | 1.98        | 2.05     |
| 22  | Z     | 607  | CLA  | MG-ND   | -3.76 | 1.98        | 2.05     |
| 25  | B     | 4003 | BCR  | C10-C9  | 3.76  | 1.44        | 1.35     |
| 22  | B     | 1239 | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | F     | 1301 | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | G     | 1601 | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | 6     | 603  | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | 9     | 604  | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | 7     | 606  | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | 7     | 607  | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | 4     | 601  | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 33  | B     | 5003 | DGD  | CGB-CFB | -3.75 | 1.33        | 1.51     |
| 22  | B     | 1201 | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | 5     | 608  | CLA  | MG-ND   | -3.75 | 1.98        | 2.05     |
| 22  | A     | 1129 | CLA  | MG-ND   | -3.74 | 1.98        | 2.05     |
| 22  | 5     | 609  | CLA  | MG-ND   | -3.74 | 1.98        | 2.05     |
| 25  | A     | 4002 | BCR  | C10-C9  | 3.74  | 1.44        | 1.35     |
| 22  | 7     | 604  | CLA  | MG-ND   | -3.74 | 1.98        | 2.05     |
| 33  | B     | 5003 | DGD  | CAA-C9A | -3.74 | 1.33        | 1.51     |
| 33  | B     | 5003 | DGD  | CAB-C9B | -3.74 | 1.33        | 1.51     |
| 40  | 5     | 611  | CHL  | C3A-C2A | -3.74 | 1.51        | 1.54     |
| 22  | A     | 1120 | CLA  | MG-ND   | -3.74 | 1.98        | 2.05     |
| 33  | B     | 5003 | DGD  | CDB-CCB | -3.74 | 1.33        | 1.51     |
| 22  | 7     | 616  | CLA  | MG-ND   | -3.74 | 1.98        | 2.05     |
| 37  | 5     | 505  | C7Z  | C35-C34 | 3.73  | 1.54        | 1.43     |
| 22  | 1     | 606  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 8     | 604  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 6     | 601  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | A     | 1103 | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 5     | 607  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 7     | 603  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 2     | 607  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 4     | 609  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | 4     | 602  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | B     | 1212 | CLA  | C1C-NC  | -3.73 | 1.32        | 1.37     |
| 22  | 4     | 606  | CLA  | MG-ND   | -3.73 | 1.98        | 2.05     |
| 22  | B     | 1202 | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 22  | Z     | 601  | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 22  | 1     | 611  | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 22  | 4     | 604  | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 22  | 6     | 606  | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 22  | 1     | 601  | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1108 | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 22  | B     | 1240 | CLA  | MG-ND   | -3.72 | 1.98        | 2.05     |
| 33  | B     | 5003 | DGD  | CGA-CFA | -3.71 | 1.33        | 1.51     |
| 22  | B     | 1232 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | 6     | 604  | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | A     | 1104 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | B     | 1231 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | A     | 1101 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | 3     | 602  | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | 3     | 616  | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | 1     | 603  | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | A     | 1121 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | B     | 1207 | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | 5     | 605  | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | 3     | 605  | CLA  | MG-ND   | -3.71 | 1.98        | 2.05     |
| 22  | A     | 1140 | CLA  | MG-ND   | -3.70 | 1.98        | 2.05     |
| 22  | 8     | 606  | CLA  | MG-ND   | -3.70 | 1.98        | 2.05     |
| 22  | Z     | 608  | CLA  | MG-ND   | -3.70 | 1.98        | 2.05     |
| 22  | 8     | 608  | CLA  | MG-ND   | -3.70 | 1.98        | 2.05     |
| 22  | B     | 1216 | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 22  | 4     | 605  | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 25  | A     | 4004 | BCR  | C10-C9  | 3.69  | 1.44        | 1.35     |
| 22  | 3     | 612  | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 22  | 7     | 611  | CLA  | MG-ND   | -3.69 | 1.98        | 2.05     |
| 22  | Z     | 603  | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 37  | J     | 4002 | C7Z  | C15-C14 | 3.68  | 1.54        | 1.43     |
| 22  | 4     | 612  | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 22  | 7     | 609  | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 37  | 1     | 503  | C7Z  | C35-C34 | 3.68  | 1.54        | 1.43     |
| 22  | 6     | 609  | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 22  | 5     | 612  | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 22  | 3     | 604  | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 22  | B     | 1220 | CLA  | C1C-NC  | -3.67 | 1.32        | 1.37     |
| 22  | 5     | 602  | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | 3     | 603  | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | B     | 1210 | CLA  | C1C-NC  | -3.66 | 1.32        | 1.37     |
| 22  | Z     | 605  | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | A     | 1109 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | 5     | 604  | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | B     | 1222 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 33  | B     | 5003 | DGD  | CDA-CCA | -3.65 | 1.33        | 1.51     |
| 22  | 1     | 605  | CLA  | MG-ND   | -3.65 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1110 | CLA  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 40  | 2     | 613  | CHL  | CBB-CAB | 3.65  | 1.52        | 1.29     |
| 22  | B     | 1238 | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 22  | 5     | 603  | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 22  | A     | 1106 | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 22  | 8     | 603  | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 22  | 7     | 605  | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 25  | B     | 4001 | BCR  | C10-C9  | 3.63  | 1.44        | 1.35     |
| 40  | 6     | 611  | CHL  | CBB-CAB | 3.62  | 1.52        | 1.29     |
| 37  | 5     | 505  | C7Z  | C2-C1   | 3.62  | 1.65        | 1.54     |
| 37  | 1     | 503  | C7Z  | C2-C1   | 3.62  | 1.65        | 1.54     |
| 40  | 2     | 610  | CHL  | C2C-C3C | 3.62  | 1.39        | 1.36     |
| 40  | 4     | 613  | CHL  | CBB-CAB | 3.61  | 1.52        | 1.29     |
| 37  | J     | 4002 | C7Z  | C2-C1   | 3.61  | 1.65        | 1.54     |
| 22  | Z     | 606  | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | B     | 1230 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 36  | F     | 4001 | RRX  | C4-C5   | -3.60 | 1.44        | 1.51     |
| 37  | J     | 4002 | C7Z  | C35-C34 | 3.60  | 1.54        | 1.43     |
| 40  | 5     | 611  | CHL  | CBB-CAB | 3.59  | 1.51        | 1.29     |
| 22  | A     | 1122 | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 40  | 4     | 611  | CHL  | CBB-CAB | 3.59  | 1.51        | 1.29     |
| 22  | B     | 1223 | CLA  | C1C-NC  | -3.59 | 1.32        | 1.37     |
| 37  | 5     | 505  | C7Z  | C7-C6   | 3.59  | 1.57        | 1.45     |
| 22  | A     | 1105 | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 40  | 6     | 613  | CHL  | CBB-CAB | 3.58  | 1.51        | 1.29     |
| 40  | 4     | 611  | CHL  | C3B-C4B | 3.56  | 1.44        | 1.41     |
| 22  | B     | 1225 | CLA  | C1C-NC  | -3.56 | 1.32        | 1.37     |
| 22  | 1     | 608  | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 37  | 1     | 503  | C7Z  | C38-C25 | 3.55  | 1.56        | 1.50     |
| 40  | 6     | 617  | CHL  | CBB-CAB | 3.55  | 1.51        | 1.29     |
| 40  | Z     | 613  | CHL  | CBB-CAB | 3.55  | 1.51        | 1.29     |
| 40  | 4     | 611  | CHL  | C2C-C3C | 3.54  | 1.39        | 1.36     |
| 40  | 8     | 610  | CHL  | CBB-CAB | 3.54  | 1.51        | 1.29     |
| 40  | 6     | 611  | CHL  | C3B-C4B | 3.53  | 1.44        | 1.41     |
| 40  | 4     | 617  | CHL  | CBB-CAB | 3.52  | 1.51        | 1.29     |
| 40  | 8     | 610  | CHL  | C3A-C2A | -3.52 | 1.51        | 1.54     |
| 40  | 7     | 610  | CHL  | CBB-CAB | 3.52  | 1.51        | 1.29     |
| 40  | 4     | 613  | CHL  | C2C-C3C | 3.51  | 1.39        | 1.36     |
| 40  | 2     | 610  | CHL  | CBB-CAB | 3.50  | 1.51        | 1.29     |
| 22  | B     | 1239 | CLA  | C1C-NC  | -3.50 | 1.32        | 1.37     |
| 40  | 5     | 617  | CHL  | CBB-CAB | 3.50  | 1.51        | 1.29     |
| 22  | A     | 1125 | CLA  | C1C-NC  | -3.49 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 3     | 610  | CLA  | C1C-NC  | -3.49 | 1.32        | 1.37     |
| 22  | A     | 1132 | CLA  | C1C-NC  | -3.49 | 1.32        | 1.37     |
| 37  | J     | 4002 | C7Z  | C7-C6   | 3.48  | 1.57        | 1.45     |
| 40  | 5     | 610  | CHL  | C3A-C2A | -3.48 | 1.51        | 1.54     |
| 36  | F     | 4001 | RRX  | C29-C30 | 3.48  | 1.65        | 1.54     |
| 22  | B     | 1211 | CLA  | C1C-NC  | -3.48 | 1.32        | 1.37     |
| 32  | A     | 5005 | DGA  | OG2-CB1 | 3.48  | 1.44        | 1.34     |
| 36  | F     | 4001 | RRX  | C24-C25 | 3.48  | 1.57        | 1.45     |
| 37  | 5     | 505  | C7Z  | C38-C25 | 3.48  | 1.56        | 1.50     |
| 22  | A     | 1124 | CLA  | C1C-NC  | -3.47 | 1.32        | 1.37     |
| 22  | A     | 1109 | CLA  | C1C-NC  | -3.47 | 1.32        | 1.37     |
| 22  | A     | 1111 | CLA  | C1C-NC  | -3.47 | 1.32        | 1.37     |
| 22  | 6     | 609  | CLA  | C1C-NC  | -3.47 | 1.32        | 1.37     |
| 40  | 1     | 610  | CHL  | CBB-CAB | 3.47  | 1.51        | 1.29     |
| 22  | A     | 1128 | CLA  | C1C-NC  | -3.46 | 1.32        | 1.37     |
| 40  | 9     | 610  | CHL  | CBB-CAB | 3.46  | 1.51        | 1.29     |
| 40  | 8     | 613  | CHL  | CBB-CAB | 3.45  | 1.50        | 1.29     |
| 32  | A     | 5005 | DGA  | OG1-CA1 | 3.45  | 1.43        | 1.33     |
| 22  | B     | 1204 | CLA  | C1C-NC  | -3.45 | 1.32        | 1.37     |
| 36  | F     | 4001 | RRX  | C11-C10 | 3.45  | 1.53        | 1.43     |
| 40  | Z     | 610  | CHL  | CBB-CAB | 3.44  | 1.50        | 1.29     |
| 40  | 6     | 611  | CHL  | C2C-C3C | 3.44  | 1.39        | 1.36     |
| 22  | B     | 1214 | CLA  | C1C-NC  | -3.44 | 1.32        | 1.37     |
| 40  | 4     | 610  | CHL  | CBB-CAB | 3.43  | 1.50        | 1.29     |
| 37  | 1     | 503  | C7Z  | C7-C6   | 3.43  | 1.56        | 1.45     |
| 22  | B     | 1230 | CLA  | C1C-NC  | -3.43 | 1.32        | 1.37     |
| 22  | 3     | 604  | CLA  | C1C-NC  | -3.43 | 1.32        | 1.37     |
| 40  | 9     | 613  | CHL  | CBB-CAB | 3.42  | 1.50        | 1.29     |
| 22  | B     | 1229 | CLA  | MG-ND   | -3.41 | 1.99        | 2.05     |
| 22  | B     | 1021 | CLA  | C1C-NC  | -3.41 | 1.32        | 1.37     |
| 40  | 1     | 609  | CHL  | CBB-CAB | 3.41  | 1.50        | 1.29     |
| 22  | A     | 1115 | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 22  | A     | 1127 | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 22  | B     | 1226 | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 32  | 9     | 802  | DGA  | OG2-CB1 | 3.40  | 1.43        | 1.34     |
| 22  | 4     | 609  | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 22  | B     | 1023 | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 22  | B     | 1205 | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 22  | A     | 1113 | CLA  | C1C-NC  | -3.38 | 1.32        | 1.37     |
| 22  | B     | 1234 | CLA  | C1C-NC  | -3.37 | 1.32        | 1.37     |
| 22  | A     | 1140 | CLA  | C1C-NC  | -3.37 | 1.32        | 1.37     |
| 22  | B     | 1208 | CLA  | C1C-NC  | -3.37 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 6     | 610  | CHL  | CBB-CAB | 3.37  | 1.50        | 1.29     |
| 22  | B     | 1229 | CLA  | C1C-NC  | -3.36 | 1.32        | 1.37     |
| 22  | B     | 1222 | CLA  | C1C-NC  | -3.36 | 1.32        | 1.37     |
| 22  | A     | 1108 | CLA  | C1C-NC  | -3.35 | 1.32        | 1.37     |
| 22  | A     | 1137 | CLA  | C1C-NC  | -3.35 | 1.32        | 1.37     |
| 22  | B     | 1209 | CLA  | C1C-NC  | -3.35 | 1.32        | 1.37     |
| 22  | 7     | 612  | CLA  | C1C-NC  | -3.35 | 1.32        | 1.37     |
| 22  | B     | 1203 | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 37  | J     | 4002 | C7Z  | C38-C25 | 3.34  | 1.56        | 1.50     |
| 22  | 3     | 605  | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 40  | 5     | 610  | CHL  | CBB-CAB | 3.34  | 1.50        | 1.29     |
| 22  | A     | 1110 | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 22  | 3     | 613  | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 40  | Z     | 609  | CHL  | CBB-CAB | 3.33  | 1.50        | 1.29     |
| 22  | A     | 1138 | CLA  | C1C-NC  | -3.33 | 1.32        | 1.37     |
| 22  | B     | 1219 | CLA  | C1C-NC  | -3.32 | 1.32        | 1.37     |
| 22  | 9     | 601  | CLA  | C1C-NC  | -3.32 | 1.32        | 1.37     |
| 22  | B     | 1202 | CLA  | C1C-NC  | -3.32 | 1.32        | 1.37     |
| 22  | 2     | 607  | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 22  | A     | 1103 | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 22  | 9     | 603  | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 22  | B     | 1228 | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 22  | B     | 1237 | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 22  | A     | 1107 | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 40  | 6     | 610  | CHL  | C3B-C4B | 3.30  | 1.44        | 1.41     |
| 40  | 5     | 610  | CHL  | C3B-C2B | -3.30 | 1.35        | 1.40     |
| 22  | G     | 1601 | CLA  | C1C-NC  | -3.30 | 1.32        | 1.37     |
| 22  | B     | 1217 | CLA  | C1C-NC  | -3.29 | 1.32        | 1.37     |
| 22  | B     | 1207 | CLA  | C1C-NC  | -3.29 | 1.32        | 1.37     |
| 22  | 7     | 601  | CLA  | C1C-NC  | -3.29 | 1.32        | 1.37     |
| 22  | K     | 1403 | CLA  | C1C-NC  | -3.29 | 1.32        | 1.37     |
| 40  | 5     | 611  | CHL  | C3B-C4B | 3.28  | 1.44        | 1.41     |
| 22  | B     | 1211 | CLA  | C4B-NB  | -3.28 | 1.33        | 1.37     |
| 22  | B     | 1236 | CLA  | C1C-NC  | -3.28 | 1.32        | 1.37     |
| 22  | A     | 1106 | CLA  | C1C-NC  | -3.28 | 1.32        | 1.37     |
| 22  | A     | 1135 | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 22  | A     | 1119 | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 22  | B     | 1218 | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 22  | 8     | 601  | CLA  | C1C-NC  | -3.27 | 1.32        | 1.37     |
| 40  | 6     | 611  | CHL  | C3A-C2A | -3.26 | 1.51        | 1.54     |
| 22  | 6     | 603  | CLA  | C1C-NC  | -3.26 | 1.32        | 1.37     |
| 36  | F     | 4001 | RRX  | C16-C17 | 3.25  | 1.53        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1215 | CLA  | C1C-NC  | -3.25 | 1.32        | 1.37     |
| 22  | F     | 1301 | CLA  | C1C-NC  | -3.25 | 1.32        | 1.37     |
| 22  | F     | 1302 | CLA  | C1C-NC  | -3.25 | 1.32        | 1.37     |
| 22  | A     | 1101 | CLA  | C1C-NC  | -3.25 | 1.32        | 1.37     |
| 22  | B     | 1241 | CLA  | C1C-NC  | -3.25 | 1.32        | 1.37     |
| 22  | 9     | 609  | CLA  | C1C-NC  | -3.25 | 1.32        | 1.37     |
| 22  | A     | 1112 | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | A     | 1105 | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | 2     | 604  | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | A     | 1122 | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | 3     | 606  | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | B     | 1213 | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | 5     | 615  | CLA  | C1C-NC  | -3.24 | 1.32        | 1.37     |
| 22  | 1     | 602  | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 22  | 7     | 609  | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 22  | A     | 1136 | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 22  | B     | 1238 | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 40  | 2     | 609  | CHL  | CBB-CAB | 3.23  | 1.49        | 1.29     |
| 40  | 5     | 611  | CHL  | C2C-C3C | 3.23  | 1.39        | 1.36     |
| 22  | 7     | 608  | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 22  | A     | 1139 | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 32  | 9     | 802  | DGA  | OG1-CA1 | 3.23  | 1.42        | 1.33     |
| 22  | 2     | 615  | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 22  | A     | 1133 | CLA  | C1C-NC  | -3.22 | 1.32        | 1.37     |
| 22  | 2     | 601  | CLA  | C1C-NC  | -3.22 | 1.32        | 1.37     |
| 22  | 8     | 609  | CLA  | C1C-NC  | -3.21 | 1.32        | 1.37     |
| 40  | Z     | 610  | CHL  | C3B-C4B | 3.21  | 1.44        | 1.41     |
| 22  | B     | 1201 | CLA  | C1C-NC  | -3.21 | 1.32        | 1.37     |
| 22  | L     | 1503 | CLA  | C1C-NC  | -3.21 | 1.32        | 1.37     |
| 22  | 7     | 606  | CLA  | C1C-NC  | -3.21 | 1.32        | 1.37     |
| 22  | 9     | 612  | CLA  | C1C-NC  | -3.21 | 1.32        | 1.37     |
| 22  | 5     | 602  | CLA  | C1C-NC  | -3.21 | 1.32        | 1.37     |
| 22  | Z     | 615  | CLA  | C1C-NC  | -3.20 | 1.32        | 1.37     |
| 22  | 8     | 612  | CLA  | C1C-NC  | -3.20 | 1.32        | 1.37     |
| 22  | B     | 1206 | CLA  | C1C-NC  | -3.20 | 1.32        | 1.37     |
| 22  | B     | 1224 | CLA  | C1C-NC  | -3.20 | 1.32        | 1.37     |
| 22  | 1     | 615  | CLA  | C1C-NC  | -3.20 | 1.32        | 1.37     |
| 22  | A     | 1131 | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |
| 22  | 1     | 612  | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |
| 22  | 3     | 601  | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |
| 22  | Z     | 601  | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |
| 22  | 8     | 615  | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 4     | 605  | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |
| 22  | A     | 1141 | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | A     | 1013 | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | 7     | 602  | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | A     | 1117 | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | A     | 1120 | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | 7     | 607  | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | 5     | 605  | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | 5     | 622  | CLA  | C1C-NC  | -3.17 | 1.32        | 1.37     |
| 22  | A     | 1130 | CLA  | C1C-NC  | -3.17 | 1.32        | 1.37     |
| 22  | K     | 1401 | CLA  | C1C-NC  | -3.17 | 1.32        | 1.37     |
| 22  | Z     | 604  | CLA  | C1C-NC  | -3.17 | 1.32        | 1.37     |
| 22  | 9     | 607  | CLA  | C1C-NC  | -3.17 | 1.32        | 1.37     |
| 22  | 9     | 608  | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | 6     | 618  | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | B     | 1227 | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | 8     | 606  | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | B     | 1022 | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | 4     | 603  | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | Z     | 602  | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | A     | 1012 | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | G     | 1602 | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | 5     | 612  | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | B     | 1235 | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | 1     | 603  | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | A     | 1121 | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | 2     | 606  | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | 3     | 603  | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | A     | 1118 | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | A     | 1104 | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | 8     | 602  | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | 9     | 602  | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | A     | 1126 | CLA  | C1C-NC  | -3.15 | 1.32        | 1.37     |
| 22  | 6     | 606  | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 22  | 2     | 608  | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 22  | 6     | 615  | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 22  | 1     | 601  | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 22  | 8     | 605  | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 40  | 2     | 609  | CHL  | C3B-C2B | -3.14 | 1.36        | 1.40     |
| 22  | 8     | 604  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 1     | 606  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 7     | 604  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 6     | 602  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | B     | 1231 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 5     | 603  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 6     | 601  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 2     | 603  | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | B     | 1216 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 3     | 612  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 2     | 612  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 4     | 612  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | B     | 1210 | CLA  | C4B-NB  | -3.12 | 1.33        | 1.37     |
| 22  | 6     | 608  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 8     | 607  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 1     | 604  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 5     | 608  | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | J     | 1901 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 22  | 2     | 605  | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 37  | J     | 4002 | C7Z  | C21-C26 | -3.11 | 1.49        | 1.53     |
| 22  | 1     | 611  | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 22  | 5     | 618  | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 40  | 3     | 611  | CHL  | CBB-CAB | 3.10  | 1.48        | 1.29     |
| 22  | 1     | 608  | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 22  | 7     | 611  | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 22  | 3     | 616  | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 6     | 619  | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | K     | 1404 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | B     | 1240 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 4     | 601  | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 1     | 605  | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | A     | 1134 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | Z     | 612  | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | A     | 1114 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 40  | 1     | 610  | CHL  | C3B-C4B | 3.09  | 1.44        | 1.41     |
| 22  | 3     | 607  | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 7     | 603  | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 5     | 609  | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 4     | 604  | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 4     | 602  | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 8     | 608  | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | B     | 1212 | CLA  | C4B-NB  | -3.08 | 1.33        | 1.37     |
| 22  | Z     | 611  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | 5     | 601  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | Z     | 603  | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 22  | L     | 1502 | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 7     | 613  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 8     | 603  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 5     | 606  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 6     | 612  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 7     | 605  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 4     | 608  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 9     | 606  | CLA  | C1C-NC | -3.07 | 1.33        | 1.37     |
| 22  | 7     | 616  | CLA  | C1C-NC | -3.06 | 1.33        | 1.37     |
| 22  | Z     | 606  | CLA  | C1C-NC | -3.06 | 1.33        | 1.37     |
| 22  | 4     | 615  | CLA  | C1C-NC | -3.06 | 1.33        | 1.37     |
| 22  | 9     | 605  | CLA  | C1C-NC | -3.06 | 1.33        | 1.37     |
| 22  | A     | 1132 | CLA  | C4B-NB | -3.06 | 1.33        | 1.37     |
| 22  | A     | 1136 | CLA  | C4B-NB | -3.06 | 1.33        | 1.37     |
| 22  | Z     | 608  | CLA  | C1C-NC | -3.05 | 1.33        | 1.37     |
| 22  | K     | 1402 | CLA  | C1C-NC | -3.05 | 1.33        | 1.37     |
| 22  | 4     | 607  | CLA  | C1C-NC | -3.05 | 1.33        | 1.37     |
| 22  | A     | 1125 | CLA  | C4B-NB | -3.05 | 1.33        | 1.37     |
| 22  | B     | 1221 | CLA  | C1C-NC | -3.05 | 1.33        | 1.37     |
| 22  | B     | 1204 | CLA  | C4B-NB | -3.05 | 1.33        | 1.37     |
| 22  | A     | 1123 | CLA  | C1C-NC | -3.05 | 1.33        | 1.37     |
| 22  | 2     | 602  | CLA  | C1C-NC | -3.04 | 1.33        | 1.37     |
| 22  | 4     | 606  | CLA  | C1C-NC | -3.04 | 1.33        | 1.37     |
| 22  | 3     | 608  | CLA  | C1C-NC | -3.04 | 1.33        | 1.37     |
| 22  | 5     | 607  | CLA  | C1C-NC | -3.04 | 1.33        | 1.37     |
| 22  | 6     | 605  | CLA  | C1C-NC | -3.04 | 1.33        | 1.37     |
| 36  | F     | 4001 | RRX  | C7-C6  | 3.04  | 1.55        | 1.45     |
| 22  | 8     | 611  | CLA  | C1C-NC | -3.04 | 1.33        | 1.37     |
| 22  | 6     | 604  | CLA  | C1C-NC | -3.03 | 1.33        | 1.37     |
| 22  | 3     | 602  | CLA  | C1C-NC | -3.03 | 1.33        | 1.37     |
| 22  | 6     | 607  | CLA  | C1C-NC | -3.03 | 1.33        | 1.37     |
| 22  | B     | 1022 | CLA  | C4B-NB | -3.03 | 1.33        | 1.37     |
| 22  | Z     | 605  | CLA  | C1C-NC | -3.03 | 1.33        | 1.37     |
| 22  | 7     | 615  | CLA  | C1C-NC | -3.03 | 1.33        | 1.37     |
| 22  | Z     | 607  | CLA  | C1C-NC | -3.03 | 1.33        | 1.37     |
| 22  | 3     | 604  | CLA  | C4B-NB | -3.02 | 1.33        | 1.37     |
| 22  | A     | 1129 | CLA  | C1C-NC | -3.02 | 1.33        | 1.37     |
| 22  | 5     | 613  | CLA  | C1C-NC | -3.02 | 1.33        | 1.37     |
| 22  | B     | 1232 | CLA  | C1C-NC | -3.02 | 1.33        | 1.37     |
| 22  | 3     | 618  | CLA  | C1C-NC | -3.02 | 1.33        | 1.37     |
| 22  | A     | 1116 | CLA  | C1C-NC | -3.01 | 1.33        | 1.37     |
| 22  | 9     | 604  | CLA  | C1C-NC | -3.01 | 1.33        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 1     | 607  | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | A     | 1135 | CLA  | C4B-NB  | -3.00 | 1.33        | 1.37     |
| 22  | 1     | 613  | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | A     | 1113 | CLA  | C4B-NB  | -2.98 | 1.33        | 1.37     |
| 40  | 2     | 609  | CHL  | CHB-C4A | -2.98 | 1.35        | 1.38     |
| 40  | 8     | 610  | CHL  | C3B-C4B | 2.98  | 1.44        | 1.41     |
| 22  | A     | 1126 | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 22  | A     | 1107 | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 22  | B     | 1222 | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 22  | B     | 1234 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 22  | B     | 1218 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 22  | A     | 1102 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 22  | B     | 1023 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 22  | B     | 1224 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 22  | A     | 1137 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 22  | A     | 1111 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 22  | A     | 1114 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 22  | A     | 1124 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 22  | 9     | 602  | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 22  | 5     | 604  | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 40  | 7     | 610  | CHL  | C2C-C3C | 2.92  | 1.39        | 1.36     |
| 22  | B     | 1205 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 8     | 612  | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | B     | 1215 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 2     | 604  | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 40  | 6     | 610  | CHL  | CHB-C4A | -2.91 | 1.35        | 1.38     |
| 22  | A     | 1013 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 40  | 4     | 611  | CHL  | C1B-C2B | 2.91  | 1.42        | 1.39     |
| 22  | B     | 1203 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 9     | 612  | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 22  | 7     | 612  | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 22  | A     | 1123 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 22  | 2     | 607  | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 22  | 9     | 601  | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 22  | 3     | 606  | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 45  | 8     | 803  | LPX  | P1-O1   | 2.89  | 1.70        | 1.59     |
| 40  | 4     | 613  | CHL  | C3B-C4B | 2.89  | 1.44        | 1.41     |
| 22  | A     | 1120 | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 22  | 6     | 619  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | 7     | 601  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 26  | 3     | 801  | LHG  | O7-C5   | -2.88 | 1.42        | 1.46     |
| 22  | L     | 1503 | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1228 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 22  | B     | 1241 | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 22  | 8     | 605  | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 22  | A     | 1117 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 22  | 5     | 605  | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 22  | 9     | 603  | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 22  | A     | 1109 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | A     | 1012 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | A     | 1108 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 40  | 2     | 613  | CHL  | CHB-C4A | -2.84 | 1.35        | 1.38     |
| 22  | B     | 1202 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | 5     | 612  | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | B     | 1219 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | A     | 1103 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 40  | 4     | 613  | CHL  | C1D-C2D | 2.82  | 1.42        | 1.39     |
| 40  | 8     | 610  | CHL  | C1B-C2B | 2.82  | 1.42        | 1.39     |
| 22  | 2     | 615  | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | Z     | 602  | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 22  | 8     | 601  | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 22  | 1     | 602  | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 21  | A     | 1011 | CL0  | CHB-C4A | -2.81 | 1.35        | 1.38     |
| 40  | 4     | 610  | CHL  | C1B-C2B | 2.81  | 1.42        | 1.39     |
| 22  | B     | 1208 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 40  | 5     | 611  | CHL  | C1B-C2B | 2.80  | 1.42        | 1.39     |
| 22  | B     | 1213 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 40  | Z     | 610  | CHL  | CHB-C4A | -2.80 | 1.35        | 1.38     |
| 36  | F     | 4001 | RRX  | C32-C1  | 2.80  | 1.59        | 1.53     |
| 37  | 5     | 505  | C7Z  | C21-C26 | -2.80 | 1.50        | 1.53     |
| 22  | A     | 1129 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | 9     | 605  | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | B     | 1220 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | 6     | 606  | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | Z     | 601  | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 40  | 2     | 609  | CHL  | C1D-C2D | 2.78  | 1.42        | 1.39     |
| 22  | 4     | 604  | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | 7     | 602  | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | 9     | 608  | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | B     | 1201 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | A     | 1131 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | A     | 1119 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 40  | 1     | 609  | CHL  | CHB-C4A | -2.77 | 1.35        | 1.38     |
| 40  | 6     | 617  | CHL  | C1B-C2B | 2.77  | 1.42        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 6     | 613  | CHL  | C1B-C2B | 2.77  | 1.42        | 1.39     |
| 22  | A     | 1115 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 22  | 3     | 610  | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 22  | 6     | 602  | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 22  | B     | 1226 | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 22  | A     | 1112 | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 40  | 8     | 613  | CHL  | CHB-C4A | -2.76 | 1.35        | 1.38     |
| 22  | 9     | 609  | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 40  | 3     | 611  | CHL  | CHB-C4A | -2.75 | 1.35        | 1.38     |
| 22  | 2     | 601  | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 22  | K     | 1403 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 40  | 4     | 617  | CHL  | C1D-C2D | 2.75  | 1.42        | 1.39     |
| 22  | G     | 1602 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 22  | 6     | 601  | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 40  | 9     | 613  | CHL  | CHB-C4A | -2.74 | 1.35        | 1.38     |
| 22  | A     | 1134 | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 22  | 7     | 606  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 22  | 5     | 622  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 40  | 9     | 610  | CHL  | CHB-C4A | -2.74 | 1.35        | 1.38     |
| 22  | 2     | 603  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 40  | 4     | 610  | CHL  | C3B-C4B | 2.74  | 1.44        | 1.41     |
| 40  | 5     | 610  | CHL  | CHB-C4A | -2.73 | 1.35        | 1.38     |
| 22  | A     | 1138 | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 1     | 611  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 1     | 606  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 3     | 601  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | B     | 1227 | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 5     | 606  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 8     | 607  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 40  | 4     | 617  | CHL  | CHB-C4A | -2.72 | 1.35        | 1.38     |
| 22  | 7     | 607  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 22  | 6     | 605  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 22  | 1     | 605  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 40  | 6     | 611  | CHL  | C1B-C2B | 2.72  | 1.42        | 1.39     |
| 40  | Z     | 609  | CHL  | CHB-C4A | -2.71 | 1.35        | 1.38     |
| 40  | 7     | 610  | CHL  | C1B-C2B | 2.71  | 1.42        | 1.39     |
| 22  | A     | 1102 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 40  | 9     | 613  | CHL  | C1A-CHA | -2.71 | 1.36        | 1.40     |
| 40  | 6     | 613  | CHL  | C1D-C2D | 2.71  | 1.42        | 1.39     |
| 22  | 9     | 607  | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 40  | Z     | 613  | CHL  | C1D-C2D | 2.71  | 1.42        | 1.39     |
| 40  | 5     | 617  | CHL  | C1B-C2B | 2.71  | 1.42        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 9     | 613  | CHL  | C1D-C2D | 2.71  | 1.42        | 1.39     |
| 22  | 2     | 612  | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 40  | 1     | 610  | CHL  | C1B-C2B | 2.70  | 1.42        | 1.39     |
| 40  | 5     | 617  | CHL  | C1D-C2D | 2.70  | 1.42        | 1.39     |
| 22  | A     | 1133 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 40  | Z     | 610  | CHL  | C1B-C2B | 2.70  | 1.42        | 1.39     |
| 22  | 3     | 612  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 22  | 4     | 606  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 22  | 1     | 607  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 40  | 4     | 617  | CHL  | C1B-C2B | 2.69  | 1.42        | 1.39     |
| 22  | 2     | 608  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 22  | 1     | 603  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 27  | 8     | 802  | NKP  | OAF-CAG | -2.69 | 1.34        | 1.44     |
| 22  | 8     | 606  | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 40  | Z     | 610  | CHL  | C1D-C2D | 2.68  | 1.42        | 1.39     |
| 22  | 3     | 618  | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 22  | B     | 1238 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 22  | Z     | 606  | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 40  | 4     | 610  | CHL  | C1D-C2D | 2.68  | 1.42        | 1.39     |
| 22  | J     | 1901 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 22  | B     | 1237 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 22  | 1     | 601  | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 40  | 8     | 613  | CHL  | C1D-C2D | 2.67  | 1.42        | 1.39     |
| 37  | 1     | 503  | C7Z  | C21-C26 | -2.67 | 1.50        | 1.53     |
| 40  | Z     | 613  | CHL  | C1B-C2B | 2.67  | 1.42        | 1.39     |
| 22  | Z     | 603  | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 22  | B     | 1235 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 40  | 1     | 610  | CHL  | CHB-C4A | -2.67 | 1.35        | 1.38     |
| 22  | A     | 1141 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 22  | 7     | 608  | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 40  | 6     | 611  | CHL  | CHB-C4A | -2.67 | 1.35        | 1.38     |
| 22  | G     | 1601 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 40  | Z     | 613  | CHL  | CHB-C4A | -2.66 | 1.35        | 1.38     |
| 22  | 7     | 604  | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 22  | 5     | 618  | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 40  | 1     | 610  | CHL  | C1D-C2D | 2.66  | 1.42        | 1.39     |
| 43  | 8     | 806  | 3PH  | O21-C2  | -2.66 | 1.40        | 1.46     |
| 40  | 8     | 610  | CHL  | C1D-C2D | 2.66  | 1.42        | 1.39     |
| 22  | B     | 1221 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 22  | 4     | 612  | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 40  | 9     | 610  | CHL  | C1B-C2B | 2.66  | 1.42        | 1.39     |
| 40  | 3     | 611  | CHL  | C1D-C2D | 2.66  | 1.42        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1239 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 22  | Z     | 612  | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 22  | 8     | 604  | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 40  | 2     | 613  | CHL  | C1D-C2D | 2.66  | 1.42        | 1.39     |
| 40  | 9     | 610  | CHL  | C1D-C2D | 2.66  | 1.42        | 1.39     |
| 40  | 9     | 613  | CHL  | C1B-C2B | 2.65  | 1.42        | 1.39     |
| 22  | A     | 1122 | CLA  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 40  | 2     | 610  | CHL  | C1D-C2D | 2.65  | 1.42        | 1.39     |
| 40  | 6     | 613  | CHL  | CHB-C4A | -2.65 | 1.35        | 1.38     |
| 40  | 2     | 610  | CHL  | CHB-C4A | -2.65 | 1.35        | 1.38     |
| 22  | 2     | 605  | CLA  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 40  | 7     | 610  | CHL  | C1D-C2D | 2.65  | 1.42        | 1.39     |
| 40  | 2     | 613  | CHL  | C1B-C2B | 2.65  | 1.42        | 1.39     |
| 22  | 1     | 604  | CLA  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 40  | 5     | 610  | CHL  | C1B-C2B | 2.65  | 1.42        | 1.39     |
| 40  | 8     | 610  | CHL  | CHB-C4A | -2.64 | 1.35        | 1.38     |
| 22  | Z     | 608  | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 35  | B     | 5004 | T7X  | O16-C8  | -2.64 | 1.40        | 1.46     |
| 22  | 2     | 602  | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 43  | 5     | 802  | 3PH  | O21-C2  | -2.64 | 1.40        | 1.46     |
| 40  | 6     | 611  | CHL  | C1D-C2D | 2.64  | 1.42        | 1.39     |
| 22  | B     | 1240 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 22  | 6     | 618  | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 22  | B     | 1230 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 22  | 6     | 604  | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 22  | 5     | 615  | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 40  | 7     | 610  | CHL  | CHB-C4A | -2.63 | 1.35        | 1.38     |
| 22  | 8     | 615  | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 22  | 6     | 612  | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 22  | 6     | 607  | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 22  | 3     | 613  | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 22  | Z     | 605  | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 22  | Z     | 607  | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 22  | B     | 1216 | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 40  | 2     | 610  | CHL  | C1B-C2B | 2.62  | 1.42        | 1.39     |
| 22  | L     | 1502 | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 22  | 2     | 606  | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 22  | 4     | 607  | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 22  | 5     | 608  | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 40  | 6     | 610  | CHL  | C1D-C2D | 2.62  | 1.42        | 1.39     |
| 22  | K     | 1402 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 22  | 4     | 615  | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 5     | 610  | CHL  | C1D-C2D | 2.61  | 1.42        | 1.39     |
| 43  | 6     | 802  | 3PH  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 22  | Z     | 604  | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 22  | 4     | 601  | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 22  | Z     | 611  | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 40  | 4     | 610  | CHL  | CHB-C4A | -2.61 | 1.35        | 1.38     |
| 40  | 4     | 611  | CHL  | C1D-C2D | 2.60  | 1.42        | 1.39     |
| 40  | 6     | 617  | CHL  | C1D-C2D | 2.60  | 1.42        | 1.39     |
| 22  | B     | 1217 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 22  | 8     | 611  | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 27  | A     | 5004 | NKP  | OAF-CAG | -2.60 | 1.34        | 1.44     |
| 22  | 5     | 601  | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 40  | 1     | 609  | CHL  | C1D-C2D | 2.60  | 1.42        | 1.39     |
| 22  | 1     | 613  | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 22  | 8     | 602  | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 22  | 4     | 603  | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 22  | A     | 1128 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 22  | A     | 1101 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 40  | 4     | 613  | CHL  | C1B-C2B | 2.59  | 1.42        | 1.39     |
| 27  | 3     | 802  | NKP  | OAF-CAG | -2.59 | 1.34        | 1.44     |
| 22  | 3     | 608  | CLA  | C4B-NB  | -2.59 | 1.34        | 1.37     |
| 22  | 7     | 611  | CLA  | C4B-NB  | -2.59 | 1.34        | 1.37     |
| 22  | B     | 1214 | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 22  | 4     | 608  | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 40  | 5     | 617  | CHL  | CHB-C4A | -2.58 | 1.35        | 1.38     |
| 22  | B     | 1206 | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 40  | 6     | 610  | CHL  | C1B-C2B | 2.58  | 1.42        | 1.39     |
| 22  | 7     | 613  | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 22  | 7     | 616  | CLA  | C4B-NB  | -2.58 | 1.34        | 1.37     |
| 40  | 6     | 617  | CHL  | CHB-C4A | -2.57 | 1.35        | 1.38     |
| 22  | 1     | 612  | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 40  | 9     | 613  | CHL  | C3B-C2B | -2.57 | 1.36        | 1.40     |
| 37  | 5     | 505  | C7Z  | C20-C13 | 2.56  | 1.56        | 1.50     |
| 40  | 9     | 610  | CHL  | C3B-C2B | -2.56 | 1.36        | 1.40     |
| 40  | Z     | 609  | CHL  | C1B-C2B | 2.56  | 1.42        | 1.39     |
| 28  | 1     | 803  | LMT  | O3'-C3' | -2.56 | 1.36        | 1.43     |
| 22  | 4     | 602  | CLA  | C4B-NB  | -2.56 | 1.34        | 1.37     |
| 22  | 5     | 607  | CLA  | C4B-NB  | -2.55 | 1.34        | 1.37     |
| 22  | K     | 1404 | CLA  | C4B-NB  | -2.55 | 1.34        | 1.37     |
| 22  | 5     | 603  | CLA  | C4B-NB  | -2.54 | 1.34        | 1.37     |
| 40  | 4     | 613  | CHL  | CHB-C4A | -2.54 | 1.35        | 1.38     |
| 37  | J     | 4002 | C7Z  | C20-C13 | 2.54  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 28  | B     | 5005 | LMT  | O3'-C3' | -2.54 | 1.36        | 1.43     |
| 22  | 9     | 606  | CLA  | C4B-NB  | -2.54 | 1.34        | 1.37     |
| 22  | 1     | 608  | CLA  | C4B-NB  | -2.53 | 1.34        | 1.37     |
| 40  | 4     | 611  | CHL  | CHB-C4A | -2.53 | 1.35        | 1.38     |
| 22  | 5     | 613  | CLA  | C4B-NB  | -2.53 | 1.34        | 1.37     |
| 40  | 7     | 610  | CHL  | C3B-C2B | -2.53 | 1.36        | 1.40     |
| 43  | 5     | 802  | 3PH  | O31-C31 | 2.53  | 1.40        | 1.33     |
| 40  | 1     | 609  | CHL  | C1B-C2B | 2.53  | 1.42        | 1.39     |
| 40  | 1     | 609  | CHL  | C3B-C2B | -2.53 | 1.36        | 1.40     |
| 22  | A     | 1118 | CLA  | C4B-NB  | -2.53 | 1.34        | 1.37     |
| 22  | 7     | 615  | CLA  | C4B-NB  | -2.53 | 1.34        | 1.37     |
| 22  | 3     | 607  | CLA  | C4B-NB  | -2.53 | 1.34        | 1.37     |
| 40  | 2     | 609  | CHL  | C1B-C2B | 2.52  | 1.42        | 1.39     |
| 22  | F     | 1302 | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 22  | 3     | 602  | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 22  | 8     | 608  | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |
| 40  | 5     | 611  | CHL  | C1D-C2D | 2.52  | 1.42        | 1.39     |
| 22  | 5     | 609  | CLA  | C4B-NB  | -2.51 | 1.34        | 1.37     |
| 22  | A     | 1104 | CLA  | C4B-NB  | -2.51 | 1.34        | 1.37     |
| 40  | Z     | 609  | CHL  | C1D-C2D | 2.51  | 1.42        | 1.39     |
| 28  | 4     | 803  | LMT  | O3'-C3' | -2.51 | 1.36        | 1.43     |
| 22  | 1     | 615  | CLA  | C4B-NB  | -2.51 | 1.34        | 1.37     |
| 26  | B     | 5002 | LHG  | O7-C5   | -2.51 | 1.43        | 1.46     |
| 22  | 7     | 605  | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 22  | K     | 1401 | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 22  | 6     | 603  | CLA  | C4B-NB  | -2.50 | 1.34        | 1.37     |
| 28  | 9     | 803  | LMT  | O3'-C3' | -2.49 | 1.36        | 1.43     |
| 40  | 8     | 613  | CHL  | C1B-C2B | 2.49  | 1.42        | 1.39     |
| 22  | 6     | 615  | CLA  | C4B-NB  | -2.49 | 1.34        | 1.37     |
| 37  | 1     | 503  | C7Z  | C18-C5  | 2.48  | 1.54        | 1.50     |
| 28  | F     | 5001 | LMT  | O3'-C3' | -2.48 | 1.36        | 1.43     |
| 43  | 2     | 802  | 3PH  | O31-C31 | 2.48  | 1.40        | 1.33     |
| 40  | 5     | 611  | CHL  | CHB-C4A | -2.47 | 1.35        | 1.38     |
| 28  | B     | 5005 | LMT  | O2'-C2' | -2.47 | 1.36        | 1.43     |
| 22  | B     | 1231 | CLA  | C4B-NB  | -2.47 | 1.34        | 1.37     |
| 22  | A     | 1139 | CLA  | C4B-NB  | -2.47 | 1.34        | 1.37     |
| 28  | 8     | 805  | LMT  | O3'-C3' | -2.47 | 1.36        | 1.43     |
| 43  | 7     | 802  | 3PH  | O31-C31 | 2.47  | 1.40        | 1.33     |
| 22  | 7     | 603  | CLA  | C4B-NB  | -2.46 | 1.34        | 1.37     |
| 28  | B     | 6101 | LMT  | O3'-C3' | -2.46 | 1.36        | 1.43     |
| 43  | 7     | 802  | 3PH  | O21-C21 | 2.46  | 1.41        | 1.34     |
| 43  | 2     | 802  | 3PH  | O21-C2  | -2.46 | 1.40        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1226 | CLA  | C3D-C4D | -2.46 | 1.38        | 1.44     |
| 43  | 6     | 802  | 3PH  | O31-C31 | 2.46  | 1.40        | 1.33     |
| 22  | Z     | 615  | CLA  | C4B-NB  | -2.45 | 1.34        | 1.37     |
| 28  | A     | 5006 | LMT  | O3'-C3' | -2.45 | 1.36        | 1.43     |
| 36  | F     | 4001 | RRX  | C35-C13 | 2.44  | 1.55        | 1.50     |
| 22  | B     | 1225 | CLA  | C4B-NB  | -2.44 | 1.34        | 1.37     |
| 40  | 2     | 613  | CHL  | CHA-CBD | 2.44  | 1.54        | 1.51     |
| 22  | A     | 1121 | CLA  | C4B-NB  | -2.44 | 1.34        | 1.37     |
| 43  | 8     | 806  | 3PH  | O31-C31 | 2.43  | 1.40        | 1.33     |
| 22  | 6     | 608  | CLA  | C4B-NB  | -2.43 | 1.34        | 1.37     |
| 22  | 3     | 605  | CLA  | C4B-NB  | -2.43 | 1.34        | 1.37     |
| 22  | A     | 1130 | CLA  | C4B-NB  | -2.42 | 1.34        | 1.37     |
| 22  | A     | 1116 | CLA  | C4B-NB  | -2.42 | 1.34        | 1.37     |
| 22  | 3     | 603  | CLA  | C4B-NB  | -2.41 | 1.34        | 1.37     |
| 28  | A     | 5006 | LMT  | O2'-C2' | -2.41 | 1.37        | 1.43     |
| 22  | B     | 1223 | CLA  | C4B-NB  | -2.41 | 1.34        | 1.37     |
| 37  | J     | 4002 | C7Z  | C18-C5  | 2.41  | 1.54        | 1.50     |
| 40  | 8     | 613  | CHL  | C1A-CHA | -2.40 | 1.37        | 1.40     |
| 22  | B     | 1207 | CLA  | C4B-NB  | -2.40 | 1.34        | 1.37     |
| 40  | 7     | 610  | CHL  | C3A-C2A | -2.39 | 1.52        | 1.54     |
| 22  | A     | 1140 | CLA  | C4B-NB  | -2.39 | 1.34        | 1.37     |
| 22  | B     | 1021 | CLA  | C4B-NB  | -2.39 | 1.34        | 1.37     |
| 22  | B     | 1232 | CLA  | C4B-NB  | -2.38 | 1.34        | 1.37     |
| 22  | B     | 1236 | CLA  | C4B-NB  | -2.38 | 1.34        | 1.37     |
| 22  | 8     | 603  | CLA  | C4B-NB  | -2.37 | 1.34        | 1.37     |
| 40  | 5     | 617  | CHL  | C3B-C2B | -2.37 | 1.37        | 1.40     |
| 22  | 6     | 609  | CLA  | C4B-NB  | -2.37 | 1.34        | 1.37     |
| 28  | B     | 6101 | LMT  | O2'-C2' | -2.36 | 1.37        | 1.43     |
| 22  | 7     | 609  | CLA  | C4B-NB  | -2.36 | 1.34        | 1.37     |
| 22  | B     | 1229 | CLA  | C4B-NB  | -2.36 | 1.34        | 1.37     |
| 40  | 2     | 610  | CHL  | C3B-C2B | -2.36 | 1.37        | 1.40     |
| 28  | F     | 5001 | LMT  | O2'-C2' | -2.36 | 1.37        | 1.43     |
| 22  | 4     | 612  | CLA  | C1A-CHA | 2.35  | 1.52        | 1.43     |
| 45  | 8     | 803  | LPX  | P1-O2   | 2.35  | 1.68        | 1.59     |
| 22  | A     | 1105 | CLA  | C1C-C2C | 2.35  | 1.49        | 1.44     |
| 22  | K     | 1404 | CLA  | C1A-CHA | 2.35  | 1.52        | 1.43     |
| 22  | 5     | 615  | CLA  | C1A-CHA | 2.35  | 1.52        | 1.43     |
| 28  | 9     | 803  | LMT  | O3B-C3B | -2.34 | 1.37        | 1.43     |
| 22  | 1     | 607  | CLA  | C1A-CHA | 2.34  | 1.52        | 1.43     |
| 35  | B     | 5004 | T7X  | O18-C11 | 2.33  | 1.40        | 1.33     |
| 28  | 1     | 803  | LMT  | O2'-C2' | -2.33 | 1.37        | 1.43     |
| 28  | A     | 5006 | LMT  | O2B-C2B | -2.33 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 39  | 5     | 501  | LUT  | C22-C21 | -2.33 | 1.51        | 1.54     |
| 22  | 2     | 603  | CLA  | C1A-CHA | 2.33  | 1.52        | 1.43     |
| 40  | 3     | 611  | CHL  | C1B-C2B | 2.33  | 1.42        | 1.39     |
| 22  | B     | 1206 | CLA  | C1A-CHA | 2.33  | 1.52        | 1.43     |
| 37  | 1     | 503  | C7Z  | C20-C13 | 2.33  | 1.55        | 1.50     |
| 22  | 2     | 607  | CLA  | C1A-CHA | 2.33  | 1.52        | 1.43     |
| 28  | 4     | 803  | LMT  | O2B-C2B | -2.33 | 1.37        | 1.43     |
| 22  | 3     | 616  | CLA  | C4B-NB  | -2.32 | 1.34        | 1.37     |
| 28  | A     | 5006 | LMT  | O1'-C1' | -2.32 | 1.36        | 1.40     |
| 22  | 3     | 607  | CLA  | C1A-CHA | 2.32  | 1.52        | 1.43     |
| 22  | A     | 1106 | CLA  | C4B-NB  | -2.32 | 1.34        | 1.37     |
| 40  | 8     | 613  | CHL  | C3B-C2B | -2.32 | 1.37        | 1.40     |
| 22  | A     | 1122 | CLA  | C1A-CHA | 2.32  | 1.52        | 1.43     |
| 22  | G     | 1601 | CLA  | C1A-CHA | 2.32  | 1.52        | 1.43     |
| 22  | 9     | 604  | CLA  | C1C-C2C | 2.32  | 1.49        | 1.44     |
| 28  | B     | 5005 | LMT  | O3B-C3B | -2.32 | 1.37        | 1.43     |
| 40  | 4     | 611  | CHL  | CHA-CBD | 2.31  | 1.54        | 1.51     |
| 22  | A     | 1105 | CLA  | C4B-NB  | -2.31 | 1.34        | 1.37     |
| 40  | 5     | 617  | CHL  | CHA-CBD | 2.30  | 1.54        | 1.51     |
| 22  | 7     | 615  | CLA  | C1A-CHA | 2.30  | 1.52        | 1.43     |
| 40  | 2     | 610  | CHL  | C3A-C2A | -2.30 | 1.52        | 1.54     |
| 22  | Z     | 607  | CLA  | C1A-CHA | 2.30  | 1.52        | 1.43     |
| 22  | B     | 1220 | CLA  | C1A-CHA | 2.29  | 1.52        | 1.43     |
| 28  | 1     | 803  | LMT  | O2B-C2B | -2.29 | 1.37        | 1.43     |
| 22  | 1     | 612  | CLA  | C1A-CHA | 2.29  | 1.52        | 1.43     |
| 22  | F     | 1301 | CLA  | C1A-CHA | 2.29  | 1.52        | 1.43     |
| 40  | 5     | 611  | CHL  | CHA-CBD | 2.29  | 1.54        | 1.51     |
| 22  | B     | 1022 | CLA  | C3D-C4D | -2.29 | 1.39        | 1.44     |
| 40  | Z     | 609  | CHL  | CHA-CBD | 2.29  | 1.54        | 1.51     |
| 22  | 3     | 616  | CLA  | C1A-CHA | 2.29  | 1.52        | 1.43     |
| 22  | 5     | 601  | CLA  | C1A-CHA | 2.29  | 1.52        | 1.43     |
| 22  | A     | 1134 | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 22  | 5     | 604  | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 22  | A     | 1116 | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 22  | A     | 1123 | CLA  | MG-NC   | 2.28  | 2.11        | 2.06     |
| 22  | A     | 1108 | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 22  | 8     | 609  | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 22  | 4     | 607  | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 22  | 1     | 603  | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 40  | Z     | 613  | CHL  | CHA-CBD | 2.28  | 1.54        | 1.51     |
| 22  | 8     | 607  | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 22  | 3     | 610  | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | A     | 1141 | CLA  | C1A-CHA | 2.28  | 1.52        | 1.43     |
| 28  | 8     | 805  | LMT  | O2B-C2B | -2.27 | 1.37        | 1.43     |
| 40  | 6     | 613  | CHL  | CHA-CBD | 2.27  | 1.54        | 1.51     |
| 22  | 9     | 607  | CLA  | C1A-CHA | 2.27  | 1.52        | 1.43     |
| 22  | 8     | 601  | CLA  | C1A-CHA | 2.27  | 1.52        | 1.43     |
| 43  | 6     | 802  | 3PH  | O21-C21 | 2.27  | 1.40        | 1.34     |
| 37  | 5     | 505  | C7Z  | C18-C5  | 2.27  | 1.54        | 1.50     |
| 22  | 5     | 622  | CLA  | C1A-CHA | 2.27  | 1.52        | 1.43     |
| 28  | F     | 5001 | LMT  | O2B-C2B | -2.27 | 1.37        | 1.43     |
| 22  | A     | 1121 | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 22  | F     | 1301 | CLA  | C4B-NB  | -2.27 | 1.34        | 1.37     |
| 22  | 5     | 603  | CLA  | C1A-CHA | 2.27  | 1.52        | 1.43     |
| 28  | B     | 6101 | LMT  | O2B-C2B | -2.27 | 1.37        | 1.43     |
| 40  | 6     | 611  | CHL  | CHA-CBD | 2.27  | 1.54        | 1.51     |
| 22  | 2     | 608  | CLA  | C1A-CHA | 2.26  | 1.52        | 1.43     |
| 22  | Z     | 606  | CLA  | C1A-CHA | 2.26  | 1.52        | 1.43     |
| 22  | 7     | 607  | CLA  | C1A-CHA | 2.26  | 1.52        | 1.43     |
| 22  | 8     | 615  | CLA  | C1A-CHA | 2.26  | 1.52        | 1.43     |
| 40  | 1     | 610  | CHL  | CHA-CBD | 2.26  | 1.54        | 1.51     |
| 22  | A     | 1110 | CLA  | C1A-CHA | 2.26  | 1.52        | 1.43     |
| 28  | A     | 5006 | LMT  | O3B-C3B | -2.26 | 1.37        | 1.43     |
| 42  | Z     | 504  | QTB  | C14-C12 | -2.26 | 1.47        | 1.53     |
| 28  | B     | 6101 | LMT  | O3B-C3B | -2.26 | 1.37        | 1.43     |
| 22  | K     | 1402 | CLA  | C1A-CHA | 2.25  | 1.52        | 1.43     |
| 22  | 4     | 605  | CLA  | C4B-NB  | -2.25 | 1.34        | 1.37     |
| 22  | B     | 1023 | CLA  | C1A-CHA | 2.25  | 1.52        | 1.43     |
| 22  | 3     | 603  | CLA  | C1A-CHA | 2.25  | 1.52        | 1.43     |
| 22  | 9     | 606  | CLA  | C1C-C2C | 2.25  | 1.49        | 1.44     |
| 22  | 6     | 615  | CLA  | C1A-CHA | 2.25  | 1.52        | 1.43     |
| 22  | Z     | 603  | CLA  | C1A-CHA | 2.25  | 1.52        | 1.43     |
| 22  | B     | 1213 | CLA  | C1A-CHA | 2.25  | 1.52        | 1.43     |
| 43  | 8     | 806  | 3PH  | O21-C21 | 2.24  | 1.40        | 1.34     |
| 22  | A     | 1102 | CLA  | C1C-C2C | 2.24  | 1.49        | 1.44     |
| 32  | 9     | 802  | DGA  | OG2-CG2 | -2.24 | 1.41        | 1.46     |
| 22  | 5     | 618  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | 6     | 605  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 35  | B     | 5004 | T7X  | O18-C9  | -2.24 | 1.40        | 1.45     |
| 22  | A     | 1123 | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | Z     | 612  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | 4     | 615  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | A     | 1117 | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | A     | 1127 | CLA  | C4B-NB  | -2.24 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 4     | 601  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | 1     | 601  | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | A     | 1139 | CLA  | C1A-CHA | 2.24  | 1.52        | 1.43     |
| 22  | 6     | 619  | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 22  | 6     | 607  | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 22  | B     | 1239 | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 40  | 4     | 617  | CHL  | CHA-CBD | 2.23  | 1.54        | 1.51     |
| 22  | 7     | 603  | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 28  | B     | 5005 | LMT  | O2B-C2B | -2.23 | 1.37        | 1.43     |
| 22  | L     | 1502 | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 22  | B     | 1209 | CLA  | C1A-CHA | 2.23  | 1.52        | 1.43     |
| 40  | 6     | 617  | CHL  | CHA-CBD | 2.23  | 1.54        | 1.51     |
| 22  | 4     | 609  | CLA  | C4B-NB  | -2.23 | 1.34        | 1.37     |
| 28  | 8     | 805  | LMT  | O2'-C2' | -2.23 | 1.37        | 1.43     |
| 43  | 2     | 802  | 3PH  | O21-C21 | 2.23  | 1.40        | 1.34     |
| 32  | A     | 5005 | DGA  | OG2-CG2 | -2.23 | 1.41        | 1.46     |
| 22  | A     | 1136 | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | B     | 1212 | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 40  | 4     | 610  | CHL  | CHA-CBD | 2.22  | 1.54        | 1.51     |
| 22  | 5     | 607  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | 6     | 606  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | 4     | 602  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | 1     | 611  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | 2     | 606  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | 1     | 613  | CLA  | C1C-C2C | 2.22  | 1.49        | 1.44     |
| 40  | 6     | 610  | CHL  | CHA-CBD | 2.22  | 1.54        | 1.51     |
| 28  | 4     | 803  | LMT  | O3B-C3B | -2.22 | 1.37        | 1.43     |
| 22  | Z     | 601  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 40  | 4     | 613  | CHL  | CHA-CBD | 2.22  | 1.54        | 1.51     |
| 22  | 4     | 604  | CLA  | C1A-CHA | 2.22  | 1.52        | 1.43     |
| 22  | B     | 1219 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 40  | 2     | 610  | CHL  | CHA-CBD | 2.21  | 1.54        | 1.51     |
| 40  | 2     | 609  | CHL  | C1A-CHA | -2.21 | 1.37        | 1.40     |
| 22  | 2     | 615  | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | B     | 1224 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | B     | 1209 | CLA  | C4B-NB  | -2.21 | 1.35        | 1.37     |
| 22  | B     | 1217 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | B     | 1240 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | 9     | 603  | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | K     | 1403 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | 6     | 608  | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | Z     | 615  | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 35  | B     | 5004 | T7X  | O16-C10 | 2.21  | 1.40        | 1.34     |
| 40  | Z     | 609  | CHL  | C3B-C2B | -2.21 | 1.37        | 1.40     |
| 22  | B     | 1232 | CLA  | C1A-CHA | 2.21  | 1.52        | 1.43     |
| 22  | B     | 1208 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 9     | 601  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | A     | 1138 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 40  | 1     | 609  | CHL  | CHA-CBD | 2.20  | 1.54        | 1.51     |
| 40  | 5     | 610  | CHL  | CHA-CBD | 2.20  | 1.54        | 1.51     |
| 22  | A     | 1133 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | A     | 1109 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 28  | 4     | 803  | LMT  | O2'-C2' | -2.20 | 1.37        | 1.43     |
| 22  | A     | 1106 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 4     | 603  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | A     | 1113 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 3     | 601  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 7     | 608  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 37  | J     | 4002 | C7Z  | C40-C33 | 2.20  | 1.55        | 1.50     |
| 28  | 9     | 803  | LMT  | O2B-C2B | -2.20 | 1.37        | 1.43     |
| 22  | A     | 1124 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 5     | 606  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 27  | 3     | 802  | NKP  | CAG-CAH | 2.20  | 1.58        | 1.51     |
| 22  | 3     | 605  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 28  | 1     | 803  | LMT  | O3B-C3B | -2.20 | 1.37        | 1.43     |
| 22  | B     | 1230 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 27  | A     | 5004 | NKP  | CAG-CAH | 2.20  | 1.58        | 1.51     |
| 22  | A     | 1126 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 6     | 601  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | A     | 1107 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | B     | 1205 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | B     | 1226 | CLA  | CHD-C1D | 2.20  | 1.42        | 1.38     |
| 22  | 1     | 605  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | A     | 1132 | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 3     | 608  | CLA  | C1A-CHA | 2.20  | 1.52        | 1.43     |
| 22  | 9     | 609  | CLA  | C1A-CHA | 2.19  | 1.52        | 1.43     |
| 28  | B     | 5005 | LMT  | O1'-C1' | -2.19 | 1.36        | 1.40     |
| 22  | L     | 1503 | CLA  | C1A-CHA | 2.19  | 1.52        | 1.43     |
| 22  | B     | 1218 | CLA  | C1A-CHA | 2.19  | 1.52        | 1.43     |
| 22  | A     | 1012 | CLA  | C1C-C2C | 2.19  | 1.49        | 1.44     |
| 22  | B     | 1210 | CLA  | C3D-C4D | -2.19 | 1.39        | 1.44     |
| 40  | 8     | 610  | CHL  | CHA-CBD | 2.19  | 1.54        | 1.51     |
| 22  | 8     | 612  | CLA  | C1A-CHA | 2.19  | 1.52        | 1.43     |
| 22  | 3     | 618  | CLA  | C1A-CHA | 2.19  | 1.52        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 4     | 617  | CHL  | C3B-C2B | -2.19 | 1.37        | 1.40     |
| 22  | B     | 1214 | CLA  | C1A-CHA | 2.19  | 1.52        | 1.43     |
| 22  | 1     | 601  | CLA  | C1C-C2C | 2.18  | 1.49        | 1.44     |
| 22  | B     | 1228 | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 40  | 6     | 617  | CHL  | C3B-C2B | -2.18 | 1.37        | 1.40     |
| 22  | 1     | 613  | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 22  | B     | 1203 | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 43  | 5     | 802  | 3PH  | O21-C21 | 2.18  | 1.40        | 1.34     |
| 22  | B     | 1221 | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 28  | 8     | 805  | LMT  | O3B-C3B | -2.18 | 1.37        | 1.43     |
| 40  | 3     | 611  | CHL  | CHA-CBD | 2.18  | 1.54        | 1.51     |
| 22  | A     | 1102 | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 22  | 9     | 609  | CLA  | C1C-C2C | 2.18  | 1.48        | 1.44     |
| 22  | 6     | 602  | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 22  | B     | 1241 | CLA  | C1A-CHA | 2.18  | 1.52        | 1.43     |
| 22  | B     | 1238 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | A     | 1130 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | A     | 1125 | CLA  | C3D-C4D | -2.17 | 1.39        | 1.44     |
| 22  | 4     | 605  | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | 3     | 610  | CLA  | CHD-C1D | 2.17  | 1.42        | 1.38     |
| 22  | B     | 1222 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 37  | 1     | 503  | C7Z  | C40-C33 | 2.17  | 1.55        | 1.50     |
| 22  | G     | 1602 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | B     | 1223 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | A     | 1127 | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | 5     | 613  | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 22  | 3     | 606  | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | 5     | 608  | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | 7     | 605  | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 40  | Z     | 610  | CHL  | CHA-CBD | 2.17  | 1.54        | 1.51     |
| 22  | Z     | 602  | CLA  | C1A-CHA | 2.17  | 1.52        | 1.43     |
| 22  | A     | 1118 | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | F     | 1302 | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 1     | 615  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 6     | 603  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 7     | 601  | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 22  | 5     | 605  | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 22  | Z     | 611  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | A     | 1131 | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | K     | 1401 | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 7     | 611  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 28  | F     | 5001 | LMT  | O3B-C3B | -2.16 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 43  | 2     | 802  | 3PH  | O31-C3  | -2.16 | 1.40        | 1.45     |
| 22  | A     | 1119 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 22  | A     | 1106 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 22  | 5     | 609  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 7     | 602  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 9     | 602  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 5     | 613  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 9     | 605  | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 22  | 7     | 616  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 2     | 605  | CLA  | C1A-CHA | 2.16  | 1.52        | 1.43     |
| 22  | 5     | 604  | CLA  | C4B-NB  | -2.16 | 1.35        | 1.37     |
| 22  | 9     | 606  | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 22  | 7     | 603  | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | 6     | 618  | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | 8     | 606  | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 22  | 4     | 608  | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 22  | 7     | 612  | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 22  | A     | 1118 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 22  | A     | 1129 | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 22  | A     | 1110 | CLA  | C4B-NB  | -2.15 | 1.35        | 1.37     |
| 22  | A     | 1103 | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 22  | 9     | 605  | CLA  | C1A-CHA | 2.15  | 1.52        | 1.43     |
| 40  | 2     | 609  | CHL  | CHA-CBD | 2.15  | 1.54        | 1.51     |
| 22  | 8     | 605  | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 22  | 8     | 611  | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 22  | B     | 1225 | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 22  | 3     | 612  | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 22  | A     | 1125 | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 22  | 3     | 613  | CLA  | C1A-CHA | 2.15  | 1.51        | 1.43     |
| 22  | 7     | 601  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 22  | 2     | 604  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 22  | A     | 1111 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 22  | 5     | 602  | CLA  | C4B-NB  | -2.14 | 1.35        | 1.37     |
| 43  | 8     | 806  | 3PH  | O31-C3  | -2.14 | 1.40        | 1.45     |
| 22  | 8     | 603  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 22  | 6     | 618  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 40  | 7     | 610  | CHL  | CHA-CBD | 2.14  | 1.54        | 1.51     |
| 22  | 1     | 604  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 22  | 6     | 612  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 22  | A     | 1012 | CLA  | C3D-C4D | -2.14 | 1.39        | 1.44     |
| 22  | B     | 1232 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 22  | Z     | 605  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 3     | 602  | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 28  | 8     | 805  | LMT  | O4'-C4B | -2.14 | 1.37        | 1.43     |
| 40  | 8     | 613  | CHL  | CHA-CBD | 2.14  | 1.54        | 1.51     |
| 22  | A     | 1137 | CLA  | C1A-CHA | 2.14  | 1.51        | 1.43     |
| 22  | B     | 1204 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 22  | 7     | 613  | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | J     | 1901 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | 8     | 602  | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | 1     | 603  | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | A     | 1140 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | A     | 1013 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | A     | 1120 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | 4     | 606  | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | A     | 1101 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 22  | B     | 1201 | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | 9     | 608  | CLA  | C1A-CHA | 2.13  | 1.51        | 1.43     |
| 22  | 7     | 613  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 22  | 6     | 609  | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 28  | A     | 5006 | LMT  | O4'-C4B | -2.12 | 1.37        | 1.43     |
| 22  | 2     | 612  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 40  | 9     | 613  | CHL  | CHA-CBD | 2.12  | 1.54        | 1.51     |
| 22  | B     | 1229 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 22  | 5     | 602  | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 43  | 7     | 802  | 3PH  | O31-C3  | -2.12 | 1.40        | 1.45     |
| 22  | A     | 1105 | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 25  | B     | 4001 | BCR  | C12-C13 | -2.12 | 1.41        | 1.46     |
| 22  | 7     | 609  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 22  | 7     | 609  | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 22  | 7     | 606  | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 22  | 4     | 606  | CLA  | C1A-CHA | 2.12  | 1.51        | 1.43     |
| 22  | 9     | 612  | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 28  | 9     | 803  | LMT  | O2'-C2' | -2.12 | 1.37        | 1.43     |
| 28  | F     | 5001 | LMT  | O1'-C1' | -2.12 | 1.36        | 1.40     |
| 43  | 7     | 802  | 3PH  | O21-C2  | -2.12 | 1.41        | 1.46     |
| 22  | K     | 1402 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | 5     | 601  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | 9     | 606  | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 22  | 2     | 601  | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 22  | B     | 1207 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 22  | Z     | 608  | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 28  | 8     | 805  | LMT  | O1'-C1' | -2.11 | 1.36        | 1.40     |
| 22  | J     | 1901 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1225 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 22  | K     | 1404 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | Z     | 603  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | B     | 1231 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 22  | Z     | 604  | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 22  | A     | 1114 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 22  | A     | 1128 | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 22  | A     | 1115 | CLA  | C3D-C4D | -2.11 | 1.39        | 1.44     |
| 22  | 9     | 604  | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 22  | 5     | 602  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | 8     | 601  | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 22  | A     | 1135 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 22  | 1     | 608  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | B     | 1223 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 22  | 1     | 602  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | 7     | 606  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | B     | 1215 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | 2     | 612  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | 7     | 615  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | 7     | 616  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | 9     | 612  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | B     | 1211 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 22  | 1     | 602  | CLA  | MG-NC   | 2.10  | 2.11        | 2.06     |
| 22  | B     | 1237 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | A     | 1109 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 22  | A     | 1112 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | B     | 1216 | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | 1     | 606  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | 8     | 606  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | B     | 1236 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 22  | B     | 1236 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 22  | A     | 1114 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 22  | 5     | 612  | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 22  | A     | 1104 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 22  | B     | 1234 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 25  | 5     | 504  | BCR  | C12-C13 | -2.09 | 1.41        | 1.46     |
| 22  | B     | 1219 | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 30  | A     | 5007 | DAO  | C2-C1   | 2.09  | 1.55        | 1.50     |
| 22  | 3     | 605  | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 22  | 9     | 604  | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 22  | 6     | 608  | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 22  | B     | 1235 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 40  | 9     | 610  | CHL  | C1A-CHA | -2.08 | 1.37        | 1.40     |
| 22  | 1     | 607  | CLA  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 22  | B     | 1021 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | B     | 1204 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | A     | 1126 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | Z     | 604  | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | A     | 1124 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 3     | 603  | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | B     | 1226 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | L     | 1502 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | B     | 1229 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | B     | 1221 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | 4     | 615  | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 5     | 604  | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | B     | 1202 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 28  | 9     | 803  | LMT  | O4'-C4B | -2.08 | 1.37        | 1.43     |
| 22  | 3     | 604  | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | B     | 1224 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | A     | 1116 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | A     | 1112 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | B     | 1215 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | 3     | 601  | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 25  | B     | 4003 | BCR  | C12-C13 | -2.08 | 1.41        | 1.46     |
| 22  | 4     | 603  | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 28  | 1     | 803  | LMT  | O4'-C4B | -2.08 | 1.37        | 1.43     |
| 25  | 3     | 504  | BCR  | C12-C13 | -2.08 | 1.41        | 1.46     |
| 22  | B     | 1227 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 43  | 6     | 802  | 3PH  | O31-C3  | -2.07 | 1.40        | 1.45     |
| 22  | 2     | 608  | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 6     | 604  | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 28  | 4     | 803  | LMT  | O4'-C4B | -2.07 | 1.37        | 1.43     |
| 22  | B     | 1214 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 40  | 9     | 610  | CHL  | CHA-CBD | 2.07  | 1.54        | 1.51     |
| 22  | 1     | 606  | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 6     | 607  | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 2     | 605  | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 22  | B     | 1227 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 22  | A     | 1129 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | B     | 1236 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 22  | B     | 1216 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 22  | A     | 1116 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 22  | Z     | 605  | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 1221 | CLA  | MG-NC   | 2.06  | 2.11        | 2.06     |
| 22  | Z     | 604  | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 4     | 609  | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 22  | B     | 1234 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 22  | A     | 1135 | CLA  | MG-NC   | 2.06  | 2.11        | 2.06     |
| 22  | 1     | 611  | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | 8     | 603  | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 2     | 604  | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | B     | 1201 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | A     | 1126 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | B     | 1235 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 35  | B     | 5004 | T7X  | P1-O1   | 2.06  | 1.65        | 1.59     |
| 22  | A     | 1117 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | F     | 1302 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | A     | 1136 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | 8     | 604  | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | 1     | 615  | CLA  | CHD-C1D | 2.05  | 1.42        | 1.38     |
| 22  | B     | 1203 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | A     | 1140 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | B     | 1240 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 7     | 604  | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | 9     | 604  | CLA  | C4B-NB  | -2.05 | 1.35        | 1.37     |
| 22  | 4     | 607  | CLA  | MG-NC   | 2.05  | 2.11        | 2.06     |
| 22  | A     | 1111 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | B     | 1208 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 5     | 609  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 6     | 612  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | Z     | 601  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 3     | 608  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 4     | 604  | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 25  | A     | 4004 | BCR  | C12-C13 | -2.05 | 1.41        | 1.46     |
| 22  | B     | 1210 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | B     | 1217 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | B     | 1021 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | A     | 1116 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 25  | A     | 4002 | BCR  | C12-C13 | -2.05 | 1.41        | 1.46     |
| 22  | A     | 1110 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 2     | 607  | CLA  | MG-NC   | 2.04  | 2.11        | 2.06     |
| 28  | B     | 6101 | LMT  | O4'-C4B | -2.04 | 1.37        | 1.43     |
| 22  | 6     | 619  | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 4     | 605  | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 38  | 7     | 803  | SPH  | C3-C4   | 2.04  | 1.53        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 7     | 608  | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 28  | 1     | 803  | LMT  | O1'-C1' | -2.04 | 1.36        | 1.40     |
| 43  | 5     | 802  | 3PH  | O31-C3  | -2.04 | 1.40        | 1.45     |
| 22  | B     | 1202 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 22  | A     | 1135 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 22  | 6     | 605  | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | B     | 1237 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | A     | 1104 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | 3     | 604  | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | 3     | 618  | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 5     | 607  | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 1     | 605  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | B     | 1201 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | Z     | 608  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 3     | 606  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 2     | 602  | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 22  | A     | 1116 | CLA  | MG-NC   | 2.03  | 2.11        | 2.06     |
| 22  | 8     | 605  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | Z     | 607  | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | 1     | 613  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | B     | 1241 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 9     | 608  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 5     | 605  | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | B     | 1231 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 22  | 2     | 601  | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | B     | 1241 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 2     | 604  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 3     | 612  | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 1     | 608  | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 1     | 606  | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 8     | 611  | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 8     | 601  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 8     | 604  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 9     | 612  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | A     | 1129 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 3     | 616  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | A     | 1106 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | B     | 1208 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 7     | 611  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 1     | 602  | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 5     | 605  | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 22  | 4     | 602  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 4     | 607  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 5     | 613  | CLA  | MG-NC   | 2.02  | 2.11        | 2.06     |
| 22  | 2     | 603  | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 6     | 602  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 1     | 604  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 8     | 612  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 4     | 609  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | B     | 1218 | CLA  | MG-NC   | 2.01  | 2.11        | 2.06     |
| 22  | 2     | 605  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 5     | 608  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | B     | 1212 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 3     | 618  | CLA  | MG-NC   | 2.01  | 2.11        | 2.06     |
| 37  | 5     | 505  | C7Z  | C40-C33 | 2.01  | 1.54        | 1.50     |
| 22  | 4     | 615  | CLA  | MG-NC   | 2.01  | 2.11        | 2.06     |
| 22  | 7     | 606  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 5     | 602  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | B     | 1235 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | Z     | 611  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | G     | 1602 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 7     | 612  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | A     | 1139 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 4     | 601  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 27  | 8     | 802  | NKP  | CAG-CAH | 2.01  | 1.57        | 1.51     |
| 22  | 7     | 607  | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 8     | 609  | CLA  | C4B-NB  | -2.01 | 1.35        | 1.37     |
| 22  | B     | 1213 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 3     | 612  | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | A     | 1131 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | A     | 1141 | CLA  | MG-NC   | 2.00  | 2.11        | 2.06     |
| 22  | 3     | 603  | CLA  | MG-NC   | 2.00  | 2.11        | 2.06     |
| 22  | A     | 1132 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 5     | 622  | CLA  | MG-NC   | 2.00  | 2.11        | 2.06     |
| 22  | 3     | 613  | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 8     | 602  | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 8     | 608  | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 41  | 2     | 803  | SQD  | O47-C45 | -2.00 | 1.41        | 1.46     |
| 22  | B     | 1239 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 2     | 606  | CLA  | MG-NC   | 2.00  | 2.11        | 2.06     |
| 22  | 7     | 604  | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | B     | 1205 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | A     | 1104 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | 3     | 607  | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | 3     | 607  | CLA  | MG-NC   | 2.00  | 2.11        | 2.06     |
| 22  | B     | 1227 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | 7     | 607  | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 41  | 1     | 802  | SQD  | O47-C45 | -2.00 | 1.41        | 1.46     |
| 22  | A     | 1138 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |

All (5192) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 6     | 504  | BCR  | C10-C11-C12 | 19.44 | 179.54      | 123.20   |
| 25  | 5     | 504  | BCR  | C10-C11-C12 | 19.24 | 178.96      | 123.20   |
| 25  | 7     | 504  | BCR  | C10-C11-C12 | 19.00 | 178.24      | 123.20   |
| 25  | 3     | 504  | BCR  | C10-C11-C12 | 18.98 | 178.19      | 123.20   |
| 25  | A     | 4002 | BCR  | C10-C11-C12 | 18.93 | 178.04      | 123.20   |
| 25  | 3     | 505  | BCR  | C10-C11-C12 | 18.92 | 178.03      | 123.20   |
| 25  | 6     | 503  | BCR  | C10-C11-C12 | 18.90 | 177.97      | 123.20   |
| 25  | 5     | 503  | BCR  | C10-C11-C12 | 18.79 | 177.64      | 123.20   |
| 25  | 3     | 503  | BCR  | C10-C11-C12 | 18.78 | 177.61      | 123.20   |
| 25  | K     | 4001 | BCR  | C10-C11-C12 | 18.65 | 177.24      | 123.20   |
| 25  | 4     | 503  | BCR  | C10-C11-C12 | 18.64 | 177.20      | 123.20   |
| 25  | 7     | 503  | BCR  | C10-C11-C12 | 18.62 | 177.16      | 123.20   |
| 25  | 8     | 503  | BCR  | C10-C11-C12 | 18.61 | 177.14      | 123.20   |
| 25  | G     | 4001 | BCR  | C10-C11-C12 | 18.52 | 176.85      | 123.20   |
| 25  | I     | 4001 | BCR  | C10-C11-C12 | 18.50 | 176.80      | 123.20   |
| 25  | B     | 4007 | BCR  | C10-C11-C12 | 18.47 | 176.72      | 123.20   |
| 25  | 3     | 506  | BCR  | C10-C11-C12 | 18.46 | 176.69      | 123.20   |
| 25  | B     | 4001 | BCR  | C10-C11-C12 | 18.46 | 176.69      | 123.20   |
| 25  | B     | 4004 | BCR  | C10-C11-C12 | 18.41 | 176.55      | 123.20   |
| 25  | K     | 4002 | BCR  | C10-C11-C12 | 18.39 | 176.47      | 123.20   |
| 25  | B     | 4002 | BCR  | C10-C11-C12 | 18.37 | 176.43      | 123.20   |
| 25  | A     | 4003 | BCR  | C10-C11-C12 | 18.32 | 176.27      | 123.20   |
| 25  | L     | 4001 | BCR  | C10-C11-C12 | 18.32 | 176.27      | 123.20   |
| 25  | B     | 4005 | BCR  | C10-C11-C12 | 18.06 | 175.54      | 123.20   |
| 25  | L     | 4002 | BCR  | C10-C11-C12 | 18.06 | 175.53      | 123.20   |
| 25  | J     | 4001 | BCR  | C10-C11-C12 | 18.01 | 175.40      | 123.20   |
| 25  | A     | 4004 | BCR  | C10-C11-C12 | 17.91 | 175.11      | 123.20   |
| 25  | A     | 4001 | BCR  | C10-C11-C12 | 17.91 | 175.08      | 123.20   |
| 25  | B     | 4006 | BCR  | C10-C11-C12 | 17.86 | 174.94      | 123.20   |
| 25  | B     | 4003 | BCR  | C10-C11-C12 | 17.82 | 174.84      | 123.20   |
| 25  | 5     | 504  | BCR  | C16-C15-C14 | 17.52 | 159.38      | 123.52   |
| 25  | A     | 4005 | BCR  | C10-C11-C12 | 17.34 | 173.45      | 123.20   |
| 25  | 7     | 504  | BCR  | C16-C15-C14 | 14.69 | 153.58      | 123.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | B     | 4005 | BCR  | C21-C20-C19 | 14.40 | 164.93      | 123.20   |
| 25  | G     | 4001 | BCR  | C21-C20-C19 | 14.37 | 164.83      | 123.20   |
| 25  | A     | 4005 | BCR  | C11-C10-C9  | 14.36 | 147.42      | 127.28   |
| 25  | J     | 4001 | BCR  | C11-C10-C9  | 14.20 | 147.20      | 127.28   |
| 21  | A     | 1011 | CL0  | C1B-CHB-C4A | 14.11 | 130.40      | 121.32   |
| 25  | B     | 4003 | BCR  | C11-C10-C9  | 14.10 | 147.05      | 127.28   |
| 25  | 3     | 506  | BCR  | C11-C10-C9  | 14.10 | 147.05      | 127.28   |
| 25  | B     | 4005 | BCR  | C11-C10-C9  | 13.98 | 146.88      | 127.28   |
| 25  | K     | 4001 | BCR  | C21-C20-C19 | 13.91 | 163.50      | 123.20   |
| 25  | A     | 4003 | BCR  | C21-C20-C19 | 13.86 | 163.37      | 123.20   |
| 25  | I     | 4001 | BCR  | C11-C10-C9  | 13.85 | 146.70      | 127.28   |
| 25  | B     | 4002 | BCR  | C11-C10-C9  | 13.83 | 146.68      | 127.28   |
| 25  | 7     | 504  | BCR  | C11-C10-C9  | 13.77 | 146.59      | 127.28   |
| 25  | B     | 4006 | BCR  | C21-C20-C19 | 13.67 | 162.82      | 123.20   |
| 25  | 3     | 505  | BCR  | C11-C10-C9  | 13.63 | 146.40      | 127.28   |
| 25  | 8     | 503  | BCR  | C11-C10-C9  | 13.60 | 146.35      | 127.28   |
| 25  | 6     | 504  | BCR  | C11-C12-C13 | 13.59 | 163.62      | 126.36   |
| 25  | 6     | 503  | BCR  | C16-C15-C14 | 13.59 | 151.32      | 123.52   |
| 25  | 7     | 503  | BCR  | C11-C10-C9  | 13.52 | 146.24      | 127.28   |
| 25  | B     | 4004 | BCR  | C11-C10-C9  | 13.50 | 146.21      | 127.28   |
| 25  | A     | 4004 | BCR  | C11-C10-C9  | 13.48 | 146.18      | 127.28   |
| 25  | K     | 4002 | BCR  | C21-C20-C19 | 13.45 | 162.18      | 123.20   |
| 25  | L     | 4001 | BCR  | C11-C10-C9  | 13.45 | 146.14      | 127.28   |
| 25  | 3     | 504  | BCR  | C21-C20-C19 | 13.43 | 162.12      | 123.20   |
| 25  | 7     | 504  | BCR  | C21-C20-C19 | 13.42 | 162.10      | 123.20   |
| 25  | 7     | 503  | BCR  | C21-C20-C19 | 13.35 | 161.87      | 123.20   |
| 25  | B     | 4001 | BCR  | C21-C20-C19 | 13.33 | 161.81      | 123.20   |
| 25  | 3     | 506  | BCR  | C21-C20-C19 | 13.32 | 161.79      | 123.20   |
| 25  | K     | 4001 | BCR  | C11-C10-C9  | 13.30 | 145.93      | 127.28   |
| 25  | 5     | 503  | BCR  | C11-C10-C9  | 13.23 | 145.83      | 127.28   |
| 25  | 3     | 506  | BCR  | C16-C15-C14 | 13.19 | 150.50      | 123.52   |
| 25  | A     | 4004 | BCR  | C21-C20-C19 | 13.14 | 161.29      | 123.20   |
| 25  | 3     | 505  | BCR  | C21-C20-C19 | 13.11 | 161.20      | 123.20   |
| 25  | 7     | 503  | BCR  | C16-C15-C14 | 13.11 | 150.33      | 123.52   |
| 25  | J     | 4001 | BCR  | C21-C20-C19 | 13.04 | 160.98      | 123.20   |
| 25  | K     | 4002 | BCR  | C11-C10-C9  | 12.99 | 145.49      | 127.28   |
| 25  | 6     | 503  | BCR  | C11-C10-C9  | 12.98 | 145.49      | 127.28   |
| 25  | A     | 4001 | BCR  | C11-C10-C9  | 12.98 | 145.47      | 127.28   |
| 25  | B     | 4007 | BCR  | C11-C10-C9  | 12.97 | 145.47      | 127.28   |
| 25  | L     | 4002 | BCR  | C11-C10-C9  | 12.93 | 145.41      | 127.28   |
| 25  | A     | 4003 | BCR  | C11-C10-C9  | 12.92 | 145.40      | 127.28   |
| 25  | 3     | 504  | BCR  | C11-C10-C9  | 12.90 | 145.37      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 3     | 505  | BCR  | C16-C15-C14 | 12.86 | 149.83      | 123.52   |
| 25  | 4     | 503  | BCR  | C11-C10-C9  | 12.84 | 145.29      | 127.28   |
| 25  | L     | 4002 | BCR  | C21-C20-C19 | 12.82 | 160.36      | 123.20   |
| 25  | G     | 4001 | BCR  | C11-C10-C9  | 12.82 | 145.26      | 127.28   |
| 25  | A     | 4005 | BCR  | C11-C12-C13 | 12.77 | 161.38      | 126.36   |
| 25  | B     | 4006 | BCR  | C11-C10-C9  | 12.75 | 145.16      | 127.28   |
| 25  | 8     | 503  | BCR  | C16-C15-C14 | 12.73 | 149.57      | 123.52   |
| 25  | 6     | 504  | BCR  | C16-C15-C14 | 12.67 | 149.44      | 123.52   |
| 25  | 5     | 503  | BCR  | C21-C20-C19 | 12.66 | 159.87      | 123.20   |
| 25  | A     | 4001 | BCR  | C21-C20-C19 | 12.58 | 159.64      | 123.20   |
| 25  | L     | 4001 | BCR  | C21-C20-C19 | 12.55 | 159.57      | 123.20   |
| 25  | K     | 4001 | BCR  | C16-C15-C14 | 12.52 | 149.13      | 123.52   |
| 39  | 2     | 501  | LUT  | C21-C26-C27 | 12.47 | 127.16      | 112.83   |
| 25  | B     | 4001 | BCR  | C11-C10-C9  | 12.35 | 144.60      | 127.28   |
| 25  | A     | 4002 | BCR  | C11-C10-C9  | 12.24 | 144.45      | 127.28   |
| 25  | A     | 4004 | BCR  | C11-C12-C13 | 12.04 | 159.37      | 126.36   |
| 25  | B     | 4003 | BCR  | C11-C12-C13 | 12.03 | 159.35      | 126.36   |
| 25  | A     | 4002 | BCR  | C21-C20-C19 | 11.98 | 157.91      | 123.20   |
| 25  | B     | 4003 | BCR  | C21-C20-C19 | 11.84 | 157.51      | 123.20   |
| 25  | 4     | 503  | BCR  | C21-C20-C19 | 11.83 | 157.47      | 123.20   |
| 25  | A     | 4003 | BCR  | C11-C12-C13 | 11.77 | 158.63      | 126.36   |
| 25  | 3     | 503  | BCR  | C16-C15-C14 | 11.76 | 147.58      | 123.52   |
| 25  | L     | 4002 | BCR  | C11-C12-C13 | 11.75 | 158.59      | 126.36   |
| 25  | B     | 4007 | BCR  | C16-C15-C14 | 11.72 | 147.50      | 123.52   |
| 25  | I     | 4001 | BCR  | C16-C15-C14 | 11.69 | 147.44      | 123.52   |
| 25  | B     | 4004 | BCR  | C21-C20-C19 | 11.64 | 156.94      | 123.20   |
| 25  | 5     | 503  | BCR  | C16-C15-C14 | 11.64 | 147.34      | 123.52   |
| 25  | L     | 4001 | BCR  | C16-C15-C14 | 11.62 | 147.29      | 123.52   |
| 25  | B     | 4004 | BCR  | C16-C15-C14 | 11.62 | 147.29      | 123.52   |
| 25  | 3     | 503  | BCR  | C11-C12-C13 | 11.53 | 157.97      | 126.36   |
| 25  | G     | 4001 | BCR  | C11-C12-C13 | 11.52 | 157.96      | 126.36   |
| 25  | 8     | 503  | BCR  | C21-C20-C19 | 11.47 | 156.45      | 123.20   |
| 25  | B     | 4001 | BCR  | C11-C12-C13 | 11.47 | 157.81      | 126.36   |
| 25  | A     | 4002 | BCR  | C16-C15-C14 | 11.45 | 146.96      | 123.52   |
| 25  | B     | 4002 | BCR  | C21-C20-C19 | 11.44 | 156.35      | 123.20   |
| 25  | B     | 4002 | BCR  | C16-C15-C14 | 11.44 | 146.93      | 123.52   |
| 25  | L     | 4001 | BCR  | C11-C12-C13 | 11.43 | 157.70      | 126.36   |
| 25  | 6     | 503  | BCR  | C21-C20-C19 | 11.42 | 156.30      | 123.20   |
| 25  | K     | 4002 | BCR  | C11-C12-C13 | 11.42 | 157.67      | 126.36   |
| 25  | A     | 4001 | BCR  | C11-C12-C13 | 11.42 | 157.66      | 126.36   |
| 25  | B     | 4004 | BCR  | C11-C12-C13 | 11.40 | 157.62      | 126.36   |
| 25  | 3     | 503  | BCR  | C11-C10-C9  | 11.37 | 143.22      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | A     | 4005 | BCR  | C21-C20-C19 | 11.37 | 156.13      | 123.20   |
| 25  | 6     | 504  | BCR  | C11-C10-C9  | 11.31 | 143.13      | 127.28   |
| 25  | 3     | 503  | BCR  | C21-C20-C19 | 11.17 | 155.57      | 123.20   |
| 25  | B     | 4005 | BCR  | C11-C12-C13 | 11.14 | 156.90      | 126.36   |
| 25  | L     | 4002 | BCR  | C16-C15-C14 | 11.12 | 146.27      | 123.52   |
| 25  | B     | 4007 | BCR  | C11-C12-C13 | 11.12 | 156.84      | 126.36   |
| 25  | K     | 4001 | BCR  | C11-C12-C13 | 11.09 | 156.78      | 126.36   |
| 25  | B     | 4006 | BCR  | C11-C12-C13 | 11.07 | 156.73      | 126.36   |
| 25  | A     | 4003 | BCR  | C16-C15-C14 | 11.07 | 146.16      | 123.52   |
| 25  | 4     | 503  | BCR  | C16-C15-C14 | 11.07 | 146.16      | 123.52   |
| 25  | B     | 4007 | BCR  | C21-C20-C19 | 11.06 | 155.25      | 123.20   |
| 25  | 3     | 504  | BCR  | C16-C15-C14 | 11.05 | 146.13      | 123.52   |
| 25  | A     | 4004 | BCR  | C16-C15-C14 | 11.03 | 146.08      | 123.52   |
| 25  | B     | 4002 | BCR  | C11-C12-C13 | 10.96 | 156.42      | 126.36   |
| 25  | 3     | 504  | BCR  | C11-C12-C13 | 10.94 | 156.36      | 126.36   |
| 25  | K     | 4002 | BCR  | C16-C15-C14 | 10.88 | 145.78      | 123.52   |
| 25  | J     | 4001 | BCR  | C11-C12-C13 | 10.87 | 156.18      | 126.36   |
| 25  | 4     | 503  | BCR  | C11-C12-C13 | 10.86 | 156.14      | 126.36   |
| 25  | A     | 4002 | BCR  | C11-C12-C13 | 10.75 | 155.84      | 126.36   |
| 25  | I     | 4001 | BCR  | C11-C12-C13 | 10.71 | 155.72      | 126.36   |
| 25  | 5     | 504  | BCR  | C21-C20-C19 | 10.68 | 154.15      | 123.20   |
| 25  | B     | 4005 | BCR  | C16-C15-C14 | 10.65 | 145.31      | 123.52   |
| 25  | I     | 4001 | BCR  | C21-C20-C19 | 10.64 | 154.03      | 123.20   |
| 25  | 6     | 504  | BCR  | C21-C20-C19 | 10.53 | 153.70      | 123.20   |
| 25  | 3     | 505  | BCR  | C11-C12-C13 | 10.50 | 155.16      | 126.36   |
| 25  | A     | 4005 | BCR  | C16-C15-C14 | 10.50 | 145.00      | 123.52   |
| 25  | 8     | 503  | BCR  | C11-C12-C13 | 10.44 | 155.00      | 126.36   |
| 25  | J     | 4001 | BCR  | C16-C15-C14 | 10.41 | 144.82      | 123.52   |
| 25  | 3     | 506  | BCR  | C11-C12-C13 | 10.33 | 154.68      | 126.36   |
| 25  | B     | 4003 | BCR  | C16-C15-C14 | 10.31 | 144.62      | 123.52   |
| 25  | 7     | 504  | BCR  | C11-C12-C13 | 10.18 | 154.28      | 126.36   |
| 25  | A     | 4001 | BCR  | C16-C15-C14 | 10.16 | 144.32      | 123.52   |
| 25  | B     | 4001 | BCR  | C16-C15-C14 | 10.11 | 144.20      | 123.52   |
| 39  | 2     | 503  | LUT  | C21-C26-C27 | 10.10 | 124.44      | 112.83   |
| 22  | B     | 1211 | CLA  | C4A-NA-C1A  | 10.01 | 111.25      | 106.68   |
| 25  | 5     | 503  | BCR  | C11-C12-C13 | 10.01 | 153.80      | 126.36   |
| 25  | G     | 4001 | BCR  | C16-C15-C14 | 10.00 | 143.98      | 123.52   |
| 22  | 2     | 603  | CLA  | C4A-NA-C1A  | 10.00 | 111.24      | 106.68   |
| 22  | B     | 1206 | CLA  | C4A-NA-C1A  | 9.99  | 111.24      | 106.68   |
| 25  | 7     | 503  | BCR  | C11-C12-C13 | 9.92  | 153.56      | 126.36   |
| 22  | A     | 1103 | CLA  | C4A-NA-C1A  | 9.90  | 111.20      | 106.68   |
| 22  | B     | 1214 | CLA  | C4A-NA-C1A  | 9.88  | 111.19      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | 4     | 612  | CLA  | C4A-NA-C1A  | 9.85 | 111.17      | 106.68   |
| 22  | 5     | 603  | CLA  | C4A-NA-C1A  | 9.81 | 111.15      | 106.68   |
| 22  | K     | 1404 | CLA  | C4A-NA-C1A  | 9.80 | 111.15      | 106.68   |
| 22  | B     | 1218 | CLA  | C4A-NA-C1A  | 9.79 | 111.14      | 106.68   |
| 22  | B     | 1023 | CLA  | C4A-NA-C1A  | 9.78 | 111.14      | 106.68   |
| 25  | B     | 4006 | BCR  | C16-C15-C14 | 9.75 | 143.47      | 123.52   |
| 22  | L     | 1502 | CLA  | C4A-NA-C1A  | 9.75 | 111.13      | 106.68   |
| 22  | B     | 1219 | CLA  | C4A-NA-C1A  | 9.65 | 111.08      | 106.68   |
| 22  | 1     | 603  | CLA  | C4A-NA-C1A  | 9.64 | 111.08      | 106.68   |
| 22  | B     | 1205 | CLA  | C4A-NA-C1A  | 9.61 | 111.06      | 106.68   |
| 22  | 7     | 611  | CLA  | C4A-NA-C1A  | 9.60 | 111.06      | 106.68   |
| 22  | 5     | 615  | CLA  | C4A-NA-C1A  | 9.59 | 111.05      | 106.68   |
| 22  | B     | 1241 | CLA  | C4A-NA-C1A  | 9.57 | 111.05      | 106.68   |
| 22  | A     | 1141 | CLA  | C4A-NA-C1A  | 9.57 | 111.04      | 106.68   |
| 39  | 2     | 501  | LUT  | C26-C27-C28 | 9.52 | 139.39      | 124.58   |
| 25  | B     | 4005 | BCR  | C20-C19-C18 | 9.50 | 152.41      | 126.36   |
| 22  | 3     | 603  | CLA  | C4A-NA-C1A  | 9.48 | 111.00      | 106.68   |
| 22  | 8     | 603  | CLA  | C4A-NA-C1A  | 9.46 | 111.00      | 106.68   |
| 22  | 8     | 615  | CLA  | C4A-NA-C1A  | 9.46 | 110.99      | 106.68   |
| 22  | A     | 1118 | CLA  | C4A-NA-C1A  | 9.44 | 110.99      | 106.68   |
| 25  | 5     | 504  | BCR  | C11-C12-C13 | 9.44 | 152.24      | 126.36   |
| 22  | 7     | 609  | CLA  | C4A-NA-C1A  | 9.42 | 110.97      | 106.68   |
| 22  | 4     | 603  | CLA  | C4A-NA-C1A  | 9.41 | 110.97      | 106.68   |
| 22  | 3     | 606  | CLA  | C4A-NA-C1A  | 9.40 | 110.97      | 106.68   |
| 22  | B     | 1230 | CLA  | C4A-NA-C1A  | 9.39 | 110.97      | 106.68   |
| 25  | 6     | 503  | BCR  | C11-C12-C13 | 9.39 | 152.12      | 126.36   |
| 22  | A     | 1123 | CLA  | C4A-NA-C1A  | 9.37 | 110.95      | 106.68   |
| 22  | B     | 1212 | CLA  | C4A-NA-C1A  | 9.36 | 110.95      | 106.68   |
| 22  | Z     | 603  | CLA  | C4A-NA-C1A  | 9.36 | 110.95      | 106.68   |
| 22  | 2     | 615  | CLA  | C4A-NA-C1A  | 9.35 | 110.94      | 106.68   |
| 22  | B     | 1221 | CLA  | C4A-NA-C1A  | 9.34 | 110.94      | 106.68   |
| 22  | F     | 1301 | CLA  | C4A-NA-C1A  | 9.34 | 110.94      | 106.68   |
| 22  | B     | 1213 | CLA  | C4A-NA-C1A  | 9.33 | 110.94      | 106.68   |
| 22  | 5     | 618  | CLA  | C4A-NA-C1A  | 9.32 | 110.93      | 106.68   |
| 22  | A     | 1108 | CLA  | C4A-NA-C1A  | 9.32 | 110.93      | 106.68   |
| 22  | A     | 1138 | CLA  | C4A-NA-C1A  | 9.31 | 110.93      | 106.68   |
| 22  | 3     | 616  | CLA  | C4A-NA-C1A  | 9.30 | 110.92      | 106.68   |
| 22  | B     | 1238 | CLA  | C4A-NA-C1A  | 9.27 | 110.91      | 106.68   |
| 22  | B     | 1217 | CLA  | C4A-NA-C1A  | 9.26 | 110.91      | 106.68   |
| 22  | 8     | 611  | CLA  | C4A-NA-C1A  | 9.21 | 110.88      | 106.68   |
| 22  | A     | 1139 | CLA  | C4A-NA-C1A  | 9.20 | 110.88      | 106.68   |
| 22  | A     | 1136 | CLA  | C4A-NA-C1A  | 9.20 | 110.88      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | A     | 1134 | CLA  | C4A-NA-C1A  | 9.19 | 110.87      | 106.68   |
| 22  | B     | 1239 | CLA  | C4A-NA-C1A  | 9.19 | 110.87      | 106.68   |
| 22  | A     | 1109 | CLA  | C4A-NA-C1A  | 9.18 | 110.87      | 106.68   |
| 22  | 9     | 601  | CLA  | C4A-NA-C1A  | 9.18 | 110.87      | 106.68   |
| 22  | B     | 1208 | CLA  | C4A-NA-C1A  | 9.18 | 110.87      | 106.68   |
| 22  | 1     | 612  | CLA  | C4A-NA-C1A  | 9.17 | 110.86      | 106.68   |
| 22  | 6     | 603  | CLA  | C4A-NA-C1A  | 9.16 | 110.86      | 106.68   |
| 22  | B     | 1237 | CLA  | C4A-NA-C1A  | 9.16 | 110.86      | 106.68   |
| 22  | 6     | 618  | CLA  | C4A-NA-C1A  | 9.16 | 110.86      | 106.68   |
| 22  | 7     | 616  | CLA  | C4A-NA-C1A  | 9.15 | 110.85      | 106.68   |
| 25  | 4     | 503  | BCR  | C20-C19-C18 | 9.15 | 151.44      | 126.36   |
| 22  | A     | 1120 | CLA  | C4A-NA-C1A  | 9.14 | 110.85      | 106.68   |
| 22  | 6     | 615  | CLA  | C4A-NA-C1A  | 9.14 | 110.85      | 106.68   |
| 22  | L     | 1503 | CLA  | C4A-NA-C1A  | 9.14 | 110.85      | 106.68   |
| 22  | 9     | 603  | CLA  | C4A-NA-C1A  | 9.14 | 110.85      | 106.68   |
| 22  | A     | 1126 | CLA  | C4A-NA-C1A  | 9.13 | 110.84      | 106.68   |
| 22  | 4     | 601  | CLA  | C4A-NA-C1A  | 9.13 | 110.84      | 106.68   |
| 25  | 3     | 503  | BCR  | C20-C19-C18 | 9.12 | 151.38      | 126.36   |
| 22  | 8     | 612  | CLA  | C4A-NA-C1A  | 9.10 | 110.83      | 106.68   |
| 25  | I     | 4001 | BCR  | C20-C19-C18 | 9.10 | 151.31      | 126.36   |
| 22  | 3     | 607  | CLA  | C4A-NA-C1A  | 9.09 | 110.83      | 106.68   |
| 22  | 2     | 608  | CLA  | C4A-NA-C1A  | 9.09 | 110.82      | 106.68   |
| 22  | 4     | 607  | CLA  | C4A-NA-C1A  | 9.08 | 110.82      | 106.68   |
| 22  | B     | 1220 | CLA  | C4A-NA-C1A  | 9.08 | 110.82      | 106.68   |
| 22  | 8     | 607  | CLA  | C4A-NA-C1A  | 9.07 | 110.82      | 106.68   |
| 22  | 1     | 607  | CLA  | C4A-NA-C1A  | 9.07 | 110.81      | 106.68   |
| 22  | 5     | 606  | CLA  | C4A-NA-C1A  | 9.06 | 110.81      | 106.68   |
| 22  | 6     | 606  | CLA  | C4A-NA-C1A  | 9.06 | 110.81      | 106.68   |
| 22  | 7     | 606  | CLA  | C4A-NA-C1A  | 9.06 | 110.81      | 106.68   |
| 22  | 3     | 612  | CLA  | C4A-NA-C1A  | 9.04 | 110.80      | 106.68   |
| 22  | 3     | 613  | CLA  | C4A-NA-C1A  | 9.02 | 110.80      | 106.68   |
| 22  | A     | 1133 | CLA  | C4A-NA-C1A  | 9.02 | 110.79      | 106.68   |
| 22  | 3     | 608  | CLA  | C4A-NA-C1A  | 9.01 | 110.79      | 106.68   |
| 22  | 6     | 612  | CLA  | C4A-NA-C1A  | 9.00 | 110.79      | 106.68   |
| 22  | 5     | 601  | CLA  | C4A-NA-C1A  | 9.00 | 110.78      | 106.68   |
| 22  | 3     | 604  | CLA  | C4A-NA-C1A  | 8.99 | 110.78      | 106.68   |
| 22  | B     | 1228 | CLA  | C4A-NA-C1A  | 8.99 | 110.78      | 106.68   |
| 22  | 7     | 607  | CLA  | C4A-NA-C1A  | 8.99 | 110.78      | 106.68   |
| 22  | B     | 1202 | CLA  | C4A-NA-C1A  | 8.98 | 110.78      | 106.68   |
| 25  | A     | 4005 | BCR  | C20-C19-C18 | 8.98 | 150.99      | 126.36   |
| 22  | 5     | 608  | CLA  | C4A-NA-C1A  | 8.98 | 110.78      | 106.68   |
| 22  | A     | 1125 | CLA  | C4A-NA-C1A  | 8.98 | 110.78      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | Z     | 612  | CLA  | C4A-NA-C1A  | 8.97 | 110.77      | 106.68   |
| 22  | Z     | 615  | CLA  | C4A-NA-C1A  | 8.97 | 110.77      | 106.68   |
| 22  | 3     | 618  | CLA  | C4A-NA-C1A  | 8.96 | 110.77      | 106.68   |
| 22  | 6     | 608  | CLA  | C4A-NA-C1A  | 8.96 | 110.77      | 106.68   |
| 22  | 1     | 608  | CLA  | C4A-NA-C1A  | 8.95 | 110.76      | 106.68   |
| 22  | 2     | 606  | CLA  | C4A-NA-C1A  | 8.95 | 110.76      | 106.68   |
| 25  | B     | 4002 | BCR  | C20-C19-C18 | 8.94 | 150.89      | 126.36   |
| 22  | 1     | 611  | CLA  | C4A-NA-C1A  | 8.94 | 110.76      | 106.68   |
| 22  | A     | 1131 | CLA  | C4A-NA-C1A  | 8.94 | 110.76      | 106.68   |
| 22  | 7     | 603  | CLA  | C4A-NA-C1A  | 8.94 | 110.76      | 106.68   |
| 22  | Z     | 601  | CLA  | C4A-NA-C1A  | 8.93 | 110.75      | 106.68   |
| 22  | 8     | 606  | CLA  | C4A-NA-C1A  | 8.93 | 110.75      | 106.68   |
| 22  | 5     | 622  | CLA  | C4A-NA-C1A  | 8.92 | 110.75      | 106.68   |
| 22  | 8     | 601  | CLA  | C4A-NA-C1A  | 8.92 | 110.75      | 106.68   |
| 25  | B     | 4004 | BCR  | C20-C19-C18 | 8.91 | 150.79      | 126.36   |
| 22  | 1     | 606  | CLA  | C4A-NA-C1A  | 8.91 | 110.74      | 106.68   |
| 22  | Z     | 606  | CLA  | C4A-NA-C1A  | 8.91 | 110.74      | 106.68   |
| 22  | G     | 1601 | CLA  | C4A-NA-C1A  | 8.91 | 110.74      | 106.68   |
| 25  | 6     | 503  | BCR  | C20-C19-C18 | 8.90 | 150.78      | 126.36   |
| 22  | 4     | 608  | CLA  | C4A-NA-C1A  | 8.90 | 110.74      | 106.68   |
| 22  | 2     | 607  | CLA  | C4A-NA-C1A  | 8.90 | 110.74      | 106.68   |
| 22  | B     | 1201 | CLA  | C4A-NA-C1A  | 8.89 | 110.74      | 106.68   |
| 22  | 3     | 601  | CLA  | C4A-NA-C1A  | 8.89 | 110.74      | 106.68   |
| 22  | K     | 1402 | CLA  | C4A-NA-C1A  | 8.89 | 110.73      | 106.68   |
| 25  | 3     | 506  | BCR  | C20-C19-C18 | 8.89 | 150.73      | 126.36   |
| 22  | Z     | 607  | CLA  | C4A-NA-C1A  | 8.88 | 110.73      | 106.68   |
| 22  | Z     | 602  | CLA  | C4A-NA-C1A  | 8.87 | 110.73      | 106.68   |
| 22  | 1     | 601  | CLA  | C4A-NA-C1A  | 8.87 | 110.72      | 106.68   |
| 22  | A     | 1127 | CLA  | C4A-NA-C1A  | 8.86 | 110.72      | 106.68   |
| 22  | 7     | 608  | CLA  | C4A-NA-C1A  | 8.85 | 110.72      | 106.68   |
| 22  | 8     | 609  | CLA  | C4A-NA-C1A  | 8.85 | 110.72      | 106.68   |
| 22  | A     | 1110 | CLA  | C4A-NA-C1A  | 8.85 | 110.72      | 106.68   |
| 22  | B     | 1224 | CLA  | C4A-NA-C1A  | 8.85 | 110.72      | 106.68   |
| 22  | B     | 1215 | CLA  | C4A-NA-C1A  | 8.84 | 110.71      | 106.68   |
| 22  | 6     | 602  | CLA  | C4A-NA-C1A  | 8.84 | 110.71      | 106.68   |
| 22  | 7     | 604  | CLA  | C4A-NA-C1A  | 8.84 | 110.71      | 106.68   |
| 22  | B     | 1222 | CLA  | C4A-NA-C1A  | 8.84 | 110.71      | 106.68   |
| 22  | B     | 1021 | CLA  | C4A-NA-C1A  | 8.83 | 110.71      | 106.68   |
| 22  | 9     | 612  | CLA  | C4A-NA-C1A  | 8.82 | 110.70      | 106.68   |
| 22  | 4     | 605  | CLA  | C4A-NA-C1A  | 8.82 | 110.70      | 106.68   |
| 22  | 2     | 604  | CLA  | C4A-NA-C1A  | 8.81 | 110.70      | 106.68   |
| 22  | A     | 1113 | CLA  | C4A-NA-C1A  | 8.81 | 110.70      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | A     | 1122 | CLA  | C4A-NA-C1A  | 8.79 | 110.69      | 106.68   |
| 22  | 2     | 612  | CLA  | C4A-NA-C1A  | 8.76 | 110.68      | 106.68   |
| 22  | 4     | 609  | CLA  | C4A-NA-C1A  | 8.76 | 110.67      | 106.68   |
| 22  | B     | 1210 | CLA  | C4A-NA-C1A  | 8.75 | 110.67      | 106.68   |
| 25  | 8     | 503  | BCR  | C20-C19-C18 | 8.74 | 150.31      | 126.36   |
| 22  | 9     | 607  | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | 1     | 605  | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | A     | 1124 | CLA  | C4A-NA-C1A  | 8.71 | 110.65      | 106.68   |
| 22  | 6     | 607  | CLA  | C4A-NA-C1A  | 8.70 | 110.65      | 106.68   |
| 22  | 7     | 612  | CLA  | C4A-NA-C1A  | 8.70 | 110.65      | 106.68   |
| 22  | 4     | 615  | CLA  | C4A-NA-C1A  | 8.70 | 110.65      | 106.68   |
| 22  | 8     | 604  | CLA  | C4A-NA-C1A  | 8.69 | 110.64      | 106.68   |
| 22  | B     | 1204 | CLA  | C4A-NA-C1A  | 8.69 | 110.64      | 106.68   |
| 22  | 2     | 601  | CLA  | C4A-NA-C1A  | 8.69 | 110.64      | 106.68   |
| 22  | A     | 1132 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | A     | 1111 | CLA  | C4A-NA-C1A  | 8.67 | 110.64      | 106.68   |
| 22  | A     | 1137 | CLA  | C4A-NA-C1A  | 8.67 | 110.64      | 106.68   |
| 22  | 4     | 602  | CLA  | C4A-NA-C1A  | 8.67 | 110.63      | 106.68   |
| 22  | A     | 1107 | CLA  | C4A-NA-C1A  | 8.66 | 110.63      | 106.68   |
| 21  | A     | 1011 | CL0  | O2D-CGD-CBD | 8.66 | 120.46      | 110.95   |
| 22  | 9     | 609  | CLA  | C4A-NA-C1A  | 8.66 | 110.63      | 106.68   |
| 22  | 2     | 602  | CLA  | C4A-NA-C1A  | 8.65 | 110.62      | 106.68   |
| 22  | 4     | 604  | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |
| 22  | 7     | 615  | CLA  | C4A-NA-C1A  | 8.63 | 110.62      | 106.68   |
| 22  | 6     | 604  | CLA  | C4A-NA-C1A  | 8.61 | 110.61      | 106.68   |
| 22  | Z     | 605  | CLA  | C4A-NA-C1A  | 8.61 | 110.61      | 106.68   |
| 22  | B     | 1223 | CLA  | C4A-NA-C1A  | 8.60 | 110.60      | 106.68   |
| 22  | 1     | 604  | CLA  | C4A-NA-C1A  | 8.59 | 110.60      | 106.68   |
| 22  | K     | 1403 | CLA  | C4A-NA-C1A  | 8.59 | 110.60      | 106.68   |
| 22  | 5     | 607  | CLA  | C4A-NA-C1A  | 8.57 | 110.59      | 106.68   |
| 22  | B     | 1203 | CLA  | C4A-NA-C1A  | 8.57 | 110.59      | 106.68   |
| 22  | A     | 1112 | CLA  | C4A-NA-C1A  | 8.55 | 110.58      | 106.68   |
| 22  | B     | 1216 | CLA  | C4A-NA-C1A  | 8.55 | 110.58      | 106.68   |
| 22  | 7     | 601  | CLA  | C4A-NA-C1A  | 8.55 | 110.58      | 106.68   |
| 22  | 4     | 606  | CLA  | C4A-NA-C1A  | 8.55 | 110.58      | 106.68   |
| 25  | B     | 4007 | BCR  | C20-C19-C18 | 8.54 | 149.78      | 126.36   |
| 22  | Z     | 604  | CLA  | C4A-NA-C1A  | 8.54 | 110.57      | 106.68   |
| 22  | 5     | 612  | CLA  | C4A-NA-C1A  | 8.54 | 110.57      | 106.68   |
| 22  | 9     | 608  | CLA  | C4A-NA-C1A  | 8.52 | 110.57      | 106.68   |
| 22  | 6     | 619  | CLA  | C4A-NA-C1A  | 8.52 | 110.57      | 106.68   |
| 22  | Z     | 611  | CLA  | C4A-NA-C1A  | 8.52 | 110.56      | 106.68   |
| 22  | 6     | 601  | CLA  | C4A-NA-C1A  | 8.52 | 110.56      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | B     | 1235 | CLA  | C4A-NA-C1A  | 8.50 | 110.56      | 106.68   |
| 22  | 7     | 602  | CLA  | C4A-NA-C1A  | 8.50 | 110.56      | 106.68   |
| 22  | A     | 1106 | CLA  | C4A-NA-C1A  | 8.47 | 110.54      | 106.68   |
| 22  | B     | 1240 | CLA  | C4A-NA-C1A  | 8.47 | 110.54      | 106.68   |
| 22  | 5     | 609  | CLA  | C4A-NA-C1A  | 8.44 | 110.53      | 106.68   |
| 22  | A     | 1012 | CLA  | C4A-NA-C1A  | 8.44 | 110.53      | 106.68   |
| 22  | 9     | 602  | CLA  | C4A-NA-C1A  | 8.44 | 110.53      | 106.68   |
| 22  | B     | 1236 | CLA  | C4A-NA-C1A  | 8.43 | 110.53      | 106.68   |
| 22  | A     | 1102 | CLA  | C4A-NA-C1A  | 8.42 | 110.52      | 106.68   |
| 25  | B     | 4003 | BCR  | C20-C19-C18 | 8.42 | 149.46      | 126.36   |
| 22  | 3     | 610  | CLA  | C4A-NA-C1A  | 8.41 | 110.52      | 106.68   |
| 22  | B     | 1225 | CLA  | C4A-NA-C1A  | 8.41 | 110.52      | 106.68   |
| 22  | 8     | 608  | CLA  | C4A-NA-C1A  | 8.40 | 110.51      | 106.68   |
| 22  | A     | 1117 | CLA  | C4A-NA-C1A  | 8.40 | 110.51      | 106.68   |
| 22  | 7     | 605  | CLA  | C4A-NA-C1A  | 8.39 | 110.51      | 106.68   |
| 22  | Z     | 608  | CLA  | C4A-NA-C1A  | 8.38 | 110.50      | 106.68   |
| 22  | B     | 1234 | CLA  | C4A-NA-C1A  | 8.38 | 110.50      | 106.68   |
| 22  | A     | 1013 | CLA  | C4A-NA-C1A  | 8.37 | 110.50      | 106.68   |
| 22  | A     | 1104 | CLA  | C4A-NA-C1A  | 8.36 | 110.49      | 106.68   |
| 22  | A     | 1121 | CLA  | C4A-NA-C1A  | 8.35 | 110.49      | 106.68   |
| 22  | G     | 1602 | CLA  | C4A-NA-C1A  | 8.35 | 110.49      | 106.68   |
| 22  | B     | 1207 | CLA  | C4A-NA-C1A  | 8.32 | 110.48      | 106.68   |
| 22  | 8     | 602  | CLA  | C4A-NA-C1A  | 8.32 | 110.47      | 106.68   |
| 22  | J     | 1901 | CLA  | C4A-NA-C1A  | 8.32 | 110.47      | 106.68   |
| 25  | A     | 4002 | BCR  | C20-C19-C18 | 8.32 | 149.16      | 126.36   |
| 22  | B     | 1229 | CLA  | C4A-NA-C1A  | 8.31 | 110.47      | 106.68   |
| 22  | 6     | 609  | CLA  | C4A-NA-C1A  | 8.30 | 110.47      | 106.68   |
| 22  | 5     | 604  | CLA  | C4A-NA-C1A  | 8.30 | 110.47      | 106.68   |
| 22  | 1     | 613  | CLA  | C4A-NA-C1A  | 8.28 | 110.46      | 106.68   |
| 22  | A     | 1105 | CLA  | C4A-NA-C1A  | 8.28 | 110.46      | 106.68   |
| 22  | 9     | 605  | CLA  | C4A-NA-C1A  | 8.28 | 110.46      | 106.68   |
| 22  | 3     | 602  | CLA  | C4A-NA-C1A  | 8.27 | 110.45      | 106.68   |
| 25  | 5     | 504  | BCR  | C11-C10-C9  | 8.27 | 138.87      | 127.28   |
| 22  | 5     | 613  | CLA  | C4A-NA-C1A  | 8.27 | 110.45      | 106.68   |
| 22  | 8     | 605  | CLA  | C4A-NA-C1A  | 8.26 | 110.45      | 106.68   |
| 22  | 1     | 602  | CLA  | C4A-NA-C1A  | 8.25 | 110.44      | 106.68   |
| 22  | B     | 1232 | CLA  | C4A-NA-C1A  | 8.24 | 110.44      | 106.68   |
| 22  | K     | 1401 | CLA  | C4A-NA-C1A  | 8.22 | 110.43      | 106.68   |
| 22  | A     | 1140 | CLA  | C4A-NA-C1A  | 8.22 | 110.43      | 106.68   |
| 22  | 1     | 615  | CLA  | C4A-NA-C1A  | 8.21 | 110.42      | 106.68   |
| 22  | A     | 1128 | CLA  | C4A-NA-C1A  | 8.19 | 110.42      | 106.68   |
| 22  | 6     | 605  | CLA  | C4A-NA-C1A  | 8.18 | 110.41      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1101 | CLA  | C4A-NA-C1A  | 8.17  | 110.41      | 106.68   |
| 22  | A     | 1129 | CLA  | C4A-NA-C1A  | 8.16  | 110.40      | 106.68   |
| 22  | F     | 1302 | CLA  | C4A-NA-C1A  | 8.16  | 110.40      | 106.68   |
| 22  | B     | 1209 | CLA  | C4A-NA-C1A  | 8.14  | 110.39      | 106.68   |
| 25  | L     | 4002 | BCR  | C20-C19-C18 | 8.11  | 148.59      | 126.36   |
| 22  | A     | 1115 | CLA  | C4A-NA-C1A  | 8.10  | 110.38      | 106.68   |
| 22  | 2     | 605  | CLA  | C4A-NA-C1A  | 8.07  | 110.36      | 106.68   |
| 22  | A     | 1114 | CLA  | C4A-NA-C1A  | 8.05  | 110.35      | 106.68   |
| 22  | 7     | 613  | CLA  | C4A-NA-C1A  | 8.05  | 110.35      | 106.68   |
| 22  | A     | 1130 | CLA  | C4A-NA-C1A  | 8.03  | 110.34      | 106.68   |
| 40  | 1     | 609  | CHL  | C1B-CHB-C4A | 8.03  | 126.49      | 121.32   |
| 22  | B     | 1231 | CLA  | C4A-NA-C1A  | 8.02  | 110.34      | 106.68   |
| 22  | 5     | 602  | CLA  | C4A-NA-C1A  | 8.01  | 110.33      | 106.68   |
| 22  | B     | 1227 | CLA  | C4A-NA-C1A  | 8.00  | 110.33      | 106.68   |
| 25  | L     | 4001 | BCR  | C20-C19-C18 | 7.98  | 148.25      | 126.36   |
| 25  | 5     | 504  | BCR  | C15-C14-C13 | -7.96 | 116.11      | 127.28   |
| 22  | 5     | 605  | CLA  | C4A-NA-C1A  | 7.93  | 110.30      | 106.68   |
| 22  | 3     | 605  | CLA  | C4A-NA-C1A  | 7.86  | 110.27      | 106.68   |
| 22  | B     | 1226 | CLA  | C4A-NA-C1A  | 7.86  | 110.27      | 106.68   |
| 22  | A     | 1119 | CLA  | C4A-NA-C1A  | 7.86  | 110.26      | 106.68   |
| 25  | A     | 4001 | BCR  | C20-C19-C18 | 7.77  | 147.67      | 126.36   |
| 22  | 9     | 606  | CLA  | C4A-NA-C1A  | 7.75  | 110.21      | 106.68   |
| 25  | 3     | 505  | BCR  | C20-C19-C18 | 7.74  | 147.60      | 126.36   |
| 25  | J     | 4001 | BCR  | C20-C19-C18 | 7.73  | 147.57      | 126.36   |
| 40  | 2     | 610  | CHL  | C1B-CHB-C4A | 7.72  | 126.29      | 121.32   |
| 25  | 5     | 503  | BCR  | C20-C19-C18 | 7.71  | 147.50      | 126.36   |
| 40  | 5     | 617  | CHL  | C1B-CHB-C4A | 7.69  | 126.27      | 121.32   |
| 22  | A     | 1135 | CLA  | C4A-NA-C1A  | 7.66  | 110.17      | 106.68   |
| 25  | 7     | 504  | BCR  | C20-C19-C18 | 7.66  | 147.36      | 126.36   |
| 22  | B     | 1022 | CLA  | C4A-NA-C1A  | 7.57  | 110.13      | 106.68   |
| 40  | 5     | 611  | CHL  | C1B-CHB-C4A | 7.51  | 126.15      | 121.32   |
| 25  | A     | 4004 | BCR  | C20-C19-C18 | 7.48  | 146.89      | 126.36   |
| 22  | A     | 1116 | CLA  | C4A-NA-C1A  | 7.45  | 110.08      | 106.68   |
| 25  | K     | 4002 | BCR  | C20-C19-C18 | 7.44  | 146.75      | 126.36   |
| 40  | 6     | 613  | CHL  | C1B-CHB-C4A | 7.42  | 126.10      | 121.32   |
| 22  | 9     | 604  | CLA  | C4A-NA-C1A  | 7.32  | 110.02      | 106.68   |
| 40  | 4     | 617  | CHL  | C1B-CHB-C4A | 7.26  | 126.00      | 121.32   |
| 40  | 5     | 610  | CHL  | C1B-CHB-C4A | 7.24  | 125.98      | 121.32   |
| 25  | 7     | 503  | BCR  | C20-C19-C18 | 7.18  | 146.06      | 126.36   |
| 40  | 4     | 613  | CHL  | C1B-CHB-C4A | 7.16  | 125.93      | 121.32   |
| 25  | 3     | 504  | BCR  | C20-C19-C18 | 7.16  | 145.99      | 126.36   |
| 40  | 4     | 611  | CHL  | C1B-CHB-C4A | 7.12  | 125.90      | 121.32   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 40  | 6     | 611  | CHL  | C1B-CHB-C4A | 7.09  | 125.88      | 121.32   |
| 22  | B     | 1210 | CLA  | O2D-CGD-CBD | 7.09  | 123.62      | 111.23   |
| 25  | A     | 4003 | BCR  | C20-C19-C18 | 7.03  | 145.65      | 126.36   |
| 40  | Z     | 613  | CHL  | C1B-CHB-C4A | 7.01  | 125.83      | 121.32   |
| 40  | 9     | 610  | CHL  | C1B-CHB-C4A | 7.01  | 125.83      | 121.32   |
| 25  | B     | 4001 | BCR  | C20-C19-C18 | 6.93  | 145.36      | 126.36   |
| 25  | K     | 4001 | BCR  | C20-C19-C18 | 6.93  | 145.36      | 126.36   |
| 40  | 8     | 613  | CHL  | C1B-CHB-C4A | 6.92  | 125.78      | 121.32   |
| 40  | 6     | 617  | CHL  | C1B-CHB-C4A | 6.91  | 125.77      | 121.32   |
| 37  | 1     | 503  | C7Z  | C35-C34-C33 | -6.87 | 117.65      | 127.28   |
| 40  | 3     | 611  | CHL  | C1B-CHB-C4A | 6.83  | 125.72      | 121.32   |
| 40  | 7     | 610  | CHL  | C1B-CHB-C4A | 6.78  | 125.68      | 121.32   |
| 25  | B     | 4006 | BCR  | C20-C19-C18 | 6.76  | 144.89      | 126.36   |
| 39  | 2     | 503  | LUT  | C31-C30-C29 | -6.67 | 117.93      | 127.28   |
| 32  | A     | 5005 | DGA  | CDB-CCB-CBB | -6.66 | 80.69       | 114.37   |
| 40  | 1     | 610  | CHL  | C1B-CHB-C4A | 6.61  | 125.58      | 121.32   |
| 25  | 6     | 504  | BCR  | C20-C19-C18 | 6.58  | 144.40      | 126.36   |
| 22  | B     | 1226 | CLA  | CMD-C2D-C1D | 6.55  | 136.26      | 124.73   |
| 32  | 9     | 802  | DGA  | CDB-CCB-CBB | -6.54 | 81.33       | 114.37   |
| 22  | 6     | 619  | CLA  | O2D-CGD-CBD | 6.42  | 122.45      | 111.23   |
| 40  | 9     | 613  | CHL  | C1B-CHB-C4A | 6.40  | 125.44      | 121.32   |
| 22  | 6     | 609  | CLA  | O2D-CGD-CBD | 6.37  | 122.37      | 111.23   |
| 22  | 2     | 604  | CLA  | CMD-C2D-C1D | 6.34  | 135.90      | 124.73   |
| 22  | B     | 1221 | CLA  | O2D-CGD-CBD | 6.32  | 122.28      | 111.23   |
| 22  | A     | 1121 | CLA  | CMD-C2D-C1D | 6.32  | 135.85      | 124.73   |
| 22  | Z     | 606  | CLA  | O2D-CGD-CBD | 6.29  | 122.23      | 111.23   |
| 40  | Z     | 609  | CHL  | C1B-CHB-C4A | 6.29  | 125.37      | 121.32   |
| 22  | A     | 1106 | CLA  | O2D-CGD-CBD | 6.24  | 122.14      | 111.23   |
| 22  | A     | 1111 | CLA  | O2D-CGD-CBD | 6.22  | 122.11      | 111.23   |
| 25  | 5     | 504  | BCR  | C20-C19-C18 | 6.17  | 143.28      | 126.36   |
| 22  | 5     | 605  | CLA  | CMD-C2D-C1D | 6.14  | 135.54      | 124.73   |
| 25  | G     | 4001 | BCR  | C20-C19-C18 | 6.14  | 143.19      | 126.36   |
| 22  | 6     | 615  | CLA  | O2D-CGD-CBD | 6.10  | 121.89      | 111.23   |
| 22  | 7     | 609  | CLA  | O2D-CGD-CBD | 6.05  | 121.81      | 111.23   |
| 22  | A     | 1135 | CLA  | O2D-CGD-CBD | 6.05  | 121.81      | 111.23   |
| 22  | 1     | 608  | CLA  | CMD-C2D-C1D | 6.04  | 135.36      | 124.73   |
| 40  | Z     | 610  | CHL  | C1B-CHB-C4A | 6.03  | 125.20      | 121.32   |
| 22  | A     | 1101 | CLA  | O2D-CGD-CBD | 6.02  | 121.75      | 111.23   |
| 22  | B     | 1212 | CLA  | O2D-CGD-CBD | 6.01  | 121.74      | 111.23   |
| 22  | A     | 1132 | CLA  | O2D-CGD-CBD | 5.99  | 121.70      | 111.23   |
| 22  | 3     | 607  | CLA  | O2D-CGD-CBD | 5.98  | 121.68      | 111.23   |
| 22  | B     | 1231 | CLA  | CMD-C2D-C1D | 5.97  | 135.23      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1120 | CLA  | O2D-CGD-CBD | 5.94  | 121.62      | 111.23   |
| 22  | 1     | 611  | CLA  | CMD-C2D-C1D | 5.92  | 135.16      | 124.73   |
| 22  | 6     | 608  | CLA  | CMD-C2D-C1D | 5.91  | 135.14      | 124.73   |
| 39  | 3     | 502  | LUT  | C21-C26-C27 | 5.91  | 119.62      | 112.83   |
| 22  | K     | 1404 | CLA  | O2D-CGD-CBD | 5.90  | 121.54      | 111.23   |
| 22  | A     | 1112 | CLA  | O2D-CGD-CBD | 5.89  | 121.53      | 111.23   |
| 22  | 8     | 601  | CLA  | CMD-C2D-C1D | 5.84  | 135.02      | 124.73   |
| 22  | Z     | 604  | CLA  | CMD-C2D-C1D | 5.83  | 134.99      | 124.73   |
| 22  | 9     | 603  | CLA  | O2D-CGD-CBD | 5.83  | 121.42      | 111.23   |
| 22  | 4     | 609  | CLA  | O2D-CGD-CBD | 5.82  | 121.41      | 111.23   |
| 22  | A     | 1109 | CLA  | CMD-C2D-C1D | 5.82  | 134.98      | 124.73   |
| 22  | 1     | 606  | CLA  | CMD-C2D-C1D | 5.81  | 134.96      | 124.73   |
| 36  | F     | 4001 | RRX  | C15-C14-C13 | -5.79 | 119.16      | 127.28   |
| 22  | 7     | 606  | CLA  | CMD-C2D-C1D | 5.78  | 134.91      | 124.73   |
| 37  | 1     | 503  | C7Z  | C31-C30-C29 | -5.78 | 119.17      | 127.28   |
| 22  | K     | 1402 | CLA  | O2D-CGD-CBD | 5.78  | 121.33      | 111.23   |
| 22  | B     | 1023 | CLA  | O2D-CGD-CBD | 5.77  | 121.32      | 111.23   |
| 22  | 5     | 622  | CLA  | CMD-C2D-C1D | 5.77  | 134.88      | 124.73   |
| 22  | A     | 1118 | CLA  | O2D-CGD-CBD | 5.76  | 121.31      | 111.23   |
| 22  | A     | 1114 | CLA  | CMD-C2D-C1D | 5.76  | 134.88      | 124.73   |
| 22  | Z     | 605  | CLA  | CMD-C2D-C1D | 5.76  | 134.87      | 124.73   |
| 22  | B     | 1202 | CLA  | O2D-CGD-CBD | 5.75  | 121.28      | 111.23   |
| 22  | 3     | 610  | CLA  | O2D-CGD-CBD | 5.73  | 121.25      | 111.23   |
| 22  | 1     | 605  | CLA  | CMD-C2D-C1D | 5.73  | 134.81      | 124.73   |
| 22  | 9     | 606  | CLA  | CMD-C2D-C1D | 5.72  | 134.81      | 124.73   |
| 22  | 5     | 601  | CLA  | CMD-C2D-C1D | 5.72  | 134.81      | 124.73   |
| 22  | Z     | 611  | CLA  | CMD-C2D-C1D | 5.72  | 134.80      | 124.73   |
| 22  | 7     | 601  | CLA  | CMD-C2D-C1D | 5.72  | 134.80      | 124.73   |
| 22  | 2     | 603  | CLA  | O2D-CGD-CBD | 5.72  | 121.22      | 111.23   |
| 22  | B     | 1221 | CLA  | CMD-C2D-C1D | 5.71  | 134.79      | 124.73   |
| 22  | 7     | 605  | CLA  | CMD-C2D-C1D | 5.71  | 134.79      | 124.73   |
| 36  | F     | 4001 | RRX  | C4-C5-C6    | -5.71 | 114.99      | 122.70   |
| 22  | 9     | 605  | CLA  | CMD-C2D-C1D | 5.70  | 134.77      | 124.73   |
| 22  | A     | 1134 | CLA  | O2D-CGD-CBD | 5.70  | 121.19      | 111.23   |
| 22  | B     | 1230 | CLA  | O2D-CGD-CBD | 5.70  | 121.19      | 111.23   |
| 22  | 3     | 613  | CLA  | CMD-C2D-C1D | 5.68  | 134.74      | 124.73   |
| 22  | A     | 1138 | CLA  | O2D-CGD-CBD | 5.66  | 121.13      | 111.23   |
| 22  | 3     | 606  | CLA  | CMD-C2D-C1D | 5.64  | 134.67      | 124.73   |
| 39  | Z     | 503  | LUT  | C35-C34-C33 | -5.64 | 119.37      | 127.28   |
| 22  | 6     | 601  | CLA  | CMD-C2D-C1D | 5.64  | 134.66      | 124.73   |
| 22  | B     | 1021 | CLA  | O2D-CGD-CBD | 5.64  | 121.08      | 111.23   |
| 22  | 8     | 609  | CLA  | O2D-CGD-CBD | 5.63  | 121.08      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 601  | CLA  | CMD-C2D-C1D | 5.63  | 134.64      | 124.73   |
| 22  | B     | 1214 | CLA  | O2D-CGD-CBD | 5.63  | 121.06      | 111.23   |
| 22  | Z     | 606  | CLA  | CMD-C2D-C1D | 5.61  | 134.61      | 124.73   |
| 40  | 2     | 613  | CHL  | C1B-CHB-C4A | 5.61  | 124.93      | 121.32   |
| 22  | 9     | 604  | CLA  | O2D-CGD-CBD | 5.61  | 121.04      | 111.23   |
| 22  | 9     | 603  | CLA  | CMD-C2D-C1D | 5.61  | 134.61      | 124.73   |
| 22  | 2     | 605  | CLA  | CMD-C2D-C1D | 5.60  | 134.60      | 124.73   |
| 22  | 1     | 604  | CLA  | CMD-C2D-C1D | 5.60  | 134.60      | 124.73   |
| 22  | 8     | 609  | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 37  | 5     | 505  | C7Z  | C38-C25-C26 | -5.60 | 118.37      | 124.48   |
| 37  | 5     | 505  | C7Z  | C15-C14-C13 | -5.60 | 119.43      | 127.28   |
| 36  | F     | 4001 | RRX  | C38-C26-C25 | -5.59 | 118.38      | 124.48   |
| 22  | Z     | 601  | CLA  | CMD-C2D-C1D | 5.59  | 134.56      | 124.73   |
| 39  | 9     | 502  | LUT  | C21-C26-C27 | 5.59  | 119.25      | 112.83   |
| 22  | 6     | 605  | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 22  | 1     | 603  | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 22  | 3     | 603  | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 22  | 1     | 615  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 22  | Z     | 608  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 22  | A     | 1120 | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 22  | 4     | 606  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 22  | 4     | 612  | CLA  | CMD-C2D-C1D | 5.57  | 134.54      | 124.73   |
| 22  | B     | 1229 | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 22  | 6     | 606  | CLA  | CMD-C2D-C1D | 5.56  | 134.52      | 124.73   |
| 22  | A     | 1122 | CLA  | CMD-C2D-C1D | 5.56  | 134.51      | 124.73   |
| 22  | 9     | 612  | CLA  | O2D-CGD-CBD | 5.55  | 120.94      | 111.23   |
| 22  | 6     | 603  | CLA  | CMD-C2D-C1D | 5.55  | 134.51      | 124.73   |
| 37  | J     | 4002 | C7Z  | C31-C30-C29 | -5.55 | 119.50      | 127.28   |
| 22  | F     | 1301 | CLA  | CMD-C2D-C1D | 5.55  | 134.50      | 124.73   |
| 42  | Z     | 504  | QTB  | C04-C03-C02 | 5.54  | 135.05      | 127.28   |
| 22  | 2     | 606  | CLA  | O2D-CGD-CBD | 5.54  | 120.92      | 111.23   |
| 22  | B     | 1224 | CLA  | O2D-CGD-CBD | 5.54  | 120.92      | 111.23   |
| 22  | 6     | 609  | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.73   |
| 42  | Z     | 504  | QTB  | C09-C02-C03 | 5.54  | 127.72      | 119.01   |
| 22  | Z     | 605  | CLA  | O2D-CGD-CBD | 5.53  | 120.91      | 111.23   |
| 22  | 6     | 619  | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 22  | 7     | 616  | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 22  | 5     | 606  | CLA  | CMD-C2D-C1D | 5.53  | 134.46      | 124.73   |
| 22  | G     | 1602 | CLA  | O2D-CGD-CBD | 5.53  | 120.89      | 111.23   |
| 22  | A     | 1105 | CLA  | CMD-C2D-C1D | 5.52  | 134.45      | 124.73   |
| 22  | A     | 1111 | CLA  | CMD-C2D-C1D | 5.52  | 134.45      | 124.73   |
| 22  | B     | 1202 | CLA  | CMD-C2D-C1D | 5.52  | 134.45      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | B     | 1235 | CLA  | CMD-C2D-C1D | 5.52 | 134.44      | 124.73   |
| 22  | B     | 1213 | CLA  | CMD-C2D-C1D | 5.51 | 134.44      | 124.73   |
| 22  | B     | 1211 | CLA  | CMD-C2D-C1D | 5.51 | 134.43      | 124.73   |
| 22  | A     | 1113 | CLA  | O2D-CGD-CBD | 5.51 | 120.86      | 111.23   |
| 22  | 5     | 603  | CLA  | CMD-C2D-C1D | 5.51 | 134.42      | 124.73   |
| 22  | A     | 1101 | CLA  | CMD-C2D-C1D | 5.50 | 134.42      | 124.73   |
| 22  | 5     | 612  | CLA  | CMD-C2D-C1D | 5.50 | 134.41      | 124.73   |
| 22  | A     | 1012 | CLA  | O2D-CGD-CBD | 5.50 | 120.85      | 111.23   |
| 25  | B     | 4005 | BCR  | C23-C22-C21 | 5.50 | 127.66      | 119.01   |
| 22  | 3     | 610  | CLA  | CMD-C2D-C1D | 5.49 | 134.40      | 124.73   |
| 22  | A     | 1137 | CLA  | CMD-C2D-C1D | 5.49 | 134.40      | 124.73   |
| 22  | 1     | 604  | CLA  | O2D-CGD-CBD | 5.49 | 120.83      | 111.23   |
| 22  | Z     | 603  | CLA  | CMD-C2D-C1D | 5.49 | 134.40      | 124.73   |
| 22  | 7     | 615  | CLA  | CMD-C2D-C1D | 5.49 | 134.39      | 124.73   |
| 22  | A     | 1102 | CLA  | CMD-C2D-C1D | 5.49 | 134.39      | 124.73   |
| 22  | A     | 1112 | CLA  | CMD-C2D-C1D | 5.49 | 134.39      | 124.73   |
| 22  | L     | 1503 | CLA  | CMD-C2D-C1D | 5.49 | 134.39      | 124.73   |
| 22  | 4     | 605  | CLA  | CMD-C2D-C1D | 5.48 | 134.38      | 124.73   |
| 22  | A     | 1130 | CLA  | CMD-C2D-C1D | 5.48 | 134.38      | 124.73   |
| 22  | Z     | 615  | CLA  | CMD-C2D-C1D | 5.48 | 134.38      | 124.73   |
| 22  | A     | 1132 | CLA  | CMD-C2D-C1D | 5.48 | 134.38      | 124.73   |
| 22  | A     | 1125 | CLA  | CMD-C2D-C1D | 5.48 | 134.38      | 124.73   |
| 22  | B     | 1216 | CLA  | CMD-C2D-C1D | 5.48 | 134.37      | 124.73   |
| 22  | 2     | 608  | CLA  | O2D-CGD-CBD | 5.48 | 120.80      | 111.23   |
| 22  | 1     | 613  | CLA  | CMD-C2D-C1D | 5.47 | 134.37      | 124.73   |
| 22  | 1     | 612  | CLA  | CMD-C2D-C1D | 5.47 | 134.37      | 124.73   |
| 22  | A     | 1108 | CLA  | CMD-C2D-C1D | 5.47 | 134.36      | 124.73   |
| 22  | B     | 1219 | CLA  | CMD-C2D-C1D | 5.46 | 134.35      | 124.73   |
| 22  | K     | 1401 | CLA  | CMD-C2D-C1D | 5.45 | 134.33      | 124.73   |
| 22  | 8     | 611  | CLA  | CMD-C2D-C1D | 5.45 | 134.33      | 124.73   |
| 22  | A     | 1141 | CLA  | CMD-C2D-C1D | 5.45 | 134.33      | 124.73   |
| 22  | B     | 1212 | CLA  | CMD-C2D-C1D | 5.45 | 134.33      | 124.73   |
| 22  | B     | 1208 | CLA  | CMD-C2D-C1D | 5.45 | 134.33      | 124.73   |
| 22  | B     | 1210 | CLA  | CMD-C2D-C1D | 5.45 | 134.32      | 124.73   |
| 22  | J     | 1901 | CLA  | CMD-C2D-C1D | 5.45 | 134.32      | 124.73   |
| 22  | A     | 1106 | CLA  | CMD-C2D-C1D | 5.45 | 134.32      | 124.73   |
| 22  | 5     | 606  | CLA  | O2D-CGD-CBD | 5.45 | 120.75      | 111.23   |
| 22  | 2     | 602  | CLA  | O2D-CGD-CBD | 5.45 | 120.75      | 111.23   |
| 22  | B     | 1231 | CLA  | O2D-CGD-CBD | 5.44 | 120.75      | 111.23   |
| 22  | 5     | 615  | CLA  | CMD-C2D-C1D | 5.44 | 134.31      | 124.73   |
| 22  | 7     | 603  | CLA  | CMD-C2D-C1D | 5.44 | 134.31      | 124.73   |
| 22  | B     | 1238 | CLA  | O2D-CGD-CBD | 5.44 | 120.74      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 602  | CLA  | O2D-CGD-CBD | 5.43  | 120.72      | 111.23   |
| 22  | B     | 1204 | CLA  | CMD-C2D-C1D | 5.43  | 134.29      | 124.73   |
| 22  | 1     | 602  | CLA  | O2D-CGD-CBD | 5.43  | 120.72      | 111.23   |
| 22  | 3     | 616  | CLA  | CMD-C2D-C1D | 5.43  | 134.29      | 124.73   |
| 22  | 2     | 607  | CLA  | CMD-C2D-C1D | 5.43  | 134.29      | 124.73   |
| 22  | A     | 1119 | CLA  | CMD-C2D-C1D | 5.43  | 134.28      | 124.73   |
| 22  | A     | 1103 | CLA  | CMD-C2D-C1D | 5.42  | 134.28      | 124.73   |
| 37  | 5     | 505  | C7Z  | C18-C5-C6   | -5.42 | 118.56      | 124.48   |
| 22  | B     | 1234 | CLA  | O2D-CGD-CBD | 5.42  | 120.71      | 111.23   |
| 36  | F     | 4001 | RRX  | C1-C6-C5    | -5.42 | 115.23      | 122.64   |
| 22  | 8     | 603  | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | 3     | 612  | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | B     | 1228 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | 8     | 604  | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | 4     | 608  | CLA  | CMD-C2D-C1D | 5.42  | 134.26      | 124.73   |
| 22  | A     | 1134 | CLA  | CMD-C2D-C1D | 5.41  | 134.26      | 124.73   |
| 22  | B     | 1203 | CLA  | CMD-C2D-C1D | 5.41  | 134.26      | 124.73   |
| 22  | 3     | 601  | CLA  | CMD-C2D-C1D | 5.41  | 134.26      | 124.73   |
| 22  | 4     | 604  | CLA  | CMD-C2D-C1D | 5.41  | 134.26      | 124.73   |
| 22  | 4     | 615  | CLA  | CMD-C2D-C1D | 5.41  | 134.26      | 124.73   |
| 22  | 1     | 601  | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | 1     | 606  | CLA  | O2D-CGD-CBD | 5.41  | 120.69      | 111.23   |
| 22  | 2     | 602  | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | 3     | 607  | CLA  | CMD-C2D-C1D | 5.40  | 134.25      | 124.73   |
| 22  | 9     | 608  | CLA  | CMD-C2D-C1D | 5.40  | 134.24      | 124.73   |
| 22  | 8     | 605  | CLA  | O2D-CGD-CBD | 5.40  | 120.67      | 111.23   |
| 22  | B     | 1240 | CLA  | CMD-C2D-C1D | 5.40  | 134.24      | 124.73   |
| 22  | A     | 1140 | CLA  | CMD-C2D-C1D | 5.39  | 134.23      | 124.73   |
| 36  | F     | 4001 | RRX  | C11-C10-C9  | -5.39 | 119.72      | 127.28   |
| 22  | K     | 1403 | CLA  | CMD-C2D-C1D | 5.39  | 134.22      | 124.73   |
| 40  | 8     | 610  | CHL  | C1B-CHB-C4A | 5.39  | 124.79      | 121.32   |
| 22  | B     | 1238 | CLA  | CMD-C2D-C1D | 5.39  | 134.22      | 124.73   |
| 22  | B     | 1211 | CLA  | O2D-CGD-CBD | 5.39  | 120.64      | 111.23   |
| 22  | B     | 1222 | CLA  | CMD-C2D-C1D | 5.38  | 134.21      | 124.73   |
| 22  | B     | 1209 | CLA  | CMD-C2D-C1D | 5.38  | 134.21      | 124.73   |
| 22  | B     | 1214 | CLA  | CMD-C2D-C1D | 5.38  | 134.21      | 124.73   |
| 22  | B     | 1218 | CLA  | O2D-CGD-CBD | 5.38  | 120.64      | 111.23   |
| 22  | 3     | 605  | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |
| 22  | B     | 1239 | CLA  | O2D-CGD-CBD | 5.38  | 120.63      | 111.23   |
| 22  | 5     | 608  | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |
| 22  | A     | 1129 | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |
| 22  | 5     | 602  | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22  | 7     | 613  | CLA  | CMD-C2D-C1D | 5.38 | 134.20      | 124.73   |
| 22  | G     | 1602 | CLA  | CMD-C2D-C1D | 5.37 | 134.19      | 124.73   |
| 22  | 7     | 611  | CLA  | CMD-C2D-C1D | 5.37 | 134.19      | 124.73   |
| 22  | 6     | 604  | CLA  | CMD-C2D-C1D | 5.37 | 134.19      | 124.73   |
| 22  | 7     | 608  | CLA  | CMD-C2D-C1D | 5.36 | 134.17      | 124.73   |
| 22  | A     | 1137 | CLA  | O2D-CGD-CBD | 5.36 | 120.60      | 111.23   |
| 22  | 9     | 606  | CLA  | O2D-CGD-CBD | 5.36 | 120.60      | 111.23   |
| 22  | 9     | 607  | CLA  | CMD-C2D-C1D | 5.36 | 134.17      | 124.73   |
| 22  | A     | 1116 | CLA  | O2D-CGD-CBD | 5.35 | 120.59      | 111.23   |
| 22  | A     | 1105 | CLA  | O2D-CGD-CBD | 5.35 | 120.58      | 111.23   |
| 22  | 8     | 606  | CLA  | CMD-C2D-C1D | 5.35 | 134.14      | 124.73   |
| 22  | 4     | 603  | CLA  | CMD-C2D-C1D | 5.34 | 134.14      | 124.73   |
| 22  | B     | 1215 | CLA  | O2D-CGD-CBD | 5.34 | 120.57      | 111.23   |
| 22  | J     | 1901 | CLA  | O2D-CGD-CBD | 5.34 | 120.56      | 111.23   |
| 22  | 2     | 608  | CLA  | CMD-C2D-C1D | 5.34 | 134.13      | 124.73   |
| 22  | 9     | 609  | CLA  | CMD-C2D-C1D | 5.34 | 134.13      | 124.73   |
| 22  | A     | 1110 | CLA  | O2D-CGD-CBD | 5.34 | 120.56      | 111.23   |
| 22  | Z     | 612  | CLA  | CMD-C2D-C1D | 5.33 | 134.12      | 124.73   |
| 22  | 9     | 601  | CLA  | CMD-C2D-C1D | 5.33 | 134.12      | 124.73   |
| 22  | 8     | 615  | CLA  | CMD-C2D-C1D | 5.33 | 134.11      | 124.73   |
| 22  | A     | 1136 | CLA  | CMD-C2D-C1D | 5.32 | 134.10      | 124.73   |
| 22  | 8     | 608  | CLA  | CMD-C2D-C1D | 5.32 | 134.10      | 124.73   |
| 22  | 4     | 602  | CLA  | CMD-C2D-C1D | 5.32 | 134.10      | 124.73   |
| 22  | A     | 1131 | CLA  | CMD-C2D-C1D | 5.32 | 134.10      | 124.73   |
| 22  | F     | 1302 | CLA  | CMD-C2D-C1D | 5.32 | 134.10      | 124.73   |
| 22  | K     | 1402 | CLA  | CMD-C2D-C1D | 5.32 | 134.10      | 124.73   |
| 22  | B     | 1236 | CLA  | CMD-C2D-C1D | 5.32 | 134.09      | 124.73   |
| 22  | 5     | 609  | CLA  | CMD-C2D-C1D | 5.32 | 134.09      | 124.73   |
| 22  | 7     | 609  | CLA  | CMD-C2D-C1D | 5.31 | 134.09      | 124.73   |
| 22  | 6     | 615  | CLA  | CMD-C2D-C1D | 5.31 | 134.09      | 124.73   |
| 22  | 1     | 605  | CLA  | O2D-CGD-CBD | 5.31 | 120.52      | 111.23   |
| 22  | 2     | 605  | CLA  | O2D-CGD-CBD | 5.31 | 120.52      | 111.23   |
| 22  | B     | 1219 | CLA  | O2D-CGD-CBD | 5.31 | 120.51      | 111.23   |
| 22  | 4     | 601  | CLA  | O2D-CGD-CBD | 5.31 | 120.51      | 111.23   |
| 22  | B     | 1207 | CLA  | CMD-C2D-C1D | 5.31 | 134.07      | 124.73   |
| 22  | 3     | 602  | CLA  | CMD-C2D-C1D | 5.31 | 134.07      | 124.73   |
| 22  | A     | 1129 | CLA  | O2D-CGD-CBD | 5.31 | 120.51      | 111.23   |
| 22  | B     | 1232 | CLA  | CMD-C2D-C1D | 5.30 | 134.07      | 124.73   |
| 22  | A     | 1116 | CLA  | CMD-C2D-C1D | 5.30 | 134.07      | 124.73   |
| 22  | A     | 1123 | CLA  | CMD-C2D-C1D | 5.30 | 134.07      | 124.73   |
| 22  | B     | 1235 | CLA  | O2D-CGD-CBD | 5.30 | 120.50      | 111.23   |
| 22  | 7     | 612  | CLA  | CMD-C2D-C1D | 5.30 | 134.06      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1218 | CLA  | CMD-C2D-C1D | 5.30  | 134.06      | 124.73   |
| 22  | A     | 1104 | CLA  | CMD-C2D-C1D | 5.30  | 134.06      | 124.73   |
| 22  | A     | 1114 | CLA  | O2D-CGD-CBD | 5.30  | 120.49      | 111.23   |
| 22  | G     | 1601 | CLA  | CMD-C2D-C1D | 5.29  | 134.05      | 124.73   |
| 22  | A     | 1139 | CLA  | CMD-C2D-C1D | 5.29  | 134.05      | 124.73   |
| 22  | B     | 1217 | CLA  | CMD-C2D-C1D | 5.29  | 134.05      | 124.73   |
| 37  | 5     | 505  | C7Z  | C11-C10-C9  | -5.29 | 119.86      | 127.28   |
| 22  | B     | 1239 | CLA  | CMD-C2D-C1D | 5.29  | 134.04      | 124.73   |
| 22  | 8     | 605  | CLA  | CMD-C2D-C1D | 5.29  | 134.04      | 124.73   |
| 22  | B     | 1209 | CLA  | O2D-CGD-CBD | 5.29  | 120.47      | 111.23   |
| 22  | 5     | 604  | CLA  | CMD-C2D-C1D | 5.28  | 134.03      | 124.73   |
| 22  | 6     | 602  | CLA  | O2D-CGD-CBD | 5.28  | 120.47      | 111.23   |
| 22  | 3     | 613  | CLA  | O2D-CGD-CBD | 5.28  | 120.46      | 111.23   |
| 22  | 7     | 601  | CLA  | O2D-CGD-CBD | 5.28  | 120.46      | 111.23   |
| 39  | 3     | 501  | LUT  | C21-C26-C27 | 5.28  | 118.89      | 112.83   |
| 22  | A     | 1121 | CLA  | O2D-CGD-CBD | 5.28  | 120.45      | 111.23   |
| 22  | 3     | 604  | CLA  | CMD-C2D-C1D | 5.26  | 134.00      | 124.73   |
| 22  | A     | 1104 | CLA  | O2D-CGD-CBD | 5.26  | 120.43      | 111.23   |
| 22  | 8     | 602  | CLA  | O2D-CGD-CBD | 5.26  | 120.43      | 111.23   |
| 22  | 2     | 603  | CLA  | CMD-C2D-C1D | 5.26  | 134.00      | 124.73   |
| 22  | 7     | 604  | CLA  | CMD-C2D-C1D | 5.26  | 133.99      | 124.73   |
| 22  | A     | 1126 | CLA  | CMD-C2D-C1D | 5.26  | 133.99      | 124.73   |
| 22  | 7     | 602  | CLA  | O2D-CGD-CBD | 5.26  | 120.42      | 111.23   |
| 22  | 5     | 613  | CLA  | O2D-CGD-CBD | 5.26  | 120.42      | 111.23   |
| 22  | 7     | 616  | CLA  | O2D-CGD-CBD | 5.26  | 120.42      | 111.23   |
| 22  | A     | 1110 | CLA  | CMD-C2D-C1D | 5.26  | 133.98      | 124.73   |
| 22  | A     | 1126 | CLA  | O2D-CGD-CBD | 5.25  | 120.42      | 111.23   |
| 21  | A     | 1011 | CL0  | O2A-CGA-O1A | -5.25 | 110.49      | 123.63   |
| 22  | 9     | 608  | CLA  | O2D-CGD-CBD | 5.25  | 120.40      | 111.23   |
| 22  | A     | 1135 | CLA  | CMD-C2D-C1D | 5.25  | 133.97      | 124.73   |
| 22  | 7     | 604  | CLA  | O2D-CGD-CBD | 5.24  | 120.40      | 111.23   |
| 22  | A     | 1131 | CLA  | O2D-CGD-CBD | 5.24  | 120.39      | 111.23   |
| 22  | 6     | 606  | CLA  | O2D-CGD-CBD | 5.24  | 120.39      | 111.23   |
| 22  | 2     | 612  | CLA  | CMD-C2D-C1D | 5.24  | 133.96      | 124.73   |
| 22  | B     | 1229 | CLA  | O2D-CGD-CBD | 5.24  | 120.39      | 111.23   |
| 22  | 1     | 613  | CLA  | O2D-CGD-CBD | 5.24  | 120.39      | 111.23   |
| 22  | 2     | 601  | CLA  | CMD-C2D-C1D | 5.24  | 133.95      | 124.73   |
| 22  | B     | 1022 | CLA  | CMD-C2D-C1D | 5.24  | 133.95      | 124.73   |
| 22  | A     | 1139 | CLA  | O2D-CGD-CBD | 5.23  | 120.38      | 111.23   |
| 22  | A     | 1133 | CLA  | CMD-C2D-C1D | 5.23  | 133.94      | 124.73   |
| 22  | A     | 1113 | CLA  | CMD-C2D-C1D | 5.23  | 133.94      | 124.73   |
| 22  | 8     | 611  | CLA  | O2D-CGD-CBD | 5.23  | 120.36      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 7     | 607  | CLA  | CMD-C2D-C1D | 5.22  | 133.93      | 124.73   |
| 22  | A     | 1138 | CLA  | CMD-C2D-C1D | 5.22  | 133.92      | 124.73   |
| 22  | B     | 1201 | CLA  | CMD-C2D-C1D | 5.22  | 133.92      | 124.73   |
| 22  | 3     | 608  | CLA  | O2D-CGD-CBD | 5.22  | 120.35      | 111.23   |
| 22  | 2     | 612  | CLA  | O2D-CGD-CBD | 5.22  | 120.35      | 111.23   |
| 22  | 5     | 608  | CLA  | O2D-CGD-CBD | 5.21  | 120.35      | 111.23   |
| 22  | K     | 1403 | CLA  | O2A-C1-C2   | 5.21  | 121.40      | 108.99   |
| 22  | Z     | 607  | CLA  | CMD-C2D-C1D | 5.20  | 133.89      | 124.73   |
| 22  | 9     | 604  | CLA  | CMD-C2D-C1D | 5.20  | 133.88      | 124.73   |
| 22  | 9     | 602  | CLA  | O2D-CGD-CBD | 5.20  | 120.31      | 111.23   |
| 37  | 5     | 505  | C7Z  | C7-C8-C9    | -5.19 | 118.56      | 126.23   |
| 22  | B     | 1215 | CLA  | CMD-C2D-C1D | 5.19  | 133.87      | 124.73   |
| 22  | B     | 1220 | CLA  | CMD-C2D-C1D | 5.19  | 133.87      | 124.73   |
| 22  | 6     | 612  | CLA  | CMD-C2D-C1D | 5.19  | 133.86      | 124.73   |
| 22  | B     | 1204 | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 22  | 3     | 602  | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 22  | B     | 1241 | CLA  | CMD-C2D-C1D | 5.18  | 133.85      | 124.73   |
| 22  | B     | 1236 | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 22  | Z     | 607  | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 22  | 2     | 601  | CLA  | O2D-CGD-CBD | 5.18  | 120.28      | 111.23   |
| 22  | 9     | 605  | CLA  | O2D-CGD-CBD | 5.18  | 120.28      | 111.23   |
| 22  | 8     | 604  | CLA  | O2D-CGD-CBD | 5.18  | 120.28      | 111.23   |
| 22  | L     | 1502 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 39  | 5     | 502  | LUT  | C21-C26-C27 | 5.17  | 118.77      | 112.83   |
| 22  | 7     | 613  | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | 5     | 602  | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | A     | 1128 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | B     | 1205 | CLA  | CMD-C2D-C1D | 5.17  | 133.83      | 124.73   |
| 22  | B     | 1230 | CLA  | CMD-C2D-C1D | 5.17  | 133.83      | 124.73   |
| 22  | 5     | 607  | CLA  | CMD-C2D-C1D | 5.16  | 133.82      | 124.73   |
| 22  | B     | 1201 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | 3     | 608  | CLA  | CMD-C2D-C1D | 5.16  | 133.81      | 124.73   |
| 22  | B     | 1206 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | B     | 1237 | CLA  | O2D-CGD-CBD | 5.15  | 120.24      | 111.23   |
| 22  | A     | 1118 | CLA  | CMD-C2D-C1D | 5.15  | 133.80      | 124.73   |
| 22  | B     | 1207 | CLA  | O2D-CGD-CBD | 5.15  | 120.23      | 111.23   |
| 22  | 5     | 607  | CLA  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 22  | 3     | 601  | CLA  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 22  | 5     | 601  | CLA  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 40  | 6     | 610  | CHL  | C1B-CHB-C4A | 5.14  | 124.63      | 121.32   |
| 22  | 1     | 601  | CLA  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 22  | K     | 1401 | CLA  | O2D-CGD-CBD | 5.14  | 120.21      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 37  | 1     | 503  | C7Z  | C38-C25-C26 | -5.13 | 118.88      | 124.48   |
| 22  | B     | 1234 | CLA  | CMD-C2D-C1D | 5.13  | 133.76      | 124.73   |
| 22  | 2     | 604  | CLA  | O2D-CGD-CBD | 5.13  | 120.20      | 111.23   |
| 22  | 4     | 605  | CLA  | O2D-CGD-CBD | 5.13  | 120.19      | 111.23   |
| 22  | B     | 1240 | CLA  | O2D-CGD-CBD | 5.12  | 120.17      | 111.23   |
| 22  | B     | 1223 | CLA  | CMD-C2D-C1D | 5.11  | 133.73      | 124.73   |
| 22  | Z     | 608  | CLA  | O2D-CGD-CBD | 5.11  | 120.17      | 111.23   |
| 22  | 6     | 602  | CLA  | CMD-C2D-C1D | 5.11  | 133.73      | 124.73   |
| 22  | 4     | 602  | CLA  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 22  | Z     | 604  | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 22  | 5     | 618  | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 22  | A     | 1117 | CLA  | CMD-C2D-C1D | 5.10  | 133.71      | 124.73   |
| 42  | Z     | 504  | QTB  | C13-C12-C11 | 5.10  | 122.21      | 112.57   |
| 22  | 1     | 611  | CLA  | O2D-CGD-CBD | 5.10  | 120.14      | 111.23   |
| 22  | 6     | 607  | CLA  | O2D-CGD-CBD | 5.09  | 120.14      | 111.23   |
| 22  | 8     | 607  | CLA  | CMD-C2D-C1D | 5.09  | 133.70      | 124.73   |
| 22  | 4     | 609  | CLA  | CMD-C2D-C1D | 5.09  | 133.69      | 124.73   |
| 22  | 8     | 606  | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 22  | 5     | 612  | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 22  | A     | 1130 | CLA  | O2D-CGD-CBD | 5.09  | 120.12      | 111.23   |
| 39  | Z     | 503  | LUT  | C11-C10-C9  | -5.08 | 120.15      | 127.28   |
| 22  | B     | 1227 | CLA  | CMD-C2D-C1D | 5.08  | 133.68      | 124.73   |
| 22  | B     | 1241 | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 22  | 3     | 616  | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 22  | 2     | 615  | CLA  | O2D-CGD-CBD | 5.07  | 120.10      | 111.23   |
| 22  | 3     | 606  | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | 4     | 607  | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | 8     | 602  | CLA  | CMD-C2D-C1D | 5.07  | 133.65      | 124.73   |
| 22  | 1     | 607  | CLA  | CMD-C2D-C1D | 5.06  | 133.65      | 124.73   |
| 26  | 3     | 801  | LHG  | O7-C7-O9    | -5.06 | 119.21      | 125.70   |
| 22  | K     | 1403 | CLA  | O2D-CGD-CBD | 5.05  | 120.06      | 111.23   |
| 22  | 7     | 607  | CLA  | O2D-CGD-CBD | 5.05  | 120.05      | 111.23   |
| 22  | 6     | 607  | CLA  | CMD-C2D-C1D | 5.04  | 133.61      | 124.73   |
| 42  | Z     | 504  | QTB  | C01-C02-C09 | -5.04 | 110.39      | 118.09   |
| 22  | 8     | 612  | CLA  | CMD-C2D-C1D | 5.04  | 133.60      | 124.73   |
| 22  | 4     | 608  | CLA  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 22  | 5     | 622  | CLA  | O2D-CGD-CBD | 5.02  | 120.01      | 111.23   |
| 22  | 3     | 612  | CLA  | O2D-CGD-CBD | 5.02  | 120.00      | 111.23   |
| 22  | 6     | 618  | CLA  | O2D-CGD-CBD | 5.02  | 120.00      | 111.23   |
| 22  | Z     | 611  | CLA  | O2D-CGD-CBD | 5.01  | 120.00      | 111.23   |
| 22  | 3     | 605  | CLA  | O2D-CGD-CBD | 5.01  | 119.99      | 111.23   |
| 22  | 2     | 606  | CLA  | CMD-C2D-C1D | 5.00  | 133.53      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 606  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 22  | Z     | 602  | CLA  | CMD-C2D-C1D | 4.99  | 133.51      | 124.73   |
| 39  | 2     | 501  | LUT  | C27-C28-C29 | 4.99  | 137.05      | 126.32   |
| 22  | 4     | 603  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 22  | A     | 1125 | CLA  | O2D-CGD-CBD | 4.97  | 119.93      | 111.23   |
| 22  | 5     | 618  | CLA  | CMD-C2D-C1D | 4.97  | 133.48      | 124.73   |
| 22  | B     | 1224 | CLA  | CMD-C2D-C1D | 4.97  | 133.48      | 124.73   |
| 22  | 4     | 607  | CLA  | CMD-C2D-C1D | 4.97  | 133.47      | 124.73   |
| 40  | Z     | 609  | CHL  | C1C-CHC-C4B | 4.96  | 133.82      | 116.07   |
| 39  | Z     | 503  | LUT  | C21-C26-C27 | 4.96  | 118.52      | 112.83   |
| 22  | 7     | 602  | CLA  | CMD-C2D-C1D | 4.95  | 133.45      | 124.73   |
| 22  | Z     | 601  | CLA  | O2D-CGD-CBD | 4.95  | 119.88      | 111.23   |
| 22  | 9     | 609  | CLA  | O2D-CGD-CBD | 4.95  | 119.88      | 111.23   |
| 22  | A     | 1107 | CLA  | CMD-C2D-C1D | 4.95  | 133.44      | 124.73   |
| 22  | A     | 1107 | CLA  | O2D-CGD-CBD | 4.95  | 119.88      | 111.23   |
| 22  | A     | 1102 | CLA  | O2D-CGD-CBD | 4.94  | 119.87      | 111.23   |
| 39  | Z     | 502  | LUT  | C21-C26-C27 | 4.94  | 118.51      | 112.83   |
| 22  | A     | 1133 | CLA  | O2D-CGD-CBD | 4.94  | 119.87      | 111.23   |
| 37  | 1     | 503  | C7Z  | C27-C28-C29 | -4.94 | 118.93      | 126.23   |
| 22  | 9     | 601  | CLA  | O2D-CGD-CBD | 4.94  | 119.86      | 111.23   |
| 22  | 3     | 618  | CLA  | O2D-CGD-CBD | 4.93  | 119.86      | 111.23   |
| 22  | 6     | 601  | CLA  | O2D-CGD-CBD | 4.93  | 119.85      | 111.23   |
| 22  | 1     | 608  | CLA  | O2D-CGD-CBD | 4.93  | 119.85      | 111.23   |
| 22  | B     | 1223 | CLA  | O2D-CGD-CBD | 4.93  | 119.85      | 111.23   |
| 22  | 5     | 613  | CLA  | CMD-C2D-C1D | 4.93  | 133.40      | 124.73   |
| 22  | 9     | 602  | CLA  | CMD-C2D-C1D | 4.92  | 133.40      | 124.73   |
| 22  | A     | 1141 | CLA  | O2D-CGD-CBD | 4.92  | 119.84      | 111.23   |
| 22  | 7     | 615  | CLA  | O2D-CGD-CBD | 4.92  | 119.84      | 111.23   |
| 22  | B     | 1226 | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 39  | 7     | 502  | LUT  | C21-C26-C27 | 4.92  | 118.48      | 112.83   |
| 22  | B     | 1208 | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 22  | 8     | 603  | CLA  | O2A-C1-C2   | 4.92  | 127.03      | 108.11   |
| 39  | 7     | 501  | LUT  | C21-C26-C27 | 4.92  | 118.48      | 112.83   |
| 40  | 2     | 609  | CHL  | C1C-CHC-C4B | 4.91  | 133.66      | 116.07   |
| 22  | B     | 1022 | CLA  | O2D-CGD-CBD | 4.91  | 119.82      | 111.23   |
| 22  | 7     | 606  | CLA  | O2D-CGD-CBD | 4.91  | 119.81      | 111.23   |
| 40  | 4     | 610  | CHL  | C1C-CHC-C4B | 4.91  | 133.64      | 116.07   |
| 22  | 8     | 601  | CLA  | O2D-CGD-CBD | 4.90  | 119.79      | 111.23   |
| 22  | 5     | 609  | CLA  | O2D-CGD-CBD | 4.90  | 119.79      | 111.23   |
| 22  | 5     | 605  | CLA  | O2D-CGD-CBD | 4.89  | 119.79      | 111.23   |
| 22  | 6     | 603  | CLA  | O2A-C1-C2   | 4.89  | 126.92      | 108.11   |
| 26  | B     | 5002 | LHG  | O7-C7-O9    | -4.89 | 119.43      | 125.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1205 | CLA  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 22  | 7     | 611  | CLA  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 40  | 2     | 613  | CHL  | C1C-CHC-C4B | 4.88  | 133.53      | 116.07   |
| 22  | 6     | 612  | CLA  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 22  | B     | 1237 | CLA  | CMD-C2D-C1D | 4.87  | 133.31      | 124.73   |
| 40  | 8     | 610  | CHL  | C1C-CHC-C4B | 4.87  | 133.50      | 116.07   |
| 22  | L     | 1502 | CLA  | CMD-C2D-C1D | 4.87  | 133.30      | 124.73   |
| 22  | 3     | 604  | CLA  | O2D-CGD-CBD | 4.86  | 119.73      | 111.23   |
| 22  | B     | 1209 | CLA  | O2A-C1-C2   | 4.86  | 126.82      | 108.11   |
| 22  | G     | 1601 | CLA  | O2D-CGD-CBD | 4.86  | 119.73      | 111.23   |
| 22  | B     | 1216 | CLA  | O2D-CGD-CBD | 4.86  | 119.72      | 111.23   |
| 22  | 4     | 612  | CLA  | O2D-CGD-CBD | 4.86  | 119.72      | 111.23   |
| 22  | 1     | 602  | CLA  | CMD-C2D-C1D | 4.85  | 133.27      | 124.73   |
| 40  | 6     | 610  | CHL  | C1C-CHC-C4B | 4.84  | 133.41      | 116.07   |
| 22  | 3     | 603  | CLA  | O2D-CGD-CBD | 4.84  | 119.70      | 111.23   |
| 22  | 4     | 604  | CLA  | O2D-CGD-CBD | 4.84  | 119.69      | 111.23   |
| 22  | 8     | 615  | CLA  | O2D-CGD-CBD | 4.83  | 119.67      | 111.23   |
| 22  | L     | 1503 | CLA  | O2D-CGD-CBD | 4.82  | 119.67      | 111.23   |
| 22  | 8     | 607  | CLA  | O2D-CGD-CBD | 4.82  | 119.66      | 111.23   |
| 22  | A     | 1124 | CLA  | O2D-CGD-CBD | 4.82  | 119.66      | 111.23   |
| 40  | 7     | 610  | CHL  | C1C-CHC-C4B | 4.82  | 133.31      | 116.07   |
| 39  | 6     | 502  | LUT  | C21-C26-C27 | 4.81  | 118.36      | 112.83   |
| 22  | A     | 1136 | CLA  | O2D-CGD-CBD | 4.81  | 119.64      | 111.23   |
| 22  | Z     | 615  | CLA  | O2D-CGD-CBD | 4.81  | 119.64      | 111.23   |
| 21  | A     | 1011 | CL0  | O2A-CGA-CBA | 4.81  | 126.49      | 111.83   |
| 22  | A     | 1109 | CLA  | O2D-CGD-CBD | 4.81  | 119.63      | 111.23   |
| 22  | B     | 1228 | CLA  | O2D-CGD-CBD | 4.80  | 119.62      | 111.23   |
| 22  | B     | 1217 | CLA  | O2D-CGD-CBD | 4.80  | 119.62      | 111.23   |
| 22  | B     | 1203 | CLA  | O2D-CGD-CBD | 4.80  | 119.61      | 111.23   |
| 22  | B     | 1213 | CLA  | O2D-CGD-CBD | 4.80  | 119.61      | 111.23   |
| 22  | A     | 1123 | CLA  | O2D-CGD-CBD | 4.79  | 119.60      | 111.23   |
| 22  | 7     | 605  | CLA  | O2D-CGD-CBD | 4.78  | 119.58      | 111.23   |
| 22  | B     | 1227 | CLA  | O2D-CGD-CBD | 4.77  | 119.56      | 111.23   |
| 22  | 7     | 608  | CLA  | O2D-CGD-CBD | 4.76  | 119.56      | 111.23   |
| 22  | 6     | 605  | CLA  | O2D-CGD-CBD | 4.76  | 119.56      | 111.23   |
| 22  | 6     | 608  | CLA  | O2D-CGD-CBD | 4.76  | 119.55      | 111.23   |
| 22  | 4     | 615  | CLA  | O2D-CGD-CBD | 4.76  | 119.55      | 111.23   |
| 40  | 9     | 613  | CHL  | C1C-CHC-C4B | 4.75  | 133.07      | 116.07   |
| 40  | Z     | 610  | CHL  | C1C-CHC-C4B | 4.75  | 133.06      | 116.07   |
| 22  | A     | 1117 | CLA  | O2D-CGD-CBD | 4.75  | 119.53      | 111.23   |
| 25  | A     | 4004 | BCR  | C27-C26-C25 | -4.74 | 116.30      | 122.70   |
| 22  | B     | 1206 | CLA  | CMD-C2D-C1D | 4.74  | 133.07      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | F     | 1302 | CLA  | O2D-CGD-CBD | 4.73  | 119.51      | 111.23   |
| 22  | 3     | 606  | CLA  | O2A-C1-C2   | 4.73  | 126.30      | 108.11   |
| 22  | 5     | 603  | CLA  | O2D-CGD-CBD | 4.73  | 119.49      | 111.23   |
| 22  | 2     | 615  | CLA  | CMD-C2D-C1D | 4.73  | 133.05      | 124.73   |
| 22  | 1     | 607  | CLA  | O2D-CGD-CBD | 4.72  | 119.49      | 111.23   |
| 25  | B     | 4005 | BCR  | C37-C22-C21 | -4.72 | 115.17      | 122.82   |
| 22  | K     | 1404 | CLA  | CMD-C2D-C1D | 4.72  | 133.04      | 124.73   |
| 40  | 6     | 617  | CHL  | C1C-CHC-C4B | 4.71  | 132.94      | 116.07   |
| 22  | B     | 1225 | CLA  | CMD-C2D-C1D | 4.71  | 133.01      | 124.73   |
| 22  | 1     | 615  | CLA  | O2D-CGD-CBD | 4.70  | 119.45      | 111.23   |
| 40  | 4     | 610  | CHL  | C1B-CHB-C4A | 4.69  | 124.34      | 121.32   |
| 39  | 8     | 501  | LUT  | C21-C26-C27 | 4.69  | 118.21      | 112.83   |
| 22  | 6     | 604  | CLA  | O2D-CGD-CBD | 4.68  | 119.42      | 111.23   |
| 22  | 6     | 618  | CLA  | CMD-C2D-C1D | 4.68  | 132.97      | 124.73   |
| 40  | 4     | 617  | CHL  | C1C-CHC-C4B | 4.67  | 132.78      | 116.07   |
| 22  | 6     | 603  | CLA  | O2D-CGD-CBD | 4.66  | 119.38      | 111.23   |
| 42  | Z     | 504  | QTB  | C17-C11-C10 | 4.66  | 120.69      | 113.07   |
| 22  | 7     | 603  | CLA  | O2A-C1-C2   | 4.66  | 126.05      | 108.11   |
| 22  | A     | 1119 | CLA  | O2D-CGD-CBD | 4.66  | 119.38      | 111.23   |
| 22  | A     | 1140 | CLA  | O2D-CGD-CBD | 4.66  | 119.38      | 111.23   |
| 22  | 1     | 603  | CLA  | O2D-CGD-CBD | 4.66  | 119.37      | 111.23   |
| 22  | 8     | 603  | CLA  | O2D-CGD-CBD | 4.66  | 119.37      | 111.23   |
| 40  | 1     | 610  | CHL  | C1C-CHC-C4B | 4.65  | 132.71      | 116.07   |
| 22  | A     | 1103 | CLA  | O2D-CGD-CBD | 4.65  | 119.36      | 111.23   |
| 40  | 2     | 609  | CHL  | C1B-CHB-C4A | 4.65  | 124.31      | 121.32   |
| 22  | 2     | 607  | CLA  | O2D-CGD-CBD | 4.63  | 119.32      | 111.23   |
| 22  | B     | 1232 | CLA  | O2D-CGD-CBD | 4.63  | 119.32      | 111.23   |
| 40  | 4     | 611  | CHL  | C1C-CHC-C4B | 4.62  | 132.62      | 116.07   |
| 40  | 2     | 610  | CHL  | C1C-CHC-C4B | 4.62  | 132.61      | 116.07   |
| 25  | 3     | 504  | BCR  | C4-C5-C6    | -4.62 | 116.46      | 122.70   |
| 40  | 6     | 613  | CHL  | C1C-CHC-C4B | 4.62  | 132.59      | 116.07   |
| 22  | 1     | 612  | CLA  | O2D-CGD-CBD | 4.61  | 119.30      | 111.23   |
| 22  | 7     | 603  | CLA  | O2D-CGD-CBD | 4.61  | 119.28      | 111.23   |
| 37  | J     | 4002 | C7Z  | C11-C12-C13 | -4.60 | 113.76      | 126.36   |
| 37  | 1     | 503  | C7Z  | C15-C14-C13 | -4.59 | 120.84      | 127.28   |
| 40  | 6     | 611  | CHL  | C1C-CHC-C4B | 4.59  | 132.50      | 116.07   |
| 40  | 9     | 610  | CHL  | C1C-CHC-C4B | 4.59  | 132.49      | 116.07   |
| 37  | J     | 4002 | C7Z  | C35-C34-C33 | -4.58 | 120.85      | 127.28   |
| 40  | Z     | 613  | CHL  | C1C-CHC-C4B | 4.58  | 132.47      | 116.07   |
| 40  | 5     | 611  | CHL  | C1C-CHC-C4B | 4.58  | 132.44      | 116.07   |
| 22  | B     | 1213 | CLA  | O2A-C1-C2   | 4.57  | 125.69      | 108.11   |
| 22  | Z     | 603  | CLA  | O2D-CGD-CBD | 4.57  | 119.22      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26  | 4     | 801  | LHG  | O7-C7-C8    | 4.57  | 121.36      | 111.48   |
| 22  | 3     | 618  | CLA  | CMD-C2D-C1D | 4.56  | 132.77      | 124.73   |
| 40  | 8     | 613  | CHL  | C1C-CHC-C4B | 4.56  | 132.38      | 116.07   |
| 37  | J     | 4002 | C7Z  | C18-C5-C6   | -4.56 | 119.51      | 124.48   |
| 37  | 1     | 503  | C7Z  | C21-C26-C25 | -4.55 | 116.42      | 122.64   |
| 22  | 8     | 612  | CLA  | O2D-CGD-CBD | 4.55  | 119.18      | 111.23   |
| 22  | 9     | 607  | CLA  | O2D-CGD-CBD | 4.54  | 119.17      | 111.23   |
| 22  | 7     | 612  | CLA  | O2D-CGD-CBD | 4.54  | 119.16      | 111.23   |
| 40  | 5     | 610  | CHL  | C1C-CHC-C4B | 4.54  | 132.30      | 116.07   |
| 40  | 5     | 617  | CHL  | C1C-CHC-C4B | 4.54  | 132.30      | 116.07   |
| 22  | A     | 1012 | CLA  | CMD-C2D-C1D | 4.54  | 132.72      | 124.73   |
| 37  | J     | 4002 | C7Z  | C27-C28-C29 | -4.53 | 119.53      | 126.23   |
| 22  | 2     | 604  | CLA  | C1-C2-C3    | -4.53 | 118.78      | 126.20   |
| 26  | 6     | 801  | LHG  | O7-C7-C8    | 4.52  | 121.26      | 111.48   |
| 22  | 2     | 604  | CLA  | O2A-C1-C2   | 4.51  | 125.48      | 108.11   |
| 22  | A     | 1127 | CLA  | O2D-CGD-CBD | 4.51  | 119.12      | 111.23   |
| 22  | 7     | 601  | CLA  | O2A-C1-C2   | 4.51  | 125.46      | 108.11   |
| 26  | 1     | 801  | LHG  | O7-C7-C8    | 4.50  | 121.22      | 111.48   |
| 22  | B     | 1023 | CLA  | CMD-C2D-C1D | 4.50  | 132.66      | 124.73   |
| 43  | 2     | 802  | 3PH  | O21-C21-C22 | 4.50  | 121.22      | 111.48   |
| 40  | 1     | 609  | CHL  | C1C-CHC-C4B | 4.50  | 132.18      | 116.07   |
| 22  | B     | 1205 | CLA  | O2A-C1-C2   | 4.50  | 125.43      | 108.11   |
| 36  | F     | 4001 | RRX  | C7-C8-C9    | -4.50 | 119.58      | 126.23   |
| 40  | 4     | 613  | CHL  | C1C-CHC-C4B | 4.50  | 132.16      | 116.07   |
| 22  | 3     | 603  | CLA  | O2A-C1-C2   | 4.50  | 125.41      | 108.11   |
| 22  | 5     | 603  | CLA  | O2A-C1-C2   | 4.49  | 125.39      | 108.11   |
| 22  | 5     | 604  | CLA  | O2D-CGD-CBD | 4.49  | 119.08      | 111.23   |
| 22  | Z     | 612  | CLA  | O2D-CGD-CBD | 4.49  | 119.08      | 111.23   |
| 25  | I     | 4001 | BCR  | C23-C24-C25 | -4.49 | 115.01      | 127.00   |
| 39  | 4     | 502  | LUT  | C21-C26-C27 | 4.48  | 117.98      | 112.83   |
| 37  | 1     | 503  | C7Z  | C18-C5-C6   | -4.48 | 119.60      | 124.48   |
| 22  | A     | 1124 | CLA  | CMD-C2D-C1D | 4.47  | 132.60      | 124.73   |
| 26  | Z     | 801  | LHG  | O7-C7-C8    | 4.47  | 121.15      | 111.48   |
| 26  | B     | 5001 | LHG  | O7-C7-C8    | 4.46  | 121.14      | 111.48   |
| 22  | B     | 1021 | CLA  | CMD-C2D-C1D | 4.46  | 132.58      | 124.73   |
| 42  | Z     | 504  | QTB  | C19-C17-C11 | -4.45 | 104.31      | 110.58   |
| 22  | A     | 1116 | CLA  | O2A-C1-C2   | 4.45  | 125.24      | 108.11   |
| 21  | A     | 1011 | CL0  | CBC-CAC-C3C | -4.45 | 106.50      | 112.87   |
| 22  | 7     | 603  | CLA  | C1-C2-C3    | -4.44 | 118.92      | 126.20   |
| 22  | 8     | 608  | CLA  | O2D-CGD-CBD | 4.43  | 118.97      | 111.23   |
| 40  | 3     | 611  | CHL  | C1C-CHC-C4B | 4.41  | 131.85      | 116.07   |
| 22  | B     | 1224 | CLA  | O2A-C1-C2   | 4.41  | 125.06      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 605  | CLA  | O2A-C1-C2   | 4.40  | 125.03      | 108.11   |
| 22  | B     | 1221 | CLA  | O2A-CGA-CBA | 4.40  | 125.24      | 111.83   |
| 25  | 3     | 504  | BCR  | C1-C6-C5    | -4.38 | 116.65      | 122.64   |
| 39  | 9     | 501  | LUT  | C7-C8-C9    | -4.38 | 119.76      | 126.23   |
| 22  | F     | 1301 | CLA  | O2D-CGD-CBD | 4.37  | 118.87      | 111.23   |
| 31  | J     | 5001 | LMG  | O7-C10-C11  | 4.37  | 120.93      | 111.48   |
| 26  | B     | 5006 | LHG  | O7-C7-C8    | 4.37  | 120.92      | 111.48   |
| 40  | 2     | 613  | CHL  | C3D-C4D-CHA | 4.37  | 115.17      | 108.54   |
| 39  | 5     | 501  | LUT  | C21-C26-C27 | 4.35  | 117.82      | 112.83   |
| 36  | F     | 4001 | RRX  | C33-C5-C6   | -4.34 | 119.74      | 124.48   |
| 26  | 2     | 801  | LHG  | O7-C7-C8    | 4.34  | 120.87      | 111.48   |
| 39  | 6     | 501  | LUT  | C35-C34-C33 | -4.34 | 121.19      | 127.28   |
| 40  | 3     | 611  | CHL  | C3D-C4D-CHA | 4.34  | 115.14      | 108.54   |
| 39  | Z     | 501  | LUT  | C21-C26-C27 | 4.32  | 117.80      | 112.83   |
| 40  | 6     | 610  | CHL  | C3D-C4D-CHA | 4.32  | 115.11      | 108.54   |
| 22  | A     | 1122 | CLA  | O2A-C1-C2   | 4.32  | 124.73      | 108.11   |
| 22  | A     | 1013 | CLA  | O2D-CGD-CBD | 4.32  | 118.78      | 111.23   |
| 40  | 5     | 611  | CHL  | C3D-C4D-CHA | 4.32  | 115.10      | 108.54   |
| 22  | 9     | 612  | CLA  | C1-C2-C3    | -4.31 | 119.78      | 126.76   |
| 22  | 7     | 604  | CLA  | O2A-C1-C2   | 4.31  | 124.70      | 108.11   |
| 22  | 4     | 603  | CLA  | O2A-C1-C2   | 4.30  | 124.67      | 108.11   |
| 22  | B     | 1235 | CLA  | O2A-C1-C2   | 4.30  | 124.67      | 108.11   |
| 39  | 9     | 501  | LUT  | C21-C26-C27 | 4.30  | 117.77      | 112.83   |
| 22  | 9     | 604  | CLA  | O2A-C1-C2   | 4.30  | 124.65      | 108.11   |
| 22  | A     | 1115 | CLA  | O2D-CGD-CBD | 4.29  | 118.73      | 111.23   |
| 22  | 2     | 601  | CLA  | O2A-C1-C2   | 4.29  | 124.61      | 108.11   |
| 39  | Z     | 503  | LUT  | C15-C14-C13 | -4.28 | 121.28      | 127.28   |
| 22  | 3     | 601  | CLA  | O2A-C1-C2   | 4.28  | 124.57      | 108.11   |
| 43  | 6     | 802  | 3PH  | O21-C21-C22 | 4.27  | 120.72      | 111.48   |
| 40  | 1     | 610  | CHL  | C3D-C4D-CHA | 4.27  | 115.03      | 108.54   |
| 40  | 2     | 609  | CHL  | C3D-C4D-CHA | 4.27  | 115.03      | 108.54   |
| 22  | A     | 1125 | CLA  | O2A-C1-C2   | 4.26  | 124.51      | 108.11   |
| 39  | 2     | 502  | LUT  | C21-C26-C27 | 4.26  | 117.72      | 112.83   |
| 22  | B     | 1214 | CLA  | O2A-C1-C2   | 4.26  | 124.50      | 108.11   |
| 32  | 9     | 802  | DGA  | OG2-CB1-CB2 | 4.26  | 120.69      | 111.48   |
| 40  | 4     | 610  | CHL  | C3D-C4D-CHA | 4.25  | 115.00      | 108.54   |
| 22  | 5     | 604  | CLA  | O2A-C1-C2   | 4.24  | 124.42      | 108.11   |
| 22  | 5     | 615  | CLA  | O2D-CGD-CBD | 4.24  | 118.64      | 111.23   |
| 21  | A     | 1011 | CL0  | CHA-C1A-C2A | -4.24 | 123.36      | 133.31   |
| 26  | 7     | 801  | LHG  | O7-C7-C8    | 4.24  | 120.65      | 111.48   |
| 22  | A     | 1110 | CLA  | O2A-C1-C2   | 4.24  | 124.41      | 108.11   |
| 40  | 1     | 609  | CHL  | C3D-C4D-CHA | 4.24  | 114.98      | 108.54   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | 2     | 501  | LUT  | C39-C29-C28 | 4.23  | 124.55      | 118.09   |
| 40  | Z     | 610  | CHL  | C3D-C4D-CHA | 4.23  | 114.97      | 108.54   |
| 39  | 7     | 502  | LUT  | C7-C8-C9    | -4.23 | 119.98      | 126.23   |
| 40  | 4     | 611  | CHL  | C3D-C4D-CHA | 4.23  | 114.97      | 108.54   |
| 40  | 5     | 617  | CHL  | C3D-C4D-CHA | 4.22  | 114.96      | 108.54   |
| 37  | J     | 4002 | C7Z  | C8-C7-C6    | -4.22 | 115.72      | 127.00   |
| 40  | 6     | 617  | CHL  | C3D-C4D-CHA | 4.22  | 114.96      | 108.54   |
| 22  | B     | 1211 | CLA  | O2A-C1-C2   | 4.22  | 124.33      | 108.11   |
| 40  | Z     | 609  | CHL  | C3D-C4D-CHA | 4.21  | 114.95      | 108.54   |
| 22  | B     | 1210 | CLA  | O2A-C1-C2   | 4.21  | 124.31      | 108.11   |
| 40  | 4     | 617  | CHL  | C3D-C4D-CHA | 4.21  | 114.94      | 108.54   |
| 26  | 5     | 801  | LHG  | O7-C7-C8    | 4.20  | 120.58      | 111.48   |
| 31  | A     | 5003 | LMG  | O7-C10-C11  | 4.20  | 120.57      | 111.48   |
| 22  | 6     | 601  | CLA  | O2A-C1-C2   | 4.20  | 124.26      | 108.11   |
| 22  | A     | 1128 | CLA  | O2A-C1-C2   | 4.20  | 124.25      | 108.11   |
| 22  | 6     | 604  | CLA  | O2A-C1-C2   | 4.19  | 124.22      | 108.11   |
| 22  | 9     | 601  | CLA  | O2A-C1-C2   | 4.19  | 124.22      | 108.11   |
| 22  | 2     | 601  | CLA  | C1-C2-C3    | -4.19 | 119.34      | 126.20   |
| 22  | 3     | 607  | CLA  | O2A-C1-C2   | 4.18  | 124.21      | 108.11   |
| 39  | 2     | 502  | LUT  | C11-C10-C9  | -4.18 | 121.41      | 127.28   |
| 26  | A     | 5001 | LHG  | O7-C7-C8    | 4.18  | 120.52      | 111.48   |
| 22  | 9     | 612  | CLA  | CMD-C2D-C1D | 4.17  | 132.08      | 124.73   |
| 22  | A     | 1012 | CLA  | O2A-C1-C2   | 4.17  | 124.16      | 108.11   |
| 22  | B     | 1225 | CLA  | O2D-CGD-CBD | 4.17  | 118.52      | 111.23   |
| 39  | 8     | 502  | LUT  | C21-C26-C27 | 4.16  | 117.61      | 112.83   |
| 37  | J     | 4002 | C7Z  | C21-C26-C25 | -4.16 | 116.95      | 122.64   |
| 40  | 5     | 610  | CHL  | C3D-C4D-CHA | 4.15  | 114.85      | 108.54   |
| 43  | 5     | 802  | 3PH  | O21-C21-C22 | 4.15  | 120.46      | 111.48   |
| 22  | B     | 1021 | CLA  | C1-C2-C3    | -4.14 | 119.41      | 126.20   |
| 39  | 2     | 503  | LUT  | C26-C27-C28 | 4.13  | 131.01      | 124.58   |
| 39  | Z     | 502  | LUT  | C7-C8-C9    | -4.13 | 120.13      | 126.23   |
| 40  | 6     | 611  | CHL  | C3D-C4D-CHA | 4.13  | 114.81      | 108.54   |
| 40  | 6     | 613  | CHL  | C3D-C4D-CHA | 4.13  | 114.81      | 108.54   |
| 22  | A     | 1122 | CLA  | O2D-CGD-CBD | 4.13  | 118.44      | 111.23   |
| 22  | A     | 1101 | CLA  | O2A-C1-C2   | 4.12  | 123.96      | 108.11   |
| 22  | 4     | 615  | CLA  | CAA-C2A-C3A | -4.12 | 106.78      | 116.23   |
| 40  | 2     | 610  | CHL  | C3D-C4D-CHA | 4.11  | 114.79      | 108.54   |
| 37  | 5     | 505  | C7Z  | C1-C6-C5    | -4.11 | 117.02      | 122.64   |
| 40  | 8     | 613  | CHL  | C3D-C4D-CHA | 4.10  | 114.78      | 108.54   |
| 22  | A     | 1115 | CLA  | CMD-C2D-C1D | 4.09  | 131.94      | 124.73   |
| 39  | 8     | 502  | LUT  | C35-C34-C33 | -4.09 | 121.54      | 127.28   |
| 22  | 8     | 609  | CLA  | O2A-C1-C2   | 4.09  | 123.85      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1204 | CLA  | O2A-C1-C2   | 4.09  | 123.85      | 108.11   |
| 39  | 8     | 501  | LUT  | C7-C8-C9    | -4.09 | 120.19      | 126.23   |
| 22  | A     | 1128 | CLA  | CMD-C2D-C1D | 4.08  | 131.92      | 124.73   |
| 37  | 5     | 505  | C7Z  | C35-C34-C33 | -4.08 | 121.55      | 127.28   |
| 39  | 1     | 502  | LUT  | C7-C8-C9    | -4.08 | 120.20      | 126.23   |
| 40  | 7     | 610  | CHL  | C3D-C4D-CHA | 4.07  | 114.73      | 108.54   |
| 22  | B     | 1023 | CLA  | O2A-C1-C2   | 4.06  | 123.74      | 108.11   |
| 25  | G     | 4001 | BCR  | C19-C18-C17 | 4.06  | 125.39      | 119.01   |
| 40  | 9     | 613  | CHL  | C3D-C4D-CHA | 4.05  | 114.70      | 108.54   |
| 40  | Z     | 613  | CHL  | C3D-C4D-CHA | 4.03  | 114.67      | 108.54   |
| 22  | A     | 1127 | CLA  | C1-C2-C3    | -4.03 | 119.59      | 126.20   |
| 39  | 2     | 503  | LUT  | C15-C14-C13 | -4.03 | 121.63      | 127.28   |
| 33  | B     | 5003 | DGD  | O2G-C1B-C2B | 4.03  | 120.19      | 111.48   |
| 22  | 9     | 603  | CLA  | O2A-C1-C2   | 4.02  | 123.59      | 108.11   |
| 25  | A     | 4003 | BCR  | C28-C27-C26 | -4.02 | 106.89      | 114.06   |
| 22  | 3     | 616  | CLA  | O2A-C1-C2   | 4.02  | 123.56      | 108.11   |
| 22  | A     | 1134 | CLA  | O2A-C1-C2   | 4.01  | 123.53      | 108.11   |
| 22  | 9     | 604  | CLA  | C3B-C4B-NB  | -4.00 | 106.95      | 110.53   |
| 21  | A     | 1011 | CL0  | CAA-C2A-C3A | -4.00 | 102.18      | 113.00   |
| 22  | Z     | 604  | CLA  | O2A-C1-C2   | 4.00  | 123.50      | 108.11   |
| 40  | 9     | 610  | CHL  | C3D-C4D-CHA | 4.00  | 114.61      | 108.54   |
| 39  | 1     | 502  | LUT  | C21-C26-C27 | 3.99  | 117.42      | 112.83   |
| 22  | 8     | 604  | CLA  | O2A-C1-C2   | 3.99  | 123.48      | 108.11   |
| 40  | 4     | 613  | CHL  | C3D-C4D-CHA | 3.99  | 114.61      | 108.54   |
| 40  | 8     | 610  | CHL  | C3D-C4D-CHA | 3.98  | 114.59      | 108.54   |
| 22  | B     | 1221 | CLA  | O2A-C1-C2   | 3.98  | 123.41      | 108.11   |
| 22  | 8     | 611  | CLA  | O2A-C1-C2   | 3.98  | 123.41      | 108.11   |
| 22  | B     | 1218 | CLA  | O2A-C1-C2   | 3.97  | 123.39      | 108.11   |
| 22  | B     | 1228 | CLA  | O2A-C1-C2   | 3.97  | 123.39      | 108.11   |
| 22  | 7     | 615  | CLA  | O2A-C1-C2   | 3.97  | 123.38      | 108.11   |
| 22  | B     | 1216 | CLA  | O2A-C1-C2   | 3.96  | 123.36      | 108.11   |
| 26  | 9     | 801  | LHG  | O7-C7-C8    | 3.95  | 120.03      | 111.48   |
| 35  | B     | 5004 | T7X  | O16-C10-C12 | 3.95  | 120.02      | 111.48   |
| 39  | 8     | 502  | LUT  | C26-C27-C28 | -3.94 | 118.44      | 124.58   |
| 22  | A     | 1117 | CLA  | O2A-C1-C2   | 3.94  | 123.28      | 108.11   |
| 22  | A     | 1108 | CLA  | O2D-CGD-CBD | 3.93  | 118.10      | 111.23   |
| 39  | 2     | 503  | LUT  | C27-C28-C29 | -3.92 | 117.88      | 126.32   |
| 39  | 7     | 502  | LUT  | C35-C34-C33 | -3.92 | 121.78      | 127.28   |
| 22  | 5     | 605  | CLA  | O2A-C1-C2   | 3.92  | 123.19      | 108.11   |
| 39  | 1     | 501  | LUT  | C21-C26-C27 | 3.92  | 117.33      | 112.83   |
| 22  | Z     | 611  | CLA  | O2A-C1-C2   | 3.91  | 123.17      | 108.11   |
| 26  | 8     | 801  | LHG  | O7-C7-C8    | 3.91  | 119.95      | 111.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1105 | CLA  | O2A-C1-C2   | 3.91  | 123.17      | 108.11   |
| 22  | 9     | 606  | CLA  | O2A-C1-C2   | 3.91  | 123.16      | 108.11   |
| 22  | 8     | 602  | CLA  | O2A-C1-C2   | 3.91  | 123.14      | 108.11   |
| 22  | A     | 1108 | CLA  | O2A-C1-C2   | 3.90  | 123.12      | 108.11   |
| 22  | L     | 1502 | CLA  | O2A-C1-C2   | 3.90  | 123.11      | 108.11   |
| 39  | 6     | 502  | LUT  | C15-C14-C13 | -3.89 | 121.82      | 127.28   |
| 39  | 2     | 502  | LUT  | C15-C14-C13 | -3.89 | 121.82      | 127.28   |
| 22  | A     | 1137 | CLA  | O2A-C1-C2   | 3.89  | 123.07      | 108.11   |
| 21  | A     | 1011 | CL0  | C1C-CHC-C4B | 3.89  | 129.98      | 116.07   |
| 25  | 5     | 504  | BCR  | C34-C9-C10  | -3.88 | 116.52      | 122.82   |
| 22  | 6     | 615  | CLA  | O2A-C1-C2   | 3.88  | 123.05      | 108.11   |
| 22  | 8     | 601  | CLA  | O2A-C1-C2   | 3.88  | 123.04      | 108.11   |
| 25  | I     | 4001 | BCR  | C27-C26-C25 | -3.88 | 117.46      | 122.70   |
| 39  | 7     | 501  | LUT  | C35-C34-C33 | -3.88 | 121.84      | 127.28   |
| 39  | 5     | 502  | LUT  | C15-C14-C13 | -3.88 | 121.84      | 127.28   |
| 22  | 8     | 605  | CLA  | O2A-C1-C2   | 3.87  | 123.02      | 108.11   |
| 22  | 6     | 606  | CLA  | O2A-C1-C2   | 3.87  | 123.02      | 108.11   |
| 27  | 3     | 802  | NKP  | OAA-PAC-OAF | -3.86 | 96.59       | 106.67   |
| 22  | 7     | 606  | CLA  | O2A-C1-C2   | 3.86  | 122.98      | 108.11   |
| 22  | B     | 1238 | CLA  | O2A-C1-C2   | 3.86  | 122.97      | 108.11   |
| 22  | B     | 1222 | CLA  | O2D-CGD-CBD | 3.86  | 117.98      | 111.23   |
| 22  | 5     | 615  | CLA  | O2A-C1-C2   | 3.86  | 122.96      | 108.11   |
| 32  | A     | 5005 | DGA  | OG2-CB1-CB2 | 3.86  | 119.83      | 111.48   |
| 22  | 2     | 605  | CLA  | O2A-C1-C2   | 3.86  | 122.96      | 108.11   |
| 22  | B     | 1208 | CLA  | O2A-C1-C2   | 3.86  | 122.95      | 108.11   |
| 39  | 8     | 502  | LUT  | C7-C8-C9    | -3.85 | 120.54      | 126.23   |
| 22  | B     | 1220 | CLA  | O2D-CGD-CBD | 3.85  | 117.95      | 111.23   |
| 22  | 4     | 604  | CLA  | O2A-C1-C2   | 3.84  | 122.90      | 108.11   |
| 22  | F     | 1301 | CLA  | C1-C2-C3    | -3.84 | 119.90      | 126.20   |
| 22  | 3     | 604  | CLA  | O2A-C1-C2   | 3.84  | 122.90      | 108.11   |
| 39  | 4     | 501  | LUT  | C35-C34-C33 | -3.84 | 121.89      | 127.28   |
| 22  | 4     | 602  | CLA  | O2A-C1-C2   | 3.84  | 122.87      | 108.11   |
| 26  | 4     | 802  | LHG  | O7-C7-C8    | 3.83  | 119.77      | 111.48   |
| 22  | A     | 1121 | CLA  | O2A-C1-C2   | 3.81  | 122.79      | 108.11   |
| 36  | F     | 4001 | RRX  | C20-C21-C22 | -3.81 | 121.93      | 127.28   |
| 22  | A     | 1104 | CLA  | O2A-C1-C2   | 3.81  | 122.78      | 108.11   |
| 22  | B     | 1212 | CLA  | O2A-C1-C2   | 3.80  | 122.75      | 108.11   |
| 22  | A     | 1013 | CLA  | CMD-C2D-C1D | 3.80  | 131.42      | 124.73   |
| 22  | B     | 1217 | CLA  | O2A-C1-C2   | 3.80  | 122.71      | 108.11   |
| 39  | 6     | 501  | LUT  | C7-C8-C9    | -3.79 | 120.62      | 126.23   |
| 39  | 7     | 502  | LUT  | C15-C14-C13 | -3.79 | 121.96      | 127.28   |
| 22  | B     | 1237 | CLA  | O2A-C1-C2   | 3.79  | 122.71      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1236 | CLA  | O2A-C1-C2   | 3.79  | 122.69      | 108.11   |
| 37  | J     | 4002 | C7Z  | C1-C6-C5    | -3.79 | 117.46      | 122.64   |
| 39  | Z     | 503  | LUT  | C31-C30-C29 | -3.79 | 121.96      | 127.28   |
| 22  | B     | 1226 | CLA  | O2A-C1-C2   | 3.79  | 122.68      | 108.11   |
| 22  | A     | 1138 | CLA  | O2A-C1-C2   | 3.78  | 122.67      | 108.11   |
| 39  | 2     | 501  | LUT  | C30-C31-C32 | -3.77 | 112.26      | 123.20   |
| 22  | B     | 1226 | CLA  | CMD-C2D-C3D | -3.77 | 119.03      | 127.69   |
| 21  | A     | 1011 | CL0  | O2A-C1-C2   | 3.77  | 122.61      | 108.11   |
| 37  | J     | 4002 | C7Z  | C38-C25-C26 | -3.77 | 120.38      | 124.48   |
| 22  | A     | 1130 | CLA  | O2A-C1-C2   | 3.75  | 122.54      | 108.11   |
| 42  | Z     | 504  | QTB  | C10-C09-C02 | -3.74 | 118.27      | 126.32   |
| 22  | B     | 1207 | CLA  | O2A-C1-C2   | 3.74  | 122.51      | 108.11   |
| 22  | 5     | 612  | CLA  | O2A-C1-C2   | 3.74  | 122.51      | 108.11   |
| 39  | Z     | 503  | LUT  | C18-C5-C6   | -3.74 | 120.40      | 124.48   |
| 22  | K     | 1402 | CLA  | O2A-C1-C2   | 3.74  | 122.50      | 108.11   |
| 22  | B     | 1230 | CLA  | O2A-C1-C2   | 3.73  | 122.48      | 108.11   |
| 36  | F     | 4001 | RRX  | C30-C25-C26 | -3.73 | 117.54      | 122.64   |
| 22  | 5     | 618  | CLA  | O2A-C1-C2   | 3.73  | 122.44      | 108.11   |
| 22  | A     | 1111 | CLA  | O2A-C1-C2   | 3.73  | 122.44      | 108.11   |
| 22  | A     | 1123 | CLA  | CMA-C3A-C4A | 3.72  | 121.78      | 111.77   |
| 22  | 5     | 603  | CLA  | O2A-CGA-CBA | 3.72  | 123.18      | 111.83   |
| 26  | A     | 5002 | LHG  | O7-C7-C8    | 3.72  | 119.53      | 111.48   |
| 39  | 9     | 501  | LUT  | C35-C34-C33 | -3.72 | 122.06      | 127.28   |
| 39  | 6     | 501  | LUT  | C35-C15-C14 | -3.72 | 115.91      | 123.52   |
| 22  | A     | 1115 | CLA  | O2A-C1-C2   | 3.72  | 122.41      | 108.11   |
| 39  | 3     | 501  | LUT  | C35-C34-C33 | -3.72 | 122.07      | 127.28   |
| 25  | B     | 4006 | BCR  | C19-C18-C17 | 3.72  | 124.85      | 119.01   |
| 22  | A     | 1132 | CLA  | O2A-C1-C2   | 3.71  | 122.40      | 108.11   |
| 40  | 6     | 610  | CHL  | C1-O2A-CGA  | 3.71  | 125.64      | 116.65   |
| 22  | B     | 1022 | CLA  | O2A-C1-C2   | 3.71  | 122.37      | 108.11   |
| 22  | 7     | 612  | CLA  | O2A-C1-C2   | 3.70  | 122.36      | 108.11   |
| 22  | 9     | 606  | CLA  | C1-C2-C3    | -3.70 | 120.77      | 126.76   |
| 22  | B     | 1240 | CLA  | O2A-C1-C2   | 3.70  | 122.36      | 108.11   |
| 22  | 4     | 608  | CLA  | O2A-C1-C2   | 3.70  | 122.35      | 108.11   |
| 22  | B     | 1210 | CLA  | C1-C2-C3    | -3.70 | 120.14      | 126.20   |
| 22  | 5     | 606  | CLA  | O2A-C1-C2   | 3.70  | 122.34      | 108.11   |
| 22  | A     | 1135 | CLA  | O2A-C1-C2   | 3.69  | 122.31      | 108.11   |
| 39  | 4     | 501  | LUT  | C7-C8-C9    | -3.69 | 120.78      | 126.23   |
| 43  | 7     | 802  | 3PH  | O21-C21-C22 | 3.69  | 119.46      | 111.48   |
| 22  | 2     | 603  | CLA  | O2A-C1-C2   | 3.69  | 122.30      | 108.11   |
| 22  | 7     | 616  | CLA  | O2A-C1-C2   | 3.68  | 122.28      | 108.11   |
| 22  | 1     | 605  | CLA  | O2A-C1-C2   | 3.68  | 122.27      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 37  | J     | 4002 | C7Z  | C31-C32-C33 | -3.68 | 116.28      | 126.36   |
| 22  | 6     | 609  | CLA  | O2A-C1-C2   | 3.68  | 122.26      | 108.11   |
| 22  | G     | 1601 | CLA  | C1-C2-C3    | -3.68 | 120.81      | 126.76   |
| 22  | 9     | 601  | CLA  | CAA-C2A-C3A | -3.68 | 103.06      | 113.00   |
| 22  | 4     | 601  | CLA  | O2A-C1-C2   | 3.67  | 122.25      | 108.11   |
| 22  | 8     | 603  | CLA  | C1-C2-C3    | -3.67 | 120.18      | 126.20   |
| 39  | 9     | 502  | LUT  | C26-C27-C28 | -3.67 | 118.86      | 124.58   |
| 22  | 1     | 605  | CLA  | C1-C2-C3    | -3.67 | 120.18      | 126.20   |
| 22  | A     | 1116 | CLA  | C3B-C4B-NB  | -3.67 | 107.25      | 110.53   |
| 22  | A     | 1102 | CLA  | O2A-CGA-CBA | 3.67  | 123.03      | 111.83   |
| 22  | A     | 1117 | CLA  | C1-C2-C3    | -3.67 | 120.19      | 126.20   |
| 39  | 1     | 502  | LUT  | C35-C34-C33 | -3.67 | 122.14      | 127.28   |
| 40  | 5     | 611  | CHL  | C4D-CHA-CBD | -3.67 | 105.27      | 108.97   |
| 22  | 7     | 602  | CLA  | C1-C2-C3    | -3.67 | 120.83      | 126.76   |
| 22  | 6     | 619  | CLA  | O2A-C1-C2   | 3.66  | 122.21      | 108.11   |
| 22  | 9     | 603  | CLA  | CAA-C2A-C3A | -3.66 | 103.10      | 113.00   |
| 22  | B     | 1241 | CLA  | C1-C2-C3    | -3.66 | 120.20      | 126.20   |
| 27  | A     | 5004 | NKP  | OAF-PAC-OAD | -3.66 | 96.55       | 106.44   |
| 22  | 9     | 604  | CLA  | CMA-C3A-C4A | 3.66  | 121.60      | 111.77   |
| 22  | 4     | 601  | CLA  | C1-C2-C3    | -3.66 | 120.21      | 126.20   |
| 22  | 7     | 612  | CLA  | C1-C2-C3    | -3.66 | 120.85      | 126.76   |
| 39  | Z     | 503  | LUT  | C26-C27-C28 | -3.65 | 118.89      | 124.58   |
| 22  | B     | 1241 | CLA  | CAA-C2A-C3A | -3.65 | 103.13      | 113.00   |
| 22  | 1     | 601  | CLA  | O2A-C1-C2   | 3.65  | 122.15      | 108.11   |
| 22  | 6     | 607  | CLA  | O2A-C1-C2   | 3.65  | 122.14      | 108.11   |
| 22  | 1     | 604  | CLA  | O2A-C1-C2   | 3.64  | 122.12      | 108.11   |
| 22  | B     | 1235 | CLA  | C1-O2A-CGA  | 3.64  | 125.45      | 116.65   |
| 40  | 4     | 610  | CHL  | C1A-CHA-C4D | 3.64  | 125.05      | 118.98   |
| 27  | 8     | 802  | NKP  | OAF-PAC-OAD | -3.63 | 96.62       | 106.44   |
| 22  | 1     | 612  | CLA  | O2A-C1-C2   | 3.63  | 122.09      | 108.11   |
| 22  | 7     | 602  | CLA  | O2A-C1-C2   | 3.63  | 122.09      | 108.11   |
| 22  | B     | 1202 | CLA  | O2A-C1-C2   | 3.63  | 122.08      | 108.11   |
| 22  | 9     | 603  | CLA  | CBA-CAA-C2A | 3.63  | 124.59      | 113.79   |
| 22  | 7     | 605  | CLA  | O2A-C1-C2   | 3.62  | 122.06      | 108.11   |
| 22  | L     | 1503 | CLA  | O2A-C1-C2   | 3.62  | 122.05      | 108.11   |
| 22  | 5     | 607  | CLA  | O2A-C1-C2   | 3.62  | 122.05      | 108.11   |
| 22  | A     | 1141 | CLA  | O2A-C1-C2   | 3.62  | 122.04      | 108.11   |
| 22  | A     | 1120 | CLA  | O2A-C1-C2   | 3.62  | 122.03      | 108.11   |
| 22  | B     | 1239 | CLA  | C2C-C1C-NC  | 3.62  | 113.78      | 109.98   |
| 39  | 5     | 501  | LUT  | C35-C15-C14 | -3.62 | 116.12      | 123.52   |
| 22  | Z     | 601  | CLA  | O2A-C1-C2   | 3.62  | 122.02      | 108.11   |
| 39  | 4     | 502  | LUT  | C35-C34-C33 | -3.61 | 122.22      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 2     | 612  | CLA  | O2A-C1-C2   | 3.61  | 122.00      | 108.11   |
| 22  | 1     | 607  | CLA  | O2A-C1-C2   | 3.61  | 121.99      | 108.11   |
| 22  | Z     | 612  | CLA  | O2A-C1-C2   | 3.61  | 121.99      | 108.11   |
| 22  | 8     | 607  | CLA  | O2A-C1-C2   | 3.60  | 121.98      | 108.11   |
| 22  | Z     | 608  | CLA  | O2A-C1-C2   | 3.60  | 121.97      | 108.11   |
| 25  | A     | 4004 | BCR  | C28-C27-C26 | -3.60 | 107.63      | 114.06   |
| 39  | 1     | 501  | LUT  | C35-C34-C33 | -3.60 | 122.23      | 127.28   |
| 39  | 2     | 503  | LUT  | C22-C23-C24 | -3.60 | 105.84      | 111.18   |
| 22  | 6     | 612  | CLA  | O2A-C1-C2   | 3.60  | 121.95      | 108.11   |
| 22  | Z     | 601  | CLA  | C1-C2-C3    | -3.59 | 120.31      | 126.20   |
| 22  | 4     | 607  | CLA  | O2A-C1-C2   | 3.59  | 121.92      | 108.11   |
| 22  | 9     | 607  | CLA  | O2A-C1-C2   | 3.59  | 121.92      | 108.11   |
| 22  | 7     | 611  | CLA  | O2A-C1-C2   | 3.59  | 121.91      | 108.11   |
| 22  | 6     | 608  | CLA  | O2A-C1-C2   | 3.58  | 121.90      | 108.11   |
| 22  | A     | 1107 | CLA  | O2A-C1-C2   | 3.58  | 121.89      | 108.11   |
| 22  | 4     | 612  | CLA  | O2A-C1-C2   | 3.58  | 121.89      | 108.11   |
| 39  | 9     | 502  | LUT  | C15-C14-C13 | -3.58 | 122.26      | 127.28   |
| 22  | B     | 1220 | CLA  | O2A-C1-C2   | 3.58  | 121.87      | 108.11   |
| 22  | A     | 1106 | CLA  | O2A-C1-C2   | 3.57  | 121.86      | 108.11   |
| 22  | 2     | 606  | CLA  | CMA-C3A-C4A | 3.57  | 121.38      | 111.77   |
| 22  | Z     | 606  | CLA  | O2A-C1-C2   | 3.57  | 121.85      | 108.11   |
| 22  | 1     | 606  | CLA  | O2A-C1-C2   | 3.57  | 121.84      | 108.11   |
| 25  | 7     | 504  | BCR  | C15-C14-C13 | -3.57 | 122.28      | 127.28   |
| 39  | Z     | 502  | LUT  | C35-C34-C33 | -3.57 | 122.28      | 127.28   |
| 22  | 5     | 609  | CLA  | O2A-C1-C2   | 3.56  | 121.81      | 108.11   |
| 22  | 3     | 603  | CLA  | O2A-CGA-CBA | 3.56  | 122.69      | 111.83   |
| 22  | B     | 1239 | CLA  | C1-C2-C3    | -3.56 | 120.37      | 126.20   |
| 22  | 8     | 606  | CLA  | O2A-C1-C2   | 3.56  | 121.80      | 108.11   |
| 22  | 6     | 612  | CLA  | C1-C2-C3    | -3.56 | 121.01      | 126.76   |
| 22  | 5     | 603  | CLA  | C1-C2-C3    | -3.56 | 120.37      | 126.20   |
| 22  | G     | 1601 | CLA  | O2A-C1-C2   | 3.55  | 121.78      | 108.11   |
| 22  | A     | 1104 | CLA  | C1-C2-C3    | -3.55 | 120.38      | 126.20   |
| 22  | 1     | 601  | CLA  | C1-C2-C3    | -3.55 | 120.38      | 126.20   |
| 39  | 2     | 501  | LUT  | C15-C14-C13 | -3.55 | 122.30      | 127.28   |
| 39  | Z     | 501  | LUT  | C7-C8-C9    | -3.55 | 120.98      | 126.23   |
| 25  | B     | 4006 | BCR  | C12-C13-C14 | -3.55 | 113.43      | 119.01   |
| 22  | 5     | 604  | CLA  | CMA-C3A-C4A | 3.55  | 121.31      | 111.77   |
| 22  | B     | 1239 | CLA  | C1C-C2C-C3C | -3.55 | 103.25      | 106.98   |
| 22  | B     | 1219 | CLA  | O2A-C1-C2   | 3.54  | 121.75      | 108.11   |
| 22  | Z     | 607  | CLA  | O2A-C1-C2   | 3.54  | 121.74      | 108.11   |
| 39  | Z     | 502  | LUT  | C26-C27-C28 | -3.54 | 119.07      | 124.58   |
| 39  | 3     | 501  | LUT  | C7-C8-C9    | -3.54 | 121.00      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1135 | CLA  | C3B-C4B-NB  | -3.54 | 107.37      | 110.53   |
| 22  | B     | 1202 | CLA  | CAA-C2A-C3A | -3.54 | 103.44      | 113.00   |
| 22  | 9     | 604  | CLA  | O2A-CGA-CBA | 3.53  | 122.61      | 111.83   |
| 22  | A     | 1140 | CLA  | C1-C2-C3    | -3.53 | 120.41      | 126.20   |
| 25  | A     | 4005 | BCR  | C23-C24-C25 | -3.53 | 117.56      | 127.00   |
| 22  | A     | 1106 | CLA  | C1-C2-C3    | -3.53 | 120.41      | 126.20   |
| 22  | 7     | 609  | CLA  | O2A-C1-C2   | 3.53  | 121.69      | 108.11   |
| 22  | A     | 1140 | CLA  | O2A-C1-C2   | 3.53  | 121.69      | 108.11   |
| 39  | 5     | 501  | LUT  | C35-C34-C33 | -3.53 | 122.33      | 127.28   |
| 22  | 9     | 606  | CLA  | C3B-C4B-NB  | -3.53 | 107.38      | 110.53   |
| 22  | 9     | 605  | CLA  | O2A-C1-C2   | 3.52  | 121.67      | 108.11   |
| 22  | B     | 1241 | CLA  | O2A-C1-C2   | 3.52  | 121.67      | 108.11   |
| 39  | Z     | 502  | LUT  | C15-C14-C13 | -3.52 | 122.34      | 127.28   |
| 22  | 6     | 603  | CLA  | O2A-CGA-CBA | 3.52  | 122.56      | 111.83   |
| 22  | 1     | 607  | CLA  | CAA-C2A-C3A | -3.51 | 103.50      | 113.00   |
| 22  | 4     | 603  | CLA  | C1-C2-C3    | -3.51 | 120.44      | 126.20   |
| 22  | A     | 1127 | CLA  | O2A-C1-C2   | 3.51  | 121.62      | 108.11   |
| 22  | A     | 1136 | CLA  | O2A-C1-C2   | 3.51  | 121.61      | 108.11   |
| 22  | A     | 1135 | CLA  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 22  | B     | 1212 | CLA  | C1-C2-C3    | -3.51 | 120.45      | 126.20   |
| 22  | A     | 1114 | CLA  | O2A-C1-C2   | 3.51  | 121.61      | 108.11   |
| 39  | 2     | 503  | LUT  | C31-C32-C33 | -3.51 | 116.75      | 126.36   |
| 22  | A     | 1122 | CLA  | C1-O2A-CGA  | 3.51  | 125.14      | 116.65   |
| 25  | L     | 4002 | BCR  | C33-C5-C6   | -3.50 | 120.66      | 124.48   |
| 37  | 5     | 505  | C7Z  | C27-C28-C29 | -3.50 | 121.05      | 126.23   |
| 22  | L     | 1502 | CLA  | CMA-C3A-C4A | 3.50  | 121.18      | 111.77   |
| 22  | Z     | 603  | CLA  | O2A-C1-C2   | 3.49  | 121.54      | 108.11   |
| 25  | B     | 4007 | BCR  | C23-C24-C25 | -3.49 | 117.68      | 127.00   |
| 22  | 5     | 602  | CLA  | O2A-C1-C2   | 3.48  | 121.51      | 108.11   |
| 22  | 3     | 604  | CLA  | CAA-C2A-C3A | -3.48 | 103.59      | 113.00   |
| 22  | A     | 1131 | CLA  | O2A-C1-C2   | 3.48  | 121.50      | 108.11   |
| 40  | 2     | 613  | CHL  | C1-C2-C3    | -3.48 | 121.13      | 126.76   |
| 22  | A     | 1112 | CLA  | O2A-C1-C2   | 3.48  | 121.49      | 108.11   |
| 22  | 6     | 602  | CLA  | O2A-C1-C2   | 3.48  | 121.48      | 108.11   |
| 22  | 4     | 609  | CLA  | O2A-C1-C2   | 3.48  | 121.48      | 108.11   |
| 22  | B     | 1231 | CLA  | O2A-C1-C2   | 3.47  | 121.48      | 108.11   |
| 22  | B     | 1223 | CLA  | O2A-C1-C2   | 3.47  | 121.47      | 108.11   |
| 22  | A     | 1102 | CLA  | O2A-C1-C2   | 3.47  | 121.47      | 108.11   |
| 22  | 5     | 604  | CLA  | C3B-C4B-NB  | -3.47 | 107.43      | 110.53   |
| 22  | 7     | 611  | CLA  | C1-C2-C3    | -3.47 | 121.15      | 126.76   |
| 22  | B     | 1240 | CLA  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 39  | Z     | 501  | LUT  | C35-C34-C33 | -3.47 | 122.42      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 5     | 618  | CLA  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 22  | 8     | 601  | CLA  | C1-C2-C3    | -3.46 | 120.52      | 126.20   |
| 22  | 6     | 604  | CLA  | O2A-CGA-CBA | 3.46  | 122.40      | 111.83   |
| 22  | 3     | 606  | CLA  | C1-O2A-CGA  | 3.46  | 125.03      | 116.65   |
| 22  | 1     | 611  | CLA  | O2A-C1-C2   | 3.46  | 121.43      | 108.11   |
| 25  | B     | 4005 | BCR  | C35-C13-C12 | 3.46  | 123.37      | 118.09   |
| 22  | 5     | 613  | CLA  | O2A-C1-C2   | 3.46  | 121.42      | 108.11   |
| 22  | 7     | 607  | CLA  | O2A-C1-C2   | 3.46  | 121.41      | 108.11   |
| 39  | 7     | 501  | LUT  | C7-C8-C9    | -3.46 | 121.12      | 126.23   |
| 22  | B     | 1206 | CLA  | O2A-C1-C2   | 3.45  | 121.40      | 108.11   |
| 22  | Z     | 605  | CLA  | O2A-C1-C2   | 3.45  | 121.39      | 108.11   |
| 22  | 6     | 607  | CLA  | C1-C2-C3    | -3.45 | 120.54      | 126.20   |
| 22  | A     | 1118 | CLA  | O2A-C1-C2   | 3.45  | 121.39      | 108.11   |
| 22  | 2     | 605  | CLA  | C1-C2-C3    | -3.45 | 121.18      | 126.76   |
| 25  | B     | 4002 | BCR  | C33-C5-C6   | -3.45 | 120.72      | 124.48   |
| 22  | 3     | 604  | CLA  | O2A-CGA-CBA | 3.45  | 122.34      | 111.83   |
| 39  | 3     | 502  | LUT  | C15-C14-C13 | -3.45 | 122.44      | 127.28   |
| 22  | B     | 1234 | CLA  | O2A-C1-C2   | 3.44  | 121.34      | 108.11   |
| 36  | F     | 4001 | RRX  | C24-C23-C22 | -3.44 | 121.15      | 126.23   |
| 36  | F     | 4001 | RRX  | C16-C17-C18 | -3.44 | 122.46      | 127.28   |
| 22  | 6     | 609  | CLA  | C1-C2-C3    | -3.43 | 120.57      | 126.20   |
| 22  | 3     | 613  | CLA  | O2A-C1-C2   | 3.43  | 121.31      | 108.11   |
| 22  | A     | 1129 | CLA  | O2A-C1-C2   | 3.43  | 121.31      | 108.11   |
| 22  | 4     | 606  | CLA  | O2A-C1-C2   | 3.43  | 121.31      | 108.11   |
| 22  | 1     | 608  | CLA  | O2A-C1-C2   | 3.43  | 121.30      | 108.11   |
| 37  | 1     | 503  | C7Z  | C8-C7-C6    | -3.43 | 117.84      | 127.00   |
| 22  | 6     | 603  | CLA  | CBA-CAA-C2A | 3.43  | 123.99      | 113.79   |
| 22  | B     | 1226 | CLA  | C2C-C1C-NC  | 3.42  | 113.58      | 109.98   |
| 22  | B     | 1225 | CLA  | O2A-C1-C2   | 3.42  | 121.28      | 108.11   |
| 22  | A     | 1130 | CLA  | C1-C2-C3    | -3.42 | 120.60      | 126.20   |
| 22  | 5     | 606  | CLA  | C1-C2-C3    | -3.42 | 121.23      | 126.76   |
| 22  | B     | 1229 | CLA  | C3B-C4B-NB  | -3.42 | 107.48      | 110.53   |
| 22  | 3     | 605  | CLA  | O2A-C1-C2   | 3.42  | 121.25      | 108.11   |
| 25  | A     | 4003 | BCR  | C27-C26-C25 | -3.41 | 118.09      | 122.70   |
| 39  | 5     | 501  | LUT  | C7-C8-C9    | -3.41 | 121.18      | 126.23   |
| 37  | 5     | 505  | C7Z  | C31-C30-C29 | -3.41 | 122.50      | 127.28   |
| 25  | 5     | 504  | BCR  | C19-C18-C17 | 3.41  | 124.37      | 119.01   |
| 22  | B     | 1223 | CLA  | C1-C2-C3    | -3.41 | 120.62      | 126.20   |
| 40  | 8     | 610  | CHL  | CHA-C1A-C2A | -3.40 | 125.32      | 133.31   |
| 22  | A     | 1127 | CLA  | CMD-C2D-C1D | 3.40  | 130.72      | 124.73   |
| 22  | A     | 1121 | CLA  | CMA-C3A-C4A | 3.40  | 120.92      | 111.77   |
| 22  | 9     | 607  | CLA  | C1-C2-C3    | -3.40 | 120.62      | 126.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 1     | 603  | CLA  | CMA-C3A-C4A | 3.40  | 120.92      | 111.77   |
| 22  | A     | 1115 | CLA  | C1-C2-C3    | -3.40 | 120.63      | 126.20   |
| 22  | 1     | 615  | CLA  | O2A-C1-C2   | 3.39  | 121.17      | 108.11   |
| 22  | 9     | 612  | CLA  | O2A-C1-C2   | 3.39  | 121.17      | 108.11   |
| 22  | A     | 1110 | CLA  | O2A-CGA-CBA | 3.39  | 122.17      | 111.83   |
| 39  | 4     | 502  | LUT  | C18-C5-C6   | -3.39 | 120.79      | 124.48   |
| 22  | 5     | 601  | CLA  | O2A-C1-C2   | 3.38  | 121.12      | 108.11   |
| 25  | 3     | 506  | BCR  | C33-C5-C6   | -3.38 | 120.80      | 124.48   |
| 22  | A     | 1134 | CLA  | C1-C2-C3    | -3.38 | 120.66      | 126.20   |
| 22  | 6     | 602  | CLA  | C1-C2-C3    | -3.38 | 120.66      | 126.20   |
| 40  | 4     | 610  | CHL  | CHA-C1A-C2A | -3.38 | 125.37      | 133.31   |
| 22  | 3     | 612  | CLA  | O2A-C1-C2   | 3.38  | 121.10      | 108.11   |
| 22  | 2     | 612  | CLA  | C1-C2-C3    | -3.37 | 121.30      | 126.76   |
| 22  | K     | 1404 | CLA  | O2A-C1-C2   | 3.37  | 121.09      | 108.11   |
| 22  | A     | 1111 | CLA  | C1-C2-C3    | -3.37 | 120.67      | 126.20   |
| 22  | B     | 1229 | CLA  | O2A-C1-C2   | 3.37  | 121.08      | 108.11   |
| 39  | 2     | 501  | LUT  | C7-C8-C9    | -3.37 | 121.25      | 126.23   |
| 22  | K     | 1402 | CLA  | C1-C2-C3    | -3.37 | 120.67      | 126.20   |
| 25  | 3     | 504  | BCR  | C33-C5-C4   | 3.37  | 120.78      | 113.60   |
| 22  | 9     | 605  | CLA  | C1-C2-C3    | -3.37 | 120.68      | 126.20   |
| 25  | 5     | 504  | BCR  | C8-C9-C10   | 3.37  | 124.30      | 119.01   |
| 22  | A     | 1109 | CLA  | O2A-C1-C2   | 3.36  | 121.05      | 108.11   |
| 22  | A     | 1113 | CLA  | C1-C2-C3    | -3.36 | 120.69      | 126.20   |
| 39  | 3     | 502  | LUT  | C35-C34-C33 | -3.36 | 122.57      | 127.28   |
| 22  | A     | 1113 | CLA  | O2D-CGD-O1D | -3.36 | 117.31      | 123.85   |
| 22  | B     | 1234 | CLA  | C1-C2-C3    | -3.36 | 120.70      | 126.20   |
| 22  | A     | 1012 | CLA  | C3B-C4B-NB  | -3.35 | 107.54      | 110.53   |
| 39  | 8     | 501  | LUT  | C35-C34-C33 | -3.35 | 122.58      | 127.28   |
| 22  | 6     | 619  | CLA  | C1-C2-C3    | -3.35 | 120.71      | 126.20   |
| 22  | A     | 1123 | CLA  | C2C-C1C-NC  | 3.35  | 113.50      | 109.98   |
| 39  | 2     | 503  | LUT  | C7-C8-C9    | 3.34  | 131.18      | 126.23   |
| 40  | 8     | 610  | CHL  | C1A-CHA-C4D | 3.34  | 124.56      | 118.98   |
| 22  | 8     | 603  | CLA  | CBA-CAA-C2A | 3.34  | 123.74      | 113.79   |
| 22  | A     | 1126 | CLA  | O2A-C1-C2   | 3.34  | 120.96      | 108.11   |
| 22  | A     | 1113 | CLA  | O2A-C1-C2   | 3.34  | 120.96      | 108.11   |
| 22  | Z     | 608  | CLA  | C1-C2-C3    | -3.34 | 120.73      | 126.20   |
| 22  | 4     | 606  | CLA  | C1-C2-C3    | -3.33 | 121.38      | 126.76   |
| 39  | 4     | 502  | LUT  | C26-C27-C28 | -3.33 | 119.40      | 124.58   |
| 22  | B     | 1236 | CLA  | C1-C2-C3    | -3.33 | 120.75      | 126.20   |
| 22  | A     | 1124 | CLA  | O2A-C1-C2   | 3.33  | 120.91      | 108.11   |
| 40  | 4     | 613  | CHL  | C1-O2A-CGA  | 3.33  | 124.70      | 116.65   |
| 25  | B     | 4003 | BCR  | C23-C22-C21 | 3.32  | 124.24      | 119.01   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 604  | CLA  | C1-C2-C3    | -3.32 | 120.75      | 126.20   |
| 22  | 3     | 607  | CLA  | C1-O2A-CGA  | 3.32  | 124.69      | 116.65   |
| 39  | Z     | 503  | LUT  | C31-C32-C33 | -3.32 | 117.27      | 126.36   |
| 28  | B     | 6101 | LMT  | C1'-O5'-C5' | -3.32 | 107.24      | 113.72   |
| 22  | 8     | 608  | CLA  | O2A-C1-C2   | 3.32  | 120.87      | 108.11   |
| 39  | 5     | 502  | LUT  | C26-C27-C28 | -3.31 | 119.42      | 124.58   |
| 33  | B     | 5003 | DGD  | O1G-C1A-C2A | 3.31  | 121.93      | 111.83   |
| 25  | 6     | 504  | BCR  | C19-C18-C17 | 3.31  | 124.21      | 119.01   |
| 22  | 4     | 612  | CLA  | C1-C2-C3    | -3.31 | 121.41      | 126.76   |
| 22  | 4     | 605  | CLA  | O2A-C1-C2   | 3.31  | 120.84      | 108.11   |
| 28  | 8     | 805  | LMT  | C1'-O5'-C5' | -3.31 | 107.26      | 113.72   |
| 22  | 7     | 604  | CLA  | O2A-CGA-CBA | 3.30  | 121.91      | 111.83   |
| 25  | K     | 4001 | BCR  | C28-C27-C26 | -3.30 | 108.17      | 114.06   |
| 39  | 6     | 501  | LUT  | C18-C5-C6   | -3.30 | 120.89      | 124.48   |
| 22  | 6     | 606  | CLA  | C1-C2-C3    | -3.30 | 120.80      | 126.20   |
| 22  | 7     | 606  | CLA  | C1-C2-C3    | -3.29 | 120.80      | 126.20   |
| 22  | B     | 1215 | CLA  | C1C-C2C-C3C | -3.29 | 103.52      | 106.98   |
| 22  | A     | 1129 | CLA  | C1-C2-C3    | -3.29 | 121.44      | 126.76   |
| 22  | 7     | 616  | CLA  | O2A-CGA-CBA | 3.29  | 121.86      | 111.83   |
| 39  | 2     | 501  | LUT  | C35-C34-C33 | -3.29 | 122.67      | 127.28   |
| 39  | 7     | 502  | LUT  | C10-C11-C12 | -3.29 | 113.67      | 123.20   |
| 22  | 5     | 604  | CLA  | O2A-CGA-CBA | 3.29  | 121.86      | 111.83   |
| 22  | B     | 1215 | CLA  | O2A-C1-C2   | 3.29  | 120.75      | 108.11   |
| 25  | 5     | 504  | BCR  | C36-C18-C17 | -3.29 | 117.49      | 122.82   |
| 22  | 4     | 602  | CLA  | O2A-CGA-CBA | 3.29  | 121.85      | 111.83   |
| 22  | 7     | 603  | CLA  | CAA-C2A-C3A | -3.28 | 104.12      | 113.00   |
| 22  | 2     | 603  | CLA  | CAA-C2A-C3A | -3.28 | 104.13      | 113.00   |
| 22  | A     | 1132 | CLA  | C1-C2-C3    | -3.28 | 120.82      | 126.20   |
| 22  | 8     | 608  | CLA  | C1-C2-C3    | -3.28 | 120.82      | 126.20   |
| 22  | 3     | 612  | CLA  | C1-C2-C3    | -3.28 | 120.82      | 126.20   |
| 25  | A     | 4005 | BCR  | C12-C13-C14 | -3.28 | 113.85      | 119.01   |
| 22  | 8     | 605  | CLA  | C1-C2-C3    | -3.28 | 120.82      | 126.20   |
| 22  | 3     | 610  | CLA  | O2A-C1-C2   | 3.28  | 120.73      | 108.11   |
| 22  | A     | 1131 | CLA  | C1-C2-C3    | -3.28 | 120.83      | 126.20   |
| 22  | 3     | 610  | CLA  | C2C-C1C-NC  | 3.28  | 113.42      | 109.98   |
| 22  | B     | 1021 | CLA  | O2A-C1-C2   | 3.27  | 120.68      | 108.11   |
| 39  | 5     | 501  | LUT  | C22-C23-C24 | -3.27 | 106.33      | 111.18   |
| 39  | 7     | 502  | LUT  | C11-C10-C9  | -3.27 | 122.70      | 127.28   |
| 22  | A     | 1139 | CLA  | O2A-C1-C2   | 3.27  | 120.68      | 108.11   |
| 22  | B     | 1237 | CLA  | C1-C2-C3    | -3.27 | 120.85      | 126.20   |
| 22  | A     | 1121 | CLA  | C1-C2-C3    | -3.26 | 120.85      | 126.20   |
| 40  | 4     | 611  | CHL  | C4D-CHA-CBD | -3.26 | 105.68      | 108.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1022 | CLA  | C3B-C4B-NB  | -3.26 | 107.62      | 110.53   |
| 40  | Z     | 610  | CHL  | C1A-CHA-C4D | 3.26  | 124.43      | 118.98   |
| 25  | 3     | 503  | BCR  | C23-C24-C25 | -3.26 | 118.29      | 127.00   |
| 40  | 3     | 611  | CHL  | C3C-C4C-NC  | -3.26 | 106.68      | 114.65   |
| 22  | K     | 1404 | CLA  | CMA-C3A-C4A | 3.26  | 120.53      | 111.77   |
| 22  | A     | 1118 | CLA  | C1-C2-C3    | -3.26 | 120.86      | 126.20   |
| 22  | A     | 1109 | CLA  | CAA-C2A-C3A | -3.26 | 104.20      | 113.00   |
| 25  | 5     | 504  | BCR  | C30-C25-C26 | -3.25 | 118.19      | 122.64   |
| 22  | 7     | 603  | CLA  | CMA-C3A-C4A | 3.25  | 120.50      | 111.77   |
| 22  | A     | 1128 | CLA  | C2C-C1C-NC  | 3.25  | 113.39      | 109.98   |
| 22  | 8     | 604  | CLA  | O2A-CGA-CBA | 3.25  | 121.74      | 111.83   |
| 22  | 7     | 603  | CLA  | CBA-CAA-C2A | 3.25  | 123.45      | 113.79   |
| 40  | 6     | 610  | CHL  | C1A-CHA-C4D | 3.24  | 124.39      | 118.98   |
| 22  | B     | 1023 | CLA  | CAA-C2A-C3A | -3.24 | 104.25      | 113.00   |
| 39  | 4     | 501  | LUT  | C21-C26-C27 | 3.24  | 116.55      | 112.83   |
| 22  | L     | 1503 | CLA  | C1-C2-C3    | -3.23 | 121.53      | 126.76   |
| 25  | 8     | 503  | BCR  | C33-C5-C6   | -3.23 | 120.96      | 124.48   |
| 25  | 6     | 503  | BCR  | C33-C5-C6   | -3.23 | 120.96      | 124.48   |
| 39  | 6     | 502  | LUT  | C35-C34-C33 | -3.23 | 122.75      | 127.28   |
| 40  | 8     | 610  | CHL  | C1-O2A-CGA  | 3.23  | 124.47      | 116.65   |
| 22  | Z     | 611  | CLA  | C1-C2-C3    | -3.23 | 120.90      | 126.20   |
| 22  | B     | 1238 | CLA  | C1-C2-C3    | -3.23 | 120.91      | 126.20   |
| 22  | Z     | 606  | CLA  | O2D-CGD-O1D | -3.23 | 117.57      | 123.85   |
| 25  | A     | 4004 | BCR  | C33-C5-C6   | -3.23 | 120.96      | 124.48   |
| 22  | 3     | 604  | CLA  | C1D-ND-C4D  | -3.23 | 104.05      | 106.31   |
| 25  | 6     | 503  | BCR  | C15-C14-C13 | -3.22 | 122.76      | 127.28   |
| 22  | 8     | 603  | CLA  | CMA-C3A-C4A | 3.22  | 120.43      | 111.77   |
| 22  | B     | 1239 | CLA  | O2A-C1-C2   | 3.22  | 120.50      | 108.11   |
| 22  | 3     | 604  | CLA  | CBA-CAA-C2A | 3.22  | 123.38      | 113.79   |
| 22  | 2     | 607  | CLA  | C2C-C1C-NC  | 3.22  | 113.36      | 109.98   |
| 22  | Z     | 603  | CLA  | CMA-C3A-C4A | 3.22  | 120.42      | 111.77   |
| 25  | B     | 4001 | BCR  | C23-C24-C25 | -3.22 | 118.41      | 127.00   |
| 22  | 3     | 605  | CLA  | C1-C2-C3    | -3.22 | 120.93      | 126.20   |
| 22  | A     | 1103 | CLA  | O2A-C1-C2   | 3.21  | 120.47      | 108.11   |
| 22  | 1     | 604  | CLA  | C1-C2-C3    | -3.21 | 120.93      | 126.20   |
| 22  | B     | 1220 | CLA  | C1-C2-C3    | -3.21 | 120.93      | 126.20   |
| 22  | K     | 1402 | CLA  | O2D-CGD-O1D | -3.21 | 117.60      | 123.85   |
| 22  | B     | 1227 | CLA  | O2A-C1-C2   | 3.21  | 120.45      | 108.11   |
| 39  | 7     | 502  | LUT  | C26-C27-C28 | -3.21 | 119.59      | 124.58   |
| 22  | 1     | 606  | CLA  | C1-C2-C3    | -3.21 | 120.94      | 126.20   |
| 22  | 7     | 616  | CLA  | C1-C2-C3    | -3.21 | 120.94      | 126.20   |
| 40  | 1     | 609  | CHL  | CHA-C1A-C2A | -3.21 | 125.78      | 133.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1102 | CLA  | C1-O2A-CGA  | 3.20  | 124.41      | 116.65   |
| 40  | 6     | 617  | CHL  | CHA-C1A-C2A | -3.20 | 125.78      | 133.31   |
| 40  | 1     | 610  | CHL  | C1A-CHA-C4D | 3.20  | 124.33      | 118.98   |
| 39  | Z     | 503  | LUT  | C7-C8-C9    | -3.20 | 121.50      | 126.23   |
| 22  | 5     | 612  | CLA  | CAA-C2A-C3A | -3.20 | 104.36      | 113.00   |
| 40  | 7     | 610  | CHL  | C1A-CHA-C4D | 3.20  | 124.32      | 118.98   |
| 22  | A     | 1112 | CLA  | C1-C2-C3    | -3.20 | 120.96      | 126.20   |
| 22  | A     | 1123 | CLA  | C1-C2-C3    | -3.19 | 120.96      | 126.20   |
| 22  | 4     | 607  | CLA  | C1-C2-C3    | -3.19 | 120.96      | 126.20   |
| 40  | Z     | 613  | CHL  | CHA-C1A-C2A | -3.19 | 125.81      | 133.31   |
| 37  | 1     | 503  | C7Z  | C35-C15-C14 | -3.19 | 116.99      | 123.52   |
| 40  | 4     | 617  | CHL  | CHA-C1A-C2A | -3.19 | 125.82      | 133.31   |
| 22  | 2     | 607  | CLA  | CMA-C3A-C4A | 3.19  | 120.34      | 111.77   |
| 39  | Z     | 501  | LUT  | C18-C5-C6   | -3.18 | 121.01      | 124.48   |
| 25  | B     | 4003 | BCR  | C33-C5-C6   | -3.18 | 121.01      | 124.48   |
| 22  | 6     | 604  | CLA  | CMA-C3A-C4A | 3.18  | 120.33      | 111.77   |
| 22  | A     | 1136 | CLA  | O2A-CGA-CBA | 3.18  | 121.54      | 111.83   |
| 22  | 1     | 603  | CLA  | O2A-C1-C2   | 3.18  | 120.36      | 108.11   |
| 39  | 2     | 503  | LUT  | C18-C5-C6   | -3.18 | 121.01      | 124.48   |
| 40  | 3     | 611  | CHL  | C4D-CHA-CBD | -3.18 | 105.76      | 108.97   |
| 22  | A     | 1013 | CLA  | CAA-C2A-C3A | -3.18 | 104.40      | 113.00   |
| 22  | A     | 1125 | CLA  | C1-O2A-CGA  | 3.18  | 124.35      | 116.65   |
| 25  | A     | 4005 | BCR  | C35-C13-C12 | 3.18  | 122.94      | 118.09   |
| 22  | A     | 1133 | CLA  | O2A-C1-C2   | 3.18  | 120.34      | 108.11   |
| 40  | 8     | 613  | CHL  | C1-C2-C3    | -3.18 | 121.00      | 126.20   |
| 22  | B     | 1209 | CLA  | O2A-CGA-CBA | 3.17  | 121.51      | 111.83   |
| 22  | 5     | 622  | CLA  | C2C-C1C-NC  | 3.17  | 113.31      | 109.98   |
| 22  | B     | 1219 | CLA  | C2C-C1C-NC  | 3.17  | 113.31      | 109.98   |
| 22  | B     | 1226 | CLA  | C1C-C2C-C3C | -3.17 | 103.65      | 106.98   |
| 22  | 8     | 604  | CLA  | CMA-C3A-C4A | 3.17  | 120.28      | 111.77   |
| 22  | A     | 1123 | CLA  | O2A-C1-C2   | 3.17  | 120.29      | 108.11   |
| 22  | Z     | 603  | CLA  | C1-C2-C3    | -3.17 | 121.64      | 126.76   |
| 22  | B     | 1210 | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 39  | 6     | 501  | LUT  | C21-C26-C27 | 3.16  | 116.46      | 112.83   |
| 22  | A     | 1140 | CLA  | C3B-C4B-NB  | -3.16 | 107.71      | 110.53   |
| 23  | A     | 2001 | PQN  | C14-C13-C15 | 3.16  | 120.71      | 115.23   |
| 39  | 9     | 501  | LUT  | C18-C5-C6   | -3.16 | 121.04      | 124.48   |
| 40  | 4     | 611  | CHL  | CHA-C1A-C2A | -3.16 | 125.89      | 133.31   |
| 22  | 4     | 602  | CLA  | C1-C2-C3    | -3.16 | 121.02      | 126.20   |
| 40  | 5     | 617  | CHL  | CHA-C1A-C2A | -3.16 | 125.89      | 133.31   |
| 40  | 2     | 610  | CHL  | CHA-C1A-C2A | -3.16 | 125.89      | 133.31   |
| 22  | 3     | 613  | CLA  | C1-C2-C3    | -3.15 | 121.03      | 126.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1101 | CLA  | C1-O2A-CGA  | 3.15  | 124.29      | 116.65   |
| 40  | 2     | 609  | CHL  | CHA-C1A-C2A | -3.15 | 125.91      | 133.31   |
| 22  | 1     | 611  | CLA  | C1-C2-C3    | -3.15 | 121.04      | 126.20   |
| 22  | B     | 1207 | CLA  | C1-C2-C3    | -3.15 | 121.04      | 126.20   |
| 22  | 6     | 609  | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 22  | 8     | 607  | CLA  | C1-C2-C3    | -3.15 | 121.04      | 126.20   |
| 25  | A     | 4002 | BCR  | C23-C24-C25 | -3.14 | 118.60      | 127.00   |
| 22  | B     | 1023 | CLA  | O2D-CGD-O1D | -3.14 | 117.73      | 123.85   |
| 22  | B     | 1238 | CLA  | CMA-C3A-C4A | 3.14  | 120.22      | 111.77   |
| 22  | 4     | 605  | CLA  | C1-C2-C3    | -3.14 | 121.05      | 126.20   |
| 40  | 7     | 610  | CHL  | CHA-C1A-C2A | -3.14 | 125.94      | 133.31   |
| 39  | 4     | 501  | LUT  | C35-C15-C14 | -3.14 | 117.10      | 123.52   |
| 40  | 9     | 610  | CHL  | CHA-C1A-C2A | -3.14 | 125.94      | 133.31   |
| 22  | 7     | 601  | CLA  | C1-O2A-CGA  | 3.14  | 124.25      | 116.65   |
| 40  | 6     | 611  | CHL  | C1-C2-C3    | -3.14 | 121.69      | 126.76   |
| 22  | 8     | 602  | CLA  | C1-C2-C3    | -3.13 | 121.06      | 126.20   |
| 25  | I     | 4001 | BCR  | C33-C5-C6   | -3.13 | 121.07      | 124.48   |
| 40  | 6     | 617  | CHL  | C1A-CHA-C4D | 3.13  | 124.21      | 118.98   |
| 40  | 7     | 610  | CHL  | C4D-CHA-CBD | -3.13 | 105.81      | 108.97   |
| 22  | B     | 1241 | CLA  | CMA-C3A-C4A | 3.13  | 120.18      | 111.77   |
| 25  | 5     | 503  | BCR  | C19-C18-C17 | 3.13  | 123.93      | 119.01   |
| 22  | B     | 1206 | CLA  | C2C-C1C-NC  | 3.13  | 113.27      | 109.98   |
| 40  | 6     | 611  | CHL  | CHA-C1A-C2A | -3.13 | 125.97      | 133.31   |
| 25  | 3     | 503  | BCR  | C33-C5-C6   | -3.13 | 121.07      | 124.48   |
| 25  | A     | 4004 | BCR  | C30-C25-C26 | -3.13 | 118.36      | 122.64   |
| 40  | 4     | 610  | CHL  | CMA-C3A-C4A | 3.12  | 121.34      | 114.61   |
| 22  | A     | 1124 | CLA  | C1-C2-C3    | -3.12 | 121.08      | 126.20   |
| 40  | 4     | 611  | CHL  | C1A-CHA-C4D | 3.12  | 124.19      | 118.98   |
| 40  | 4     | 610  | CHL  | C4D-CHA-CBD | -3.12 | 105.82      | 108.97   |
| 22  | 1     | 603  | CLA  | C1-C2-C3    | -3.11 | 121.09      | 126.20   |
| 25  | 4     | 503  | BCR  | C4-C5-C6    | -3.11 | 118.50      | 122.70   |
| 22  | 1     | 611  | CLA  | C1C-C2C-C3C | -3.11 | 103.70      | 106.98   |
| 39  | 1     | 501  | LUT  | C10-C11-C12 | -3.11 | 114.18      | 123.20   |
| 25  | 6     | 504  | BCR  | C15-C14-C13 | -3.11 | 122.91      | 127.28   |
| 22  | B     | 1211 | CLA  | C1-C2-C3    | -3.11 | 121.10      | 126.20   |
| 22  | A     | 1105 | CLA  | C4B-CHC-C1C | 3.11  | 133.56      | 126.25   |
| 22  | 3     | 604  | CLA  | CMA-C3A-C4A | 3.11  | 120.13      | 111.77   |
| 22  | B     | 1225 | CLA  | C3B-C4B-NB  | -3.11 | 107.75      | 110.53   |
| 22  | 4     | 604  | CLA  | C1-C2-C3    | -3.11 | 121.11      | 126.20   |
| 22  | B     | 1208 | CLA  | O2A-CGA-CBA | 3.11  | 121.31      | 111.83   |
| 22  | 4     | 603  | CLA  | CMA-C3A-C4A | 3.11  | 120.12      | 111.77   |
| 25  | 5     | 504  | BCR  | C37-C22-C23 | 3.11  | 122.83      | 118.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 6     | 503  | BCR  | C23-C24-C25 | -3.11 | 118.70      | 127.00   |
| 25  | A     | 4003 | BCR  | C1-C6-C5    | -3.10 | 118.39      | 122.64   |
| 40  | 4     | 610  | CHL  | C1-O2A-CGA  | 3.10  | 124.16      | 116.65   |
| 22  | 3     | 603  | CLA  | CMA-C3A-C4A | 3.10  | 120.11      | 111.77   |
| 22  | 8     | 611  | CLA  | C1C-C2C-C3C | -3.10 | 103.72      | 106.98   |
| 25  | A     | 4003 | BCR  | C33-C5-C6   | -3.10 | 121.10      | 124.48   |
| 40  | 1     | 610  | CHL  | CHA-C1A-C2A | -3.10 | 126.03      | 133.31   |
| 40  | Z     | 613  | CHL  | C3C-C4C-NC  | -3.10 | 107.08      | 114.65   |
| 40  | 6     | 610  | CHL  | C3C-C4C-NC  | -3.10 | 107.08      | 114.65   |
| 22  | 5     | 604  | CLA  | C1-O2A-CGA  | 3.10  | 124.14      | 116.65   |
| 22  | B     | 1202 | CLA  | O2A-CGA-CBA | 3.09  | 121.27      | 111.83   |
| 22  | Z     | 612  | CLA  | C1-C2-C3    | -3.09 | 121.13      | 126.20   |
| 22  | 6     | 619  | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 22  | B     | 1205 | CLA  | O2A-CGA-CBA | 3.09  | 121.27      | 111.83   |
| 22  | Z     | 605  | CLA  | C1C-C2C-C3C | -3.09 | 103.73      | 106.98   |
| 25  | 3     | 504  | BCR  | C19-C18-C17 | 3.09  | 123.87      | 119.01   |
| 40  | 6     | 613  | CHL  | CHA-C1A-C2A | -3.09 | 126.05      | 133.31   |
| 22  | 6     | 605  | CLA  | C1-C2-C3    | -3.09 | 121.13      | 126.20   |
| 22  | 2     | 605  | CLA  | C1-O2A-CGA  | 3.09  | 124.12      | 116.65   |
| 22  | B     | 1219 | CLA  | C1-C2-C3    | -3.09 | 121.14      | 126.20   |
| 22  | 2     | 606  | CLA  | C2C-C1C-NC  | 3.09  | 113.22      | 109.98   |
| 37  | 5     | 505  | C7Z  | C21-C26-C25 | -3.08 | 118.42      | 122.64   |
| 22  | 8     | 615  | CLA  | C2C-C1C-NC  | 3.08  | 113.22      | 109.98   |
| 22  | B     | 1021 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 22  | A     | 1121 | CLA  | CMD-C2D-C3D | -3.08 | 120.63      | 127.69   |
| 22  | 4     | 609  | CLA  | C1-C2-C3    | -3.08 | 121.15      | 126.20   |
| 40  | 8     | 613  | CHL  | CHA-C1A-C2A | -3.08 | 126.08      | 133.31   |
| 39  | 8     | 501  | LUT  | C35-C15-C14 | -3.08 | 117.22      | 123.52   |
| 22  | 9     | 601  | CLA  | CMA-C3A-C4A | 3.08  | 120.04      | 111.77   |
| 22  | 3     | 607  | CLA  | O2D-CGD-O1D | -3.08 | 117.86      | 123.85   |
| 40  | 2     | 613  | CHL  | CHA-C1A-C2A | -3.08 | 126.08      | 133.31   |
| 39  | 3     | 501  | LUT  | C15-C14-C13 | -3.08 | 122.96      | 127.28   |
| 40  | 1     | 609  | CHL  | C3C-C4C-NC  | -3.08 | 107.13      | 114.65   |
| 25  | 5     | 504  | BCR  | C33-C5-C6   | -3.08 | 121.13      | 124.48   |
| 22  | B     | 1230 | CLA  | C1-C2-C3    | -3.07 | 121.16      | 126.20   |
| 40  | 3     | 611  | CHL  | CHA-C1A-C2A | -3.07 | 126.09      | 133.31   |
| 40  | 1     | 610  | CHL  | C4D-CHA-CBD | -3.07 | 105.87      | 108.97   |
| 22  | B     | 1222 | CLA  | CAA-C2A-C3A | -3.07 | 104.69      | 113.00   |
| 22  | B     | 1235 | CLA  | O2A-CGA-CBA | 3.07  | 121.20      | 111.83   |
| 22  | 5     | 605  | CLA  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 22  | 5     | 612  | CLA  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 22  | A     | 1119 | CLA  | O2A-C1-C2   | 3.07  | 119.91      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 5     | 602  | CLA  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 22  | 1     | 615  | CLA  | C2C-C1C-NC  | 3.07  | 113.20      | 109.98   |
| 22  | 7     | 615  | CLA  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 40  | 2     | 609  | CHL  | C3C-C4C-NC  | -3.06 | 107.16      | 114.65   |
| 22  | A     | 1138 | CLA  | O2D-CGD-O1D | -3.06 | 117.88      | 123.85   |
| 40  | 6     | 611  | CHL  | C4D-CHA-CBD | -3.06 | 105.88      | 108.97   |
| 22  | A     | 1012 | CLA  | C1-O2A-CGA  | 3.06  | 124.07      | 116.65   |
| 22  | B     | 1211 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 40  | 6     | 610  | CHL  | CHA-C1A-C2A | -3.06 | 126.11      | 133.31   |
| 25  | G     | 4001 | BCR  | C33-C5-C6   | -3.06 | 121.14      | 124.48   |
| 40  | Z     | 610  | CHL  | CHA-C1A-C2A | -3.06 | 126.12      | 133.31   |
| 25  | G     | 4001 | BCR  | C36-C18-C17 | -3.06 | 117.86      | 122.82   |
| 22  | A     | 1136 | CLA  | C2C-C1C-NC  | 3.06  | 113.19      | 109.98   |
| 40  | Z     | 610  | CHL  | C4D-CHA-CBD | -3.06 | 105.88      | 108.97   |
| 22  | Z     | 606  | CLA  | C1-C2-C3    | -3.06 | 121.19      | 126.20   |
| 22  | 5     | 615  | CLA  | C2C-C1C-NC  | 3.06  | 113.19      | 109.98   |
| 22  | Z     | 605  | CLA  | C1-C2-C3    | -3.05 | 121.19      | 126.20   |
| 40  | 6     | 611  | CHL  | C1A-CHA-C4D | 3.05  | 124.07      | 118.98   |
| 22  | A     | 1138 | CLA  | O2A-CGA-CBA | 3.05  | 121.14      | 111.83   |
| 22  | 4     | 608  | CLA  | CMA-C3A-C4A | 3.05  | 119.97      | 111.77   |
| 22  | B     | 1203 | CLA  | C1-C2-C3    | -3.05 | 121.20      | 126.20   |
| 22  | A     | 1106 | CLA  | C4B-CHC-C1C | 3.05  | 133.42      | 126.25   |
| 22  | A     | 1141 | CLA  | C2C-C1C-NC  | 3.05  | 113.18      | 109.98   |
| 22  | B     | 1206 | CLA  | C1C-C2C-C3C | -3.05 | 103.78      | 106.98   |
| 22  | 8     | 611  | CLA  | O2A-CGA-CBA | 3.04  | 121.12      | 111.83   |
| 25  | 5     | 503  | BCR  | C33-C5-C6   | -3.04 | 121.16      | 124.48   |
| 39  | 5     | 501  | LUT  | C18-C5-C6   | -3.04 | 121.16      | 124.48   |
| 22  | 2     | 603  | CLA  | C1-C2-C3    | -3.04 | 121.21      | 126.20   |
| 36  | F     | 4001 | RRX  | C33-C5-C4   | 3.04  | 120.08      | 113.60   |
| 22  | 1     | 607  | CLA  | C2C-C1C-NC  | 3.04  | 113.18      | 109.98   |
| 39  | 7     | 501  | LUT  | C35-C15-C14 | -3.04 | 117.30      | 123.52   |
| 39  | 1     | 501  | LUT  | C15-C14-C13 | -3.04 | 123.02      | 127.28   |
| 22  | B     | 1205 | CLA  | O2D-CGD-O1D | -3.04 | 117.94      | 123.85   |
| 22  | A     | 1132 | CLA  | C2C-C1C-NC  | 3.04  | 113.17      | 109.98   |
| 25  | B     | 4002 | BCR  | C23-C24-C25 | -3.04 | 118.89      | 127.00   |
| 22  | 2     | 608  | CLA  | CMA-C3A-C4A | 3.03  | 119.93      | 111.77   |
| 22  | A     | 1013 | CLA  | O2A-C1-C2   | 3.03  | 119.78      | 108.11   |
| 22  | B     | 1209 | CLA  | C1-O2A-CGA  | 3.03  | 123.99      | 116.65   |
| 40  | 4     | 613  | CHL  | C4D-CHA-CBD | -3.03 | 105.91      | 108.97   |
| 25  | 6     | 504  | BCR  | C33-C5-C4   | 3.03  | 120.06      | 113.60   |
| 22  | A     | 1140 | CLA  | C4B-CHC-C1C | 3.03  | 133.37      | 126.25   |
| 22  | A     | 1124 | CLA  | CAA-C2A-C3A | -3.03 | 104.81      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 40  | 9     | 613  | CHL  | C1A-CHA-C4D | 3.03  | 124.04      | 118.98   |
| 22  | A     | 1127 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 22  | A     | 1110 | CLA  | CMA-C3A-C4A | 3.03  | 119.91      | 111.77   |
| 22  | 1     | 612  | CLA  | C1-C2-C3    | -3.02 | 121.24      | 126.20   |
| 22  | B     | 1216 | CLA  | C1-C2-C3    | -3.02 | 121.24      | 126.20   |
| 22  | B     | 1227 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 22  | 7     | 604  | CLA  | C1-O2A-CGA  | 3.02  | 123.97      | 116.65   |
| 22  | 3     | 601  | CLA  | CAA-C2A-C3A | -3.02 | 104.83      | 113.00   |
| 22  | 5     | 613  | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 22  | 3     | 605  | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 40  | 4     | 613  | CHL  | CHA-C1A-C2A | -3.02 | 126.22      | 133.31   |
| 22  | 9     | 601  | CLA  | O2A-CGA-CBA | 3.02  | 121.04      | 111.83   |
| 22  | A     | 1137 | CLA  | C1-C2-C3    | -3.02 | 121.25      | 126.20   |
| 22  | 3     | 607  | CLA  | CMA-C3A-C4A | 3.02  | 119.88      | 111.77   |
| 22  | 9     | 609  | CLA  | CMA-C3A-C4A | 3.02  | 119.88      | 111.77   |
| 39  | 9     | 502  | LUT  | C10-C11-C12 | -3.01 | 114.47      | 123.20   |
| 22  | B     | 1215 | CLA  | C2C-C1C-NC  | 3.01  | 113.15      | 109.98   |
| 22  | B     | 1203 | CLA  | O2A-C1-C2   | 3.01  | 119.70      | 108.11   |
| 22  | L     | 1502 | CLA  | C1-C2-C3    | -3.01 | 121.27      | 126.20   |
| 22  | 4     | 603  | CLA  | CBA-CAA-C2A | 3.01  | 122.75      | 113.79   |
| 22  | 4     | 608  | CLA  | C1-C2-C3    | -3.01 | 121.27      | 126.20   |
| 22  | B     | 1209 | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 22  | 4     | 607  | CLA  | CMA-C3A-C4A | 3.01  | 119.86      | 111.77   |
| 22  | B     | 1209 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 22  | B     | 1223 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 40  | Z     | 609  | CHL  | C3C-C4C-NC  | -3.01 | 107.30      | 114.65   |
| 25  | 4     | 503  | BCR  | C1-C6-C5    | -3.00 | 118.53      | 122.64   |
| 25  | 6     | 504  | BCR  | C4-C5-C6    | -3.00 | 118.65      | 122.70   |
| 40  | 4     | 613  | CHL  | C3C-C4C-NC  | -3.00 | 107.31      | 114.65   |
| 22  | F     | 1301 | CLA  | O2A-CGA-CBA | 3.00  | 120.99      | 111.83   |
| 25  | 3     | 505  | BCR  | C38-C26-C25 | -3.00 | 121.21      | 124.48   |
| 40  | 6     | 610  | CHL  | C4D-CHA-CBD | -3.00 | 105.94      | 108.97   |
| 22  | 6     | 603  | CLA  | CMA-C3A-C4A | 3.00  | 119.84      | 111.77   |
| 22  | A     | 1132 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 26  | 8     | 801  | LHG  | O8-C23-C24  | 3.00  | 120.98      | 111.83   |
| 40  | 5     | 610  | CHL  | C1-O2A-CGA  | 3.00  | 123.91      | 116.65   |
| 22  | K     | 1403 | CLA  | C2C-C1C-NC  | 3.00  | 113.13      | 109.98   |
| 40  | 8     | 610  | CHL  | C3C-C4C-NC  | -3.00 | 107.32      | 114.65   |
| 22  | 5     | 609  | CLA  | C1-C2-C3    | -3.00 | 121.29      | 126.20   |
| 22  | A     | 1131 | CLA  | C2C-C1C-NC  | 2.99  | 113.13      | 109.98   |
| 22  | 8     | 603  | CLA  | C6-C5-C3    | -2.99 | 106.17      | 113.47   |
| 22  | B     | 1224 | CLA  | C1-O2A-CGA  | 2.99  | 123.90      | 116.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1105 | CLA  | C1-C2-C3    | -2.99 | 121.29      | 126.20   |
| 22  | 8     | 606  | CLA  | C1-C2-C3    | -2.99 | 121.29      | 126.20   |
| 40  | 2     | 609  | CHL  | C1-C2-C3    | -2.99 | 121.92      | 126.76   |
| 22  | 1     | 602  | CLA  | C2C-C1C-NC  | 2.99  | 113.12      | 109.98   |
| 22  | F     | 1302 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 22  | Z     | 612  | CLA  | C2C-C1C-NC  | 2.99  | 113.12      | 109.98   |
| 28  | 8     | 805  | LMT  | O1'-C1'-C2' | 2.99  | 112.81      | 108.27   |
| 22  | B     | 1222 | CLA  | O2A-C1-C2   | 2.99  | 119.62      | 108.11   |
| 22  | A     | 1107 | CLA  | C2C-C1C-NC  | 2.99  | 113.12      | 109.98   |
| 22  | 8     | 611  | CLA  | C1-C2-C3    | -2.99 | 121.92      | 126.76   |
| 22  | B     | 1229 | CLA  | C4B-CHC-C1C | 2.99  | 133.28      | 126.25   |
| 22  | A     | 1130 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 22  | 9     | 601  | CLA  | C1-O2A-CGA  | 2.99  | 123.88      | 116.65   |
| 29  | A     | 5008 | OCA  | O1-C1-C2    | -2.99 | 113.62      | 123.09   |
| 40  | 4     | 613  | CHL  | C1A-CHA-C4D | 2.99  | 123.97      | 118.98   |
| 22  | 5     | 603  | CLA  | CMA-C3A-C4A | 2.99  | 119.80      | 111.77   |
| 40  | 3     | 611  | CHL  | C1A-CHA-C4D | 2.99  | 123.97      | 118.98   |
| 22  | B     | 1224 | CLA  | C2C-C1C-NC  | 2.99  | 113.12      | 109.98   |
| 39  | 8     | 501  | LUT  | C10-C11-C12 | -2.98 | 114.55      | 123.20   |
| 25  | B     | 4005 | BCR  | C27-C26-C25 | -2.98 | 118.67      | 122.70   |
| 22  | 7     | 608  | CLA  | C2C-C1C-NC  | 2.98  | 113.12      | 109.98   |
| 22  | A     | 1126 | CLA  | C1-C2-C3    | -2.98 | 121.31      | 126.20   |
| 39  | Z     | 501  | LUT  | C35-C15-C14 | -2.98 | 117.42      | 123.52   |
| 22  | A     | 1110 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 22  | 7     | 611  | CLA  | C1C-C2C-C3C | -2.98 | 103.84      | 106.98   |
| 25  | B     | 4006 | BCR  | C15-C14-C13 | 2.98  | 131.46      | 127.28   |
| 22  | A     | 1108 | CLA  | CMA-C3A-C4A | 2.98  | 119.79      | 111.77   |
| 22  | 3     | 616  | CLA  | CMA-C3A-C4A | 2.98  | 119.78      | 111.77   |
| 22  | A     | 1106 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 22  | 5     | 615  | CLA  | CMA-C3A-C4A | 2.98  | 119.78      | 111.77   |
| 22  | A     | 1117 | CLA  | CMA-C3A-C4A | 2.98  | 119.78      | 111.77   |
| 22  | 7     | 605  | CLA  | C1-C2-C3    | -2.97 | 121.32      | 126.20   |
| 22  | 9     | 609  | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 22  | 9     | 605  | CLA  | C1C-C2C-C3C | -2.97 | 103.86      | 106.98   |
| 25  | B     | 4006 | BCR  | C36-C18-C17 | -2.97 | 118.01      | 122.82   |
| 40  | 2     | 610  | CHL  | C4D-CHA-CBD | -2.97 | 105.97      | 108.97   |
| 22  | B     | 1218 | CLA  | C2C-C1C-NC  | 2.97  | 113.10      | 109.98   |
| 39  | 1     | 502  | LUT  | C10-C11-C12 | -2.97 | 114.60      | 123.20   |
| 40  | Z     | 610  | CHL  | C3C-C4C-NC  | -2.97 | 107.40      | 114.65   |
| 22  | 5     | 622  | CLA  | C1C-C2C-C3C | -2.97 | 103.86      | 106.98   |
| 22  | B     | 1232 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 40  | 6     | 613  | CHL  | C4D-CHA-CBD | -2.96 | 105.98      | 108.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 615  | CLA  | C1-C2-C3    | -2.96 | 121.34      | 126.20   |
| 37  | J     | 4002 | C7Z  | C15-C14-C13 | -2.96 | 123.12      | 127.28   |
| 40  | Z     | 609  | CHL  | C4D-CHA-CBD | -2.96 | 105.98      | 108.97   |
| 40  | 6     | 617  | CHL  | C4D-CHA-CBD | -2.96 | 105.98      | 108.97   |
| 40  | 9     | 610  | CHL  | C3C-C4C-NC  | -2.96 | 107.41      | 114.65   |
| 40  | 9     | 610  | CHL  | C1-C2-C3    | -2.96 | 121.35      | 126.20   |
| 40  | 6     | 613  | CHL  | C1A-CHA-C4D | 2.96  | 123.92      | 118.98   |
| 22  | Z     | 604  | CLA  | CMA-C3A-C4A | 2.96  | 119.73      | 111.77   |
| 22  | A     | 1104 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 22  | B     | 1210 | CLA  | O1D-CGD-CBD | -2.95 | 118.69      | 124.52   |
| 22  | A     | 1110 | CLA  | C1-C2-C3    | -2.95 | 121.36      | 126.20   |
| 22  | 6     | 609  | CLA  | C4B-CHC-C1C | 2.95  | 133.19      | 126.25   |
| 22  | 7     | 603  | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 25  | A     | 4001 | BCR  | C35-C13-C12 | 2.95  | 122.59      | 118.09   |
| 40  | Z     | 609  | CHL  | CHA-C1A-C2A | -2.95 | 126.38      | 133.31   |
| 39  | 2     | 502  | LUT  | C38-C25-C24 | -2.95 | 116.38      | 123.36   |
| 22  | 4     | 612  | CLA  | C1C-C2C-C3C | -2.95 | 103.88      | 106.98   |
| 22  | 7     | 601  | CLA  | CAA-C2A-C3A | -2.95 | 105.04      | 113.00   |
| 22  | A     | 1110 | CLA  | C4B-CHC-C1C | 2.94  | 133.17      | 126.25   |
| 22  | A     | 1125 | CLA  | C1-C2-C3    | -2.94 | 121.38      | 126.20   |
| 25  | A     | 4001 | BCR  | C19-C18-C17 | 2.94  | 123.64      | 119.01   |
| 22  | 2     | 604  | CLA  | CMD-C2D-C3D | -2.94 | 120.94      | 127.69   |
| 22  | 1     | 607  | CLA  | CMA-C3A-C4A | 2.94  | 119.68      | 111.77   |
| 25  | 5     | 504  | BCR  | C27-C26-C25 | -2.94 | 118.73      | 122.70   |
| 22  | Z     | 615  | CLA  | C2C-C1C-NC  | 2.94  | 113.07      | 109.98   |
| 25  | A     | 4004 | BCR  | C12-C13-C14 | -2.94 | 114.38      | 119.01   |
| 25  | 6     | 504  | BCR  | C33-C5-C6   | -2.94 | 121.28      | 124.48   |
| 22  | 4     | 604  | CLA  | CMA-C3A-C4A | 2.94  | 119.67      | 111.77   |
| 22  | A     | 1126 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | B     | 1208 | CLA  | C1-C2-C3    | -2.94 | 121.39      | 126.20   |
| 22  | B     | 1222 | CLA  | O2A-CGA-CBA | 2.94  | 120.79      | 111.83   |
| 40  | 2     | 613  | CHL  | C4D-CHA-CBD | -2.94 | 106.01      | 108.97   |
| 22  | A     | 1105 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 39  | 2     | 502  | LUT  | C15-C35-C34 | -2.94 | 117.51      | 123.52   |
| 39  | 4     | 501  | LUT  | C10-C11-C12 | -2.93 | 114.70      | 123.20   |
| 28  | B     | 5005 | LMT  | O5'-C5'-C4' | 2.93  | 115.79      | 109.72   |
| 22  | 3     | 605  | CLA  | C4B-CHC-C1C | 2.93  | 133.14      | 126.25   |
| 39  | 2     | 503  | LUT  | C19-C9-C8   | 2.93  | 122.57      | 118.09   |
| 22  | Z     | 602  | CLA  | C2C-C1C-NC  | 2.93  | 113.06      | 109.98   |
| 22  | A     | 1117 | CLA  | C2C-C1C-NC  | 2.93  | 113.06      | 109.98   |
| 22  | 3     | 607  | CLA  | C2C-C1C-NC  | 2.93  | 113.06      | 109.98   |
| 22  | B     | 1203 | CLA  | C1C-C2C-C3C | -2.93 | 103.90      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | 2     | 502  | LUT  | C26-C27-C28 | -2.93 | 120.02      | 124.58   |
| 22  | 6     | 608  | CLA  | CAA-C2A-C3A | -2.93 | 105.09      | 113.00   |
| 22  | 5     | 602  | CLA  | C4B-CHC-C1C | 2.93  | 133.13      | 126.25   |
| 25  | A     | 4003 | BCR  | C33-C5-C4   | 2.93  | 119.84      | 113.60   |
| 40  | 8     | 613  | CHL  | CMA-C3A-C4A | 2.93  | 120.92      | 114.61   |
| 40  | Z     | 609  | CHL  | CAA-C2A-C3A | -2.93 | 105.09      | 113.00   |
| 22  | B     | 1237 | CLA  | CMA-C3A-C4A | 2.92  | 119.63      | 111.77   |
| 22  | 4     | 612  | CLA  | CMA-C3A-C4A | 2.92  | 119.63      | 111.77   |
| 22  | A     | 1109 | CLA  | CMA-C3A-C4A | 2.92  | 119.63      | 111.77   |
| 22  | 5     | 615  | CLA  | C1-O2A-CGA  | 2.92  | 123.72      | 116.65   |
| 22  | 6     | 608  | CLA  | C2C-C1C-NC  | 2.92  | 113.05      | 109.98   |
| 22  | 4     | 608  | CLA  | C2C-C1C-NC  | 2.92  | 113.05      | 109.98   |
| 22  | 3     | 601  | CLA  | C1-O2A-CGA  | 2.92  | 123.72      | 116.65   |
| 22  | B     | 1204 | CLA  | O2A-CGA-CBA | 2.92  | 120.73      | 111.83   |
| 39  | 5     | 502  | LUT  | C10-C11-C12 | -2.92 | 114.75      | 123.20   |
| 22  | A     | 1134 | CLA  | C2C-C1C-NC  | 2.92  | 113.05      | 109.98   |
| 22  | A     | 1138 | CLA  | C1-C2-C3    | -2.92 | 121.42      | 126.20   |
| 40  | Z     | 610  | CHL  | C1-O2A-CGA  | 2.92  | 123.71      | 116.65   |
| 22  | A     | 1120 | CLA  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |
| 22  | 8     | 602  | CLA  | CAA-C2A-C3A | -2.91 | 105.13      | 113.00   |
| 22  | Z     | 612  | CLA  | C1C-C2C-C3C | -2.91 | 103.92      | 106.98   |
| 22  | A     | 1136 | CLA  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |
| 22  | 3     | 601  | CLA  | O2A-CGA-CBA | 2.91  | 120.71      | 111.83   |
| 25  | B     | 4001 | BCR  | C33-C5-C6   | -2.91 | 121.31      | 124.48   |
| 39  | 3     | 501  | LUT  | C11-C10-C9  | -2.91 | 123.19      | 127.28   |
| 40  | 5     | 611  | CHL  | C1-O2A-CGA  | 2.91  | 123.70      | 116.65   |
| 22  | B     | 1223 | CLA  | C4B-CHC-C1C | 2.91  | 133.09      | 126.25   |
| 22  | 7     | 609  | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 22  | A     | 1101 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 40  | 9     | 610  | CHL  | C1-O2A-CGA  | 2.91  | 123.69      | 116.65   |
| 22  | B     | 1228 | CLA  | C1-C2-C3    | -2.91 | 121.43      | 126.20   |
| 21  | A     | 1011 | CL0  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 22  | 5     | 608  | CLA  | C2C-C1C-NC  | 2.91  | 113.03      | 109.98   |
| 22  | B     | 1213 | CLA  | O2A-CGA-CBA | 2.91  | 120.69      | 111.83   |
| 22  | A     | 1117 | CLA  | C1C-C2C-C3C | -2.91 | 103.92      | 106.98   |
| 40  | Z     | 613  | CHL  | C4D-CHA-CBD | -2.91 | 106.04      | 108.97   |
| 22  | 3     | 618  | CLA  | C2C-C1C-NC  | 2.90  | 113.03      | 109.98   |
| 22  | B     | 1202 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 22  | B     | 1218 | CLA  | C1C-C2C-C3C | -2.90 | 103.93      | 106.98   |
| 22  | 5     | 606  | CLA  | C2C-C1C-NC  | 2.90  | 113.03      | 109.98   |
| 22  | B     | 1204 | CLA  | C2C-C1C-NC  | 2.90  | 113.03      | 109.98   |
| 28  | 4     | 803  | LMT  | C3'-C4'-C5' | -2.90 | 104.51      | 110.93   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 605  | CLA  | O2A-CGA-CBA | 2.90  | 120.66      | 111.83   |
| 22  | 9     | 605  | CLA  | C2C-C1C-NC  | 2.90  | 113.02      | 109.98   |
| 40  | 5     | 610  | CHL  | C4D-CHA-CBD | -2.90 | 106.05      | 108.97   |
| 22  | B     | 1213 | CLA  | C1-O2A-CGA  | 2.90  | 123.66      | 116.65   |
| 22  | Z     | 611  | CLA  | CMA-C3A-C4A | 2.89  | 119.55      | 111.77   |
| 22  | A     | 1120 | CLA  | C1-C2-C3    | -2.89 | 121.45      | 126.20   |
| 40  | 1     | 609  | CHL  | C4D-CHA-CBD | -2.89 | 106.05      | 108.97   |
| 40  | 4     | 617  | CHL  | C1A-CHA-C4D | 2.89  | 123.81      | 118.98   |
| 22  | 6     | 609  | CLA  | C2C-C1C-NC  | 2.89  | 113.02      | 109.98   |
| 22  | B     | 1230 | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 22  | 7     | 605  | CLA  | O2A-CGA-CBA | 2.89  | 120.65      | 111.83   |
| 40  | 5     | 610  | CHL  | CHA-C1A-C2A | -2.89 | 126.52      | 133.31   |
| 22  | B     | 1227 | CLA  | C1-C2-C3    | -2.89 | 122.09      | 126.76   |
| 22  | 9     | 612  | CLA  | O2A-CGA-CBA | 2.89  | 120.64      | 111.83   |
| 22  | 6     | 603  | CLA  | C1-O2A-CGA  | 2.89  | 123.64      | 116.65   |
| 31  | J     | 5001 | LMG  | O8-C28-C29  | 2.89  | 120.64      | 111.83   |
| 22  | 9     | 607  | CLA  | C2C-C1C-NC  | 2.89  | 113.01      | 109.98   |
| 22  | A     | 1139 | CLA  | CMA-C3A-C4A | 2.88  | 119.52      | 111.77   |
| 22  | A     | 1101 | CLA  | O2A-CGA-CBA | 2.88  | 120.63      | 111.83   |
| 22  | 2     | 605  | CLA  | O2A-CGA-CBA | 2.88  | 120.63      | 111.83   |
| 22  | B     | 1204 | CLA  | C1-C2-C3    | -2.88 | 121.47      | 126.20   |
| 22  | A     | 1133 | CLA  | C1C-C2C-C3C | -2.88 | 103.95      | 106.98   |
| 25  | B     | 4007 | BCR  | C33-C5-C6   | -2.88 | 121.34      | 124.48   |
| 40  | 4     | 617  | CHL  | C4D-CHA-CBD | -2.88 | 106.06      | 108.97   |
| 22  | 3     | 616  | CLA  | C2C-C1C-NC  | 2.88  | 113.01      | 109.98   |
| 25  | B     | 4003 | BCR  | C34-C9-C10  | -2.88 | 118.15      | 122.82   |
| 22  | A     | 1114 | CLA  | C2C-C1C-NC  | 2.88  | 113.00      | 109.98   |
| 39  | 8     | 502  | LUT  | C35-C15-C14 | -2.88 | 117.63      | 123.52   |
| 22  | 3     | 618  | CLA  | C1C-C2C-C3C | -2.88 | 103.95      | 106.98   |
| 22  | 3     | 616  | CLA  | C1-C2-C3    | -2.88 | 121.49      | 126.20   |
| 22  | 2     | 604  | CLA  | CHD-C1D-ND  | -2.87 | 120.76      | 124.80   |
| 22  | A     | 1114 | CLA  | C1C-C2C-C3C | -2.87 | 103.96      | 106.98   |
| 22  | B     | 1226 | CLA  | CHA-C4D-ND  | 2.87  | 138.47      | 132.55   |
| 26  | 2     | 801  | LHG  | O8-C23-C24  | 2.87  | 120.59      | 111.83   |
| 31  | A     | 5003 | LMG  | O8-C28-C29  | 2.87  | 120.59      | 111.83   |
| 22  | 7     | 607  | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | 5     | 607  | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | B     | 1023 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 37  | 1     | 503  | C7Z  | C10-C11-C12 | -2.87 | 114.88      | 123.20   |
| 22  | A     | 1118 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | A     | 1122 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | 6     | 612  | CLA  | CMA-C3A-C4A | 2.87  | 119.48      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | 4     | 502  | LUT  | C35-C15-C14 | -2.87 | 117.65      | 123.52   |
| 22  | A     | 1137 | CLA  | C2C-C1C-NC  | 2.87  | 112.99      | 109.98   |
| 22  | A     | 1139 | CLA  | CAA-C2A-C3A | -2.87 | 105.25      | 113.00   |
| 26  | 4     | 801  | LHG  | O8-C23-C24  | 2.87  | 120.57      | 111.83   |
| 22  | 3     | 608  | CLA  | C2C-C1C-NC  | 2.87  | 112.99      | 109.98   |
| 40  | 7     | 610  | CHL  | C3C-C4C-NC  | -2.87 | 107.65      | 114.65   |
| 22  | Z     | 611  | CLA  | C1C-C2C-C3C | -2.86 | 103.97      | 106.98   |
| 25  | B     | 4004 | BCR  | C35-C13-C12 | 2.86  | 122.46      | 118.09   |
| 22  | 2     | 601  | CLA  | CMA-C3A-C4A | 2.86  | 119.47      | 111.77   |
| 22  | A     | 1013 | CLA  | CMB-C2B-C3B | 2.86  | 133.28      | 126.55   |
| 22  | B     | 1226 | CLA  | CAA-C2A-C3A | -2.86 | 105.26      | 113.00   |
| 22  | 9     | 603  | CLA  | O2A-CGA-CBA | 2.86  | 120.56      | 111.83   |
| 39  | 8     | 502  | LUT  | C15-C14-C13 | -2.86 | 123.26      | 127.28   |
| 25  | B     | 4003 | BCR  | C12-C13-C14 | -2.86 | 114.51      | 119.01   |
| 40  | 3     | 611  | CHL  | C1-C2-C3    | -2.86 | 121.51      | 126.20   |
| 22  | 6     | 603  | CLA  | C2C-C1C-NC  | 2.86  | 112.99      | 109.98   |
| 22  | 9     | 606  | CLA  | CAA-C2A-C3A | -2.86 | 105.27      | 113.00   |
| 40  | Z     | 613  | CHL  | C1A-CHA-C4D | 2.86  | 123.75      | 118.98   |
| 22  | 2     | 604  | CLA  | C1C-C2C-C3C | -2.86 | 103.97      | 106.98   |
| 22  | 5     | 602  | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 22  | B     | 1214 | CLA  | OBD-CAD-C3D | -2.86 | 121.73      | 128.42   |
| 25  | L     | 4002 | BCR  | C38-C26-C25 | -2.86 | 121.36      | 124.48   |
| 22  | 4     | 607  | CLA  | C2C-C1C-NC  | 2.86  | 112.98      | 109.98   |
| 22  | 6     | 602  | CLA  | C2C-C1C-NC  | 2.86  | 112.98      | 109.98   |
| 22  | 9     | 603  | CLA  | C2C-C1C-NC  | 2.86  | 112.98      | 109.98   |
| 22  | 1     | 608  | CLA  | C1C-C2C-C3C | -2.86 | 103.97      | 106.98   |
| 22  | A     | 1128 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 39  | 3     | 501  | LUT  | C18-C5-C6   | -2.86 | 121.37      | 124.48   |
| 22  | 4     | 605  | CLA  | C2C-C1C-NC  | 2.86  | 112.98      | 109.98   |
| 22  | 9     | 607  | CLA  | CMA-C3A-C4A | 2.86  | 119.45      | 111.77   |
| 25  | J     | 4001 | BCR  | C30-C25-C24 | 2.85  | 123.39      | 115.65   |
| 39  | 6     | 502  | LUT  | C10-C11-C12 | -2.85 | 114.93      | 123.20   |
| 39  | 8     | 502  | LUT  | C11-C10-C9  | -2.85 | 123.28      | 127.28   |
| 22  | B     | 1236 | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 39  | 6     | 502  | LUT  | C35-C15-C14 | -2.85 | 117.69      | 123.52   |
| 39  | 1     | 502  | LUT  | C11-C10-C9  | -2.85 | 123.28      | 127.28   |
| 39  | 2     | 503  | LUT  | C40-C33-C34 | -2.85 | 118.20      | 122.82   |
| 22  | 7     | 603  | CLA  | O2A-CGA-CBA | 2.85  | 120.52      | 111.83   |
| 22  | A     | 1135 | CLA  | C2C-C1C-NC  | 2.85  | 112.97      | 109.98   |
| 40  | 8     | 610  | CHL  | C4D-CHA-CBD | -2.85 | 106.09      | 108.97   |
| 22  | 9     | 603  | CLA  | CMA-C3A-C4A | 2.85  | 119.43      | 111.77   |
| 40  | 6     | 611  | CHL  | C3C-C4C-NC  | -2.85 | 107.69      | 114.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 603  | CLA  | CAA-C2A-C3A | -2.85 | 105.30      | 113.00   |
| 27  | 8     | 802  | NKP  | OAB-PAC-OAA | 2.85  | 118.48      | 107.80   |
| 22  | A     | 1136 | CLA  | C1C-C2C-C3C | -2.85 | 103.99      | 106.98   |
| 22  | A     | 1128 | CLA  | C1-C2-C3    | -2.85 | 121.53      | 126.20   |
| 39  | 1     | 502  | LUT  | C15-C14-C13 | -2.85 | 123.29      | 127.28   |
| 28  | B     | 5005 | LMT  | O5'-C1'-C2' | -2.84 | 104.53      | 110.37   |
| 22  | 6     | 618  | CLA  | C2D-C1D-ND  | 2.84  | 112.94      | 110.13   |
| 22  | A     | 1127 | CLA  | CMA-C3A-C4A | 2.84  | 119.42      | 111.77   |
| 22  | 4     | 609  | CLA  | C4B-CHC-C1C | 2.84  | 132.93      | 126.25   |
| 25  | B     | 4004 | BCR  | C33-C5-C6   | -2.84 | 121.38      | 124.48   |
| 22  | 7     | 616  | CLA  | CMA-C3A-C4A | 2.84  | 119.41      | 111.77   |
| 36  | F     | 4001 | RRX  | C30-C25-C24 | 2.84  | 123.36      | 115.65   |
| 25  | A     | 4003 | BCR  | C19-C18-C17 | 2.84  | 123.48      | 119.01   |
| 22  | L     | 1503 | CLA  | C2C-C1C-NC  | 2.84  | 112.97      | 109.98   |
| 22  | 4     | 615  | CLA  | CMA-C3A-C4A | 2.84  | 119.40      | 111.77   |
| 25  | A     | 4003 | BCR  | C1-C6-C7    | 2.84  | 123.35      | 115.65   |
| 39  | 5     | 501  | LUT  | C26-C27-C28 | -2.84 | 120.16      | 124.58   |
| 22  | A     | 1101 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 40  | 5     | 611  | CHL  | C1A-CHA-C4D | 2.84  | 123.72      | 118.98   |
| 22  | B     | 1229 | CLA  | CAA-CBA-CGA | -2.84 | 105.15      | 113.21   |
| 22  | 5     | 605  | CLA  | CMA-C3A-C4A | 2.84  | 119.40      | 111.77   |
| 22  | 8     | 603  | CLA  | C1D-ND-C4D  | -2.84 | 104.32      | 106.31   |
| 22  | 4     | 605  | CLA  | C1C-C2C-C3C | -2.84 | 104.00      | 106.98   |
| 22  | A     | 1102 | CLA  | C1-C2-C3    | -2.84 | 121.55      | 126.20   |
| 26  | 1     | 801  | LHG  | O8-C23-C24  | 2.83  | 120.47      | 111.83   |
| 22  | B     | 1238 | CLA  | C2C-C1C-NC  | 2.83  | 112.96      | 109.98   |
| 22  | 7     | 602  | CLA  | C2C-C1C-NC  | 2.83  | 112.96      | 109.98   |
| 39  | 9     | 501  | LUT  | C10-C11-C12 | -2.83 | 114.99      | 123.20   |
| 39  | 2     | 503  | LUT  | C35-C34-C33 | -2.83 | 123.31      | 127.28   |
| 22  | 5     | 618  | CLA  | C2D-C1D-ND  | 2.83  | 112.93      | 110.13   |
| 45  | 8     | 803  | LPX  | O3-P1-O4    | 2.83  | 125.61      | 112.44   |
| 25  | L     | 4001 | BCR  | C28-C27-C26 | -2.83 | 109.01      | 114.06   |
| 27  | A     | 5004 | NKP  | OAB-PAC-OAA | 2.83  | 118.41      | 107.80   |
| 22  | G     | 1601 | CLA  | C2C-C1C-NC  | 2.83  | 112.95      | 109.98   |
| 22  | B     | 1217 | CLA  | C1-C2-C3    | -2.83 | 121.56      | 126.20   |
| 22  | 7     | 608  | CLA  | C1C-C2C-C3C | -2.83 | 104.01      | 106.98   |
| 22  | 9     | 608  | CLA  | C2C-C1C-NC  | 2.83  | 112.95      | 109.98   |
| 22  | 6     | 601  | CLA  | O2A-CGA-CBA | 2.83  | 120.45      | 111.83   |
| 21  | A     | 1011 | CL0  | CMC-C2C-C1C | 2.83  | 129.82      | 124.73   |
| 22  | A     | 1013 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 22  | A     | 1122 | CLA  | C1C-C2C-C3C | -2.82 | 104.01      | 106.98   |
| 23  | B     | 2002 | PQN  | C11-C12-C13 | -2.82 | 121.97      | 126.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | G     | 1602 | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | B     | 1209 | CLA  | C4B-CHC-C1C | 2.82  | 132.88      | 126.25   |
| 32  | 9     | 802  | DGA  | OG1-CA1-CA2 | 2.82  | 120.44      | 111.83   |
| 22  | B     | 1215 | CLA  | CMA-C3A-C4A | 2.82  | 119.36      | 111.77   |
| 22  | 5     | 609  | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | B     | 1207 | CLA  | CMA-C3A-C4A | 2.82  | 119.36      | 111.77   |
| 22  | A     | 1108 | CLA  | C2C-C1C-NC  | 2.82  | 112.94      | 109.98   |
| 22  | A     | 1121 | CLA  | C2C-C1C-NC  | 2.82  | 112.94      | 109.98   |
| 25  | K     | 4001 | BCR  | C2-C1-C6    | 2.82  | 114.54      | 110.44   |
| 22  | Z     | 603  | CLA  | O2A-CGA-CBA | 2.82  | 120.43      | 111.83   |
| 22  | B     | 1226 | CLA  | CAC-C3C-C4C | 2.82  | 128.46      | 124.79   |
| 22  | B     | 1223 | CLA  | CMA-C3A-C4A | 2.82  | 119.35      | 111.77   |
| 22  | A     | 1118 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 22  | A     | 1105 | CLA  | CMA-C3A-C4A | 2.82  | 119.35      | 111.77   |
| 22  | B     | 1229 | CLA  | C1C-C2C-C3C | -2.82 | 104.02      | 106.98   |
| 22  | 2     | 615  | CLA  | C1C-C2C-C3C | -2.82 | 104.02      | 106.98   |
| 22  | A     | 1101 | CLA  | C1-C2-C3    | -2.82 | 121.58      | 126.20   |
| 32  | A     | 5005 | DGA  | OG1-CA1-CA2 | 2.82  | 120.42      | 111.83   |
| 43  | 6     | 802  | 3PH  | O31-C31-C32 | 2.82  | 120.42      | 111.83   |
| 22  | 8     | 609  | CLA  | C2C-C1C-NC  | 2.82  | 112.94      | 109.98   |
| 22  | A     | 1137 | CLA  | C1C-C2C-C3C | -2.82 | 104.02      | 106.98   |
| 22  | 7     | 603  | CLA  | C6-C5-C3    | -2.82 | 106.61      | 113.47   |
| 39  | 2     | 502  | LUT  | C40-C33-C32 | 2.82  | 122.39      | 118.09   |
| 25  | L     | 4001 | BCR  | C33-C5-C6   | -2.82 | 121.41      | 124.48   |
| 39  | 2     | 501  | LUT  | C10-C11-C12 | -2.81 | 115.05      | 123.20   |
| 22  | 6     | 615  | CLA  | C1C-C2C-C3C | -2.81 | 104.02      | 106.98   |
| 22  | B     | 1226 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 22  | 1     | 608  | CLA  | C1-C2-C3    | -2.81 | 121.59      | 126.20   |
| 22  | 6     | 607  | CLA  | C2C-C1C-NC  | 2.81  | 112.94      | 109.98   |
| 22  | 3     | 610  | CLA  | C4B-CHC-C1C | 2.81  | 132.86      | 126.25   |
| 22  | B     | 1205 | CLA  | C1-C2-C3    | -2.81 | 121.59      | 126.20   |
| 22  | Z     | 612  | CLA  | CMA-C3A-C4A | 2.81  | 119.33      | 111.77   |
| 22  | 5     | 615  | CLA  | C1-C2-C3    | -2.81 | 122.22      | 126.76   |
| 22  | A     | 1122 | CLA  | C2C-C1C-NC  | 2.81  | 112.93      | 109.98   |
| 22  | 1     | 605  | CLA  | C1C-C2C-C3C | -2.81 | 104.03      | 106.98   |
| 22  | 9     | 603  | CLA  | C1-C2-C3    | -2.81 | 121.59      | 126.20   |
| 22  | 7     | 602  | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 22  | 6     | 606  | CLA  | C2C-C1C-NC  | 2.81  | 112.93      | 109.98   |
| 22  | 3     | 612  | CLA  | C1C-C2C-C3C | -2.81 | 104.03      | 106.98   |
| 22  | A     | 1107 | CLA  | CMA-C3A-C4A | 2.81  | 119.32      | 111.77   |
| 22  | 6     | 615  | CLA  | C2C-C1C-NC  | 2.81  | 112.93      | 109.98   |
| 22  | 8     | 607  | CLA  | C2C-C1C-NC  | 2.81  | 112.93      | 109.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 40  | 5     | 610  | CHL  | C3C-C4C-NC  | -2.81 | 107.79      | 114.65   |
| 39  | 8     | 502  | LUT  | C10-C11-C12 | -2.81 | 115.07      | 123.20   |
| 40  | 2     | 610  | CHL  | C1A-CHA-C4D | 2.80  | 123.66      | 118.98   |
| 22  | B     | 1224 | CLA  | O1D-CGD-CBD | -2.80 | 118.99      | 124.52   |
| 22  | A     | 1113 | CLA  | CMA-C3A-C4A | 2.80  | 119.31      | 111.77   |
| 22  | A     | 1108 | CLA  | C1C-C2C-C3C | -2.80 | 104.03      | 106.98   |
| 22  | 8     | 603  | CLA  | O2A-CGA-CBA | 2.80  | 120.38      | 111.83   |
| 22  | 5     | 606  | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 22  | A     | 1114 | CLA  | CMA-C3A-C4A | 2.80  | 119.31      | 111.77   |
| 22  | B     | 1211 | CLA  | C1D-ND-C4D  | -2.80 | 104.35      | 106.31   |
| 22  | B     | 1241 | CLA  | C1D-ND-C4D  | -2.80 | 104.35      | 106.31   |
| 22  | 2     | 603  | CLA  | CBA-CAA-C2A | 2.80  | 122.13      | 113.79   |
| 22  | A     | 1128 | CLA  | C1C-C2C-C3C | -2.80 | 104.03      | 106.98   |
| 22  | 3     | 616  | CLA  | C1C-C2C-C3C | -2.80 | 104.03      | 106.98   |
| 22  | B     | 1240 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 22  | A     | 1140 | CLA  | C1C-C2C-C3C | -2.80 | 104.03      | 106.98   |
| 25  | 5     | 503  | BCR  | C33-C5-C4   | 2.80  | 119.57      | 113.60   |
| 39  | 2     | 502  | LUT  | C35-C34-C33 | -2.80 | 123.35      | 127.28   |
| 22  | B     | 1022 | CLA  | C2C-C1C-NC  | 2.80  | 112.92      | 109.98   |
| 22  | K     | 1403 | CLA  | CMA-C3A-C4A | 2.80  | 119.30      | 111.77   |
| 22  | B     | 1225 | CLA  | C4B-CHC-C1C | 2.80  | 132.82      | 126.25   |
| 22  | 6     | 609  | CLA  | C1C-C2C-C3C | -2.80 | 104.04      | 106.98   |
| 37  | 1     | 503  | C7Z  | C1-C6-C5    | -2.80 | 118.82      | 122.64   |
| 22  | 8     | 615  | CLA  | C1C-C2C-C3C | -2.79 | 104.04      | 106.98   |
| 22  | A     | 1116 | CLA  | O2A-CGA-CBA | 2.79  | 120.36      | 111.83   |
| 39  | 1     | 502  | LUT  | C26-C27-C28 | -2.79 | 120.23      | 124.58   |
| 22  | 6     | 618  | CLA  | CMA-C3A-C4A | 2.79  | 119.28      | 111.77   |
| 22  | 8     | 605  | CLA  | C1C-C2C-C3C | -2.79 | 104.04      | 106.98   |
| 22  | A     | 1132 | CLA  | CAA-C2A-C3A | -2.79 | 105.46      | 113.00   |
| 22  | 2     | 605  | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 22  | B     | 1218 | CLA  | CMA-C3A-C4A | 2.79  | 119.27      | 111.77   |
| 22  | 9     | 603  | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 22  | B     | 1217 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 22  | 5     | 601  | CLA  | C1-C2-C3    | -2.79 | 121.63      | 126.20   |
| 22  | 7     | 607  | CLA  | C2C-C1C-NC  | 2.79  | 112.91      | 109.98   |
| 22  | A     | 1138 | CLA  | C1C-C2C-C3C | -2.79 | 104.05      | 106.98   |
| 22  | B     | 1231 | CLA  | CMD-C2D-C3D | -2.79 | 121.30      | 127.69   |
| 22  | A     | 1107 | CLA  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 22  | 7     | 601  | CLA  | O2A-CGA-CBA | 2.79  | 120.34      | 111.83   |
| 26  | Z     | 801  | LHG  | O8-C23-C24  | 2.79  | 120.33      | 111.83   |
| 39  | 9     | 501  | LUT  | C35-C15-C14 | -2.79 | 117.82      | 123.52   |
| 40  | 5     | 617  | CHL  | C4D-CHA-CBD | -2.79 | 106.16      | 108.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1213 | CLA  | C1-C2-C3    | -2.79 | 121.63      | 126.20   |
| 22  | 7     | 605  | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 22  | 2     | 603  | CLA  | C2C-C1C-NC  | 2.79  | 112.91      | 109.98   |
| 22  | B     | 1218 | CLA  | O2A-CGA-CBA | 2.79  | 120.33      | 111.83   |
| 22  | B     | 1206 | CLA  | C1-C2-C3    | -2.79 | 121.63      | 126.20   |
| 22  | F     | 1301 | CLA  | C3B-C4B-NB  | -2.78 | 108.04      | 110.53   |
| 22  | B     | 1221 | CLA  | O1D-CGD-CBD | -2.78 | 119.03      | 124.52   |
| 40  | 7     | 610  | CHL  | C1-C2-C3    | -2.78 | 121.64      | 126.20   |
| 25  | 3     | 506  | BCR  | C37-C22-C21 | -2.78 | 118.31      | 122.82   |
| 40  | 8     | 613  | CHL  | C3C-C4C-NC  | -2.78 | 107.84      | 114.65   |
| 22  | 6     | 612  | CLA  | C2C-C1C-NC  | 2.78  | 112.91      | 109.98   |
| 22  | F     | 1301 | CLA  | C6-C5-C3    | -2.78 | 106.69      | 113.47   |
| 22  | A     | 1121 | CLA  | CHD-C1D-ND  | -2.78 | 120.89      | 124.80   |
| 22  | Z     | 607  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 3     | 605  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | B     | 1222 | CLA  | C1-O2A-CGA  | 2.78  | 123.38      | 116.65   |
| 22  | 8     | 605  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 3     | 610  | CLA  | C1-C2-C3    | -2.78 | 121.64      | 126.20   |
| 22  | A     | 1112 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 22  | 2     | 602  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 43  | 8     | 806  | 3PH  | O31-C31-C32 | 2.78  | 120.30      | 111.83   |
| 40  | 4     | 617  | CHL  | C3C-C4C-NC  | -2.78 | 107.86      | 114.65   |
| 22  | 8     | 612  | CLA  | C1C-C2C-C3C | -2.78 | 104.06      | 106.98   |
| 22  | A     | 1141 | CLA  | CMA-C3A-C4A | 2.78  | 119.23      | 111.77   |
| 22  | 6     | 612  | CLA  | C1C-C2C-C3C | -2.78 | 104.06      | 106.98   |
| 22  | A     | 1129 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 39  | 3     | 502  | LUT  | C10-C11-C12 | -2.77 | 115.16      | 123.20   |
| 40  | Z     | 609  | CHL  | CMA-C3A-C4A | 2.77  | 120.59      | 114.61   |
| 22  | 8     | 611  | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 22  | 8     | 612  | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 39  | 6     | 502  | LUT  | C26-C27-C28 | -2.77 | 120.26      | 124.58   |
| 39  | 1     | 501  | LUT  | C7-C8-C9    | -2.77 | 122.13      | 126.23   |
| 22  | 3     | 608  | CLA  | CMA-C3A-C4A | 2.77  | 119.22      | 111.77   |
| 22  | Z     | 605  | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 25  | A     | 4001 | BCR  | C12-C13-C14 | -2.77 | 114.65      | 119.01   |
| 22  | A     | 1111 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 40  | 5     | 617  | CHL  | C3C-C4C-NC  | -2.77 | 107.88      | 114.65   |
| 22  | 1     | 608  | CLA  | CMD-C2D-C3D | -2.77 | 121.33      | 127.69   |
| 25  | B     | 4003 | BCR  | C33-C5-C4   | 2.77  | 119.50      | 113.60   |
| 22  | A     | 1116 | CLA  | CMA-C3A-C4A | 2.77  | 119.22      | 111.77   |
| 22  | 3     | 603  | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 22  | 2     | 605  | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1120 | CLA  | C1C-C2C-C3C | -2.77 | 104.07      | 106.98   |
| 22  | 8     | 615  | CLA  | CMA-C3A-C4A | 2.77  | 119.21      | 111.77   |
| 25  | A     | 4002 | BCR  | C27-C26-C25 | -2.77 | 118.96      | 122.70   |
| 25  | 3     | 504  | BCR  | C36-C18-C17 | -2.77 | 118.33      | 122.82   |
| 22  | 1     | 604  | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 22  | 8     | 609  | CLA  | C4B-CHC-C1C | 2.77  | 132.75      | 126.25   |
| 22  | B     | 1206 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 37  | 5     | 505  | C7Z  | C28-C27-C26 | -2.77 | 119.61      | 127.00   |
| 22  | B     | 1238 | CLA  | O2D-CGD-O1D | -2.77 | 118.47      | 123.85   |
| 22  | 7     | 608  | CLA  | CMA-C3A-C4A | 2.77  | 119.20      | 111.77   |
| 22  | B     | 1236 | CLA  | C4B-CHC-C1C | 2.76  | 132.75      | 126.25   |
| 25  | 6     | 503  | BCR  | C33-C5-C4   | 2.76  | 119.49      | 113.60   |
| 22  | B     | 1234 | CLA  | C2C-C1C-NC  | 2.76  | 112.89      | 109.98   |
| 22  | L     | 1502 | CLA  | C2C-C1C-NC  | 2.76  | 112.89      | 109.98   |
| 22  | A     | 1119 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 22  | 8     | 602  | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 22  | A     | 1106 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 43  | 7     | 802  | 3PH  | O31-C31-C32 | 2.76  | 120.26      | 111.83   |
| 22  | A     | 1124 | CLA  | C4B-CHC-C1C | 2.76  | 132.74      | 126.25   |
| 22  | Z     | 601  | CLA  | O2A-CGA-CBA | 2.76  | 120.25      | 111.83   |
| 40  | 9     | 610  | CHL  | C1A-CHA-C4D | 2.76  | 123.59      | 118.98   |
| 22  | B     | 1224 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 26  | A     | 5002 | LHG  | O8-C23-C24  | 2.76  | 120.25      | 111.83   |
| 41  | 1     | 802  | SQD  | O7-S-C6     | -2.76 | 102.64      | 106.76   |
| 22  | B     | 1203 | CLA  | C2C-C1C-NC  | 2.76  | 112.88      | 109.98   |
| 43  | 2     | 802  | 3PH  | O31-C31-C32 | 2.76  | 120.25      | 111.83   |
| 26  | 7     | 801  | LHG  | C5-O7-C7    | -2.76 | 111.19      | 117.80   |
| 22  | B     | 1229 | CLA  | C1-C2-C3    | -2.76 | 121.68      | 126.20   |
| 22  | 1     | 612  | CLA  | CMA-C3A-C4A | 2.76  | 119.19      | 111.77   |
| 39  | 4     | 501  | LUT  | C18-C5-C6   | -2.76 | 121.47      | 124.48   |
| 22  | A     | 1134 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 22  | B     | 1205 | CLA  | C1-O2A-CGA  | 2.76  | 123.32      | 116.65   |
| 25  | A     | 4004 | BCR  | C38-C26-C27 | 2.76  | 119.47      | 113.60   |
| 26  | 6     | 801  | LHG  | O8-C23-C24  | 2.76  | 120.24      | 111.83   |
| 22  | 5     | 612  | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 22  | 1     | 611  | CLA  | C2C-C1C-NC  | 2.76  | 112.88      | 109.98   |
| 22  | 6     | 607  | CLA  | CMA-C3A-C4A | 2.76  | 119.18      | 111.77   |
| 22  | B     | 1224 | CLA  | C1-C2-C3    | -2.75 | 121.69      | 126.20   |
| 22  | 9     | 612  | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 22  | A     | 1131 | CLA  | C1C-C2C-C3C | -2.75 | 104.08      | 106.98   |
| 39  | 2     | 503  | LUT  | C18-C5-C4   | 2.75  | 119.48      | 114.42   |
| 22  | B     | 1207 | CLA  | C4B-CHC-C1C | 2.75  | 132.72      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | 2     | 502  | LUT  | C39-C29-C28 | 2.75  | 122.29      | 118.09   |
| 22  | B     | 1204 | CLA  | C1C-C2C-C3C | -2.75 | 104.08      | 106.98   |
| 22  | 5     | 618  | CLA  | C1C-C2C-C3C | -2.75 | 104.08      | 106.98   |
| 22  | 4     | 615  | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 26  | B     | 5006 | LHG  | O8-C23-C24  | 2.75  | 120.23      | 111.83   |
| 40  | 5     | 611  | CHL  | C3C-C4C-NC  | -2.75 | 107.92      | 114.65   |
| 25  | A     | 4004 | BCR  | C35-C13-C12 | 2.75  | 122.29      | 118.09   |
| 40  | 4     | 611  | CHL  | C1-O2A-CGA  | 2.75  | 123.31      | 116.65   |
| 22  | B     | 1229 | CLA  | O2A-CGA-CBA | 2.75  | 120.22      | 111.83   |
| 22  | B     | 1211 | CLA  | O2A-CGA-CBA | 2.75  | 120.22      | 111.83   |
| 22  | 9     | 603  | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 9     | 604  | CLA  | C4B-CHC-C1C | 2.75  | 132.71      | 126.25   |
| 39  | 2     | 503  | LUT  | C36-C21-C22 | -2.75 | 104.28      | 109.41   |
| 22  | 5     | 601  | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 22  | 5     | 606  | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 6     | 604  | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | 2     | 604  | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 40  | 6     | 617  | CHL  | C3C-C4C-NC  | -2.75 | 107.94      | 114.65   |
| 22  | A     | 1112 | CLA  | O2A-CGA-CBA | 2.75  | 120.21      | 111.83   |
| 22  | Z     | 607  | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 22  | 7     | 616  | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 40  | 4     | 610  | CHL  | C3C-C4C-NC  | -2.75 | 107.94      | 114.65   |
| 22  | 8     | 609  | CLA  | C1-C2-C3    | -2.75 | 121.70      | 126.20   |
| 22  | 3     | 606  | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 5     | 605  | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 5     | 622  | CLA  | CMA-C3A-C4A | 2.75  | 119.15      | 111.77   |
| 39  | 2     | 502  | LUT  | C30-C31-C32 | -2.75 | 115.25      | 123.20   |
| 22  | B     | 1238 | CLA  | C1C-C2C-C3C | -2.74 | 104.09      | 106.98   |
| 22  | A     | 1120 | CLA  | CHD-C1D-ND  | -2.74 | 120.94      | 124.80   |
| 25  | B     | 4005 | BCR  | C33-C5-C6   | -2.74 | 121.49      | 124.48   |
| 22  | 1     | 607  | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | B     | 1021 | CLA  | C4B-CHC-C1C | 2.74  | 132.69      | 126.25   |
| 22  | A     | 1132 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | 6     | 603  | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | A     | 1140 | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | 9     | 608  | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | 2     | 608  | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | 7     | 616  | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 22  | A     | 1121 | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 22  | B     | 1232 | CLA  | CMA-C3A-C4A | 2.74  | 119.13      | 111.77   |
| 22  | 7     | 607  | CLA  | C1-C2-C3    | -2.74 | 121.71      | 126.20   |
| 39  | 4     | 501  | LUT  | C15-C14-C13 | -2.74 | 123.44      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1241 | CLA  | O2A-CGA-CBA | 2.74  | 120.18      | 111.83   |
| 22  | 1     | 613  | CLA  | CMA-C3A-C4A | 2.74  | 119.13      | 111.77   |
| 22  | 5     | 615  | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | Z     | 605  | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | 4     | 609  | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | A     | 1012 | CLA  | CAA-C2A-C3A | -2.74 | 105.61      | 113.00   |
| 39  | 2     | 502  | LUT  | C7-C8-C9    | -2.73 | 122.19      | 126.23   |
| 39  | 2     | 503  | LUT  | C1-C6-C5    | -2.73 | 118.90      | 122.64   |
| 22  | B     | 1207 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | B     | 1236 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | Z     | 615  | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 22  | A     | 1135 | CLA  | CMA-C3A-C4A | 2.73  | 119.12      | 111.77   |
| 22  | 5     | 609  | CLA  | O2A-CGA-CBA | 2.73  | 120.17      | 111.83   |
| 22  | A     | 1123 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 22  | G     | 1602 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 22  | A     | 1134 | CLA  | CMA-C3A-C4A | 2.73  | 119.11      | 111.77   |
| 22  | 1     | 612  | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | 5     | 609  | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 22  | Z     | 607  | CLA  | CMA-C3A-C4A | 2.73  | 119.11      | 111.77   |
| 25  | B     | 4006 | BCR  | C35-C13-C12 | 2.73  | 122.26      | 118.09   |
| 40  | 6     | 610  | CHL  | C1-C2-C3    | -2.73 | 121.73      | 126.20   |
| 22  | 5     | 604  | CLA  | C4B-CHC-C1C | 2.73  | 132.66      | 126.25   |
| 22  | 9     | 602  | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | 2     | 605  | CLA  | CHA-C4D-ND  | 2.73  | 138.17      | 132.55   |
| 22  | A     | 1135 | CLA  | C4B-CHC-C1C | 2.73  | 132.66      | 126.25   |
| 22  | B     | 1202 | CLA  | C1-O2A-CGA  | 2.72  | 123.25      | 116.65   |
| 22  | 1     | 615  | CLA  | C1C-C2C-C3C | -2.72 | 104.11      | 106.98   |
| 22  | A     | 1109 | CLA  | O2A-CGA-CBA | 2.72  | 120.14      | 111.83   |
| 22  | A     | 1110 | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 22  | 6     | 615  | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 22  | B     | 1216 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 25  | B     | 4004 | BCR  | C37-C22-C23 | 2.72  | 122.25      | 118.09   |
| 22  | 6     | 608  | CLA  | CMD-C2D-C3D | -2.72 | 121.45      | 127.69   |
| 22  | 7     | 609  | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 40  | 9     | 613  | CHL  | C3C-C4C-NC  | -2.72 | 108.00      | 114.65   |
| 22  | 4     | 605  | CLA  | C4B-CHC-C1C | 2.72  | 132.65      | 126.25   |
| 22  | 2     | 606  | CLA  | O2D-CGD-O1D | -2.72 | 118.55      | 123.85   |
| 22  | Z     | 611  | CLA  | C1-O2A-CGA  | 2.72  | 123.24      | 116.65   |
| 22  | 3     | 607  | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | 3     | 606  | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 39  | 2     | 501  | LUT  | C28-C29-C30 | -2.72 | 114.73      | 119.01   |
| 22  | A     | 1012 | CLA  | OBD-CAD-C3D | -2.72 | 122.06      | 128.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1141 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | 4     | 608  | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 40  | 1     | 610  | CHL  | C3C-C4C-NC  | -2.72 | 108.01      | 114.65   |
| 40  | 4     | 611  | CHL  | C3C-C4C-NC  | -2.72 | 108.01      | 114.65   |
| 22  | B     | 1227 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | K     | 1404 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | 5     | 618  | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | B     | 1215 | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 22  | J     | 1901 | CLA  | CMA-C3A-C4A | 2.72  | 119.07      | 111.77   |
| 22  | 6     | 608  | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | B     | 1211 | CLA  | CHD-C1D-ND  | -2.72 | 120.98      | 124.80   |
| 40  | 4     | 613  | CHL  | C1-C2-C3    | -2.72 | 121.75      | 126.20   |
| 22  | Z     | 607  | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 39  | Z     | 502  | LUT  | C10-C11-C12 | -2.72 | 115.33      | 123.20   |
| 22  | 4     | 602  | CLA  | C2C-C1C-NC  | 2.72  | 112.83      | 109.98   |
| 22  | K     | 1404 | CLA  | C1-C2-C3    | -2.71 | 121.75      | 126.20   |
| 22  | 4     | 609  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 26  | A     | 5001 | LHG  | C5-O7-C7    | -2.71 | 111.30      | 117.80   |
| 22  | A     | 1121 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 39  | 3     | 501  | LUT  | C22-C23-C24 | -2.71 | 107.16      | 111.18   |
| 22  | B     | 1231 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | 7     | 615  | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | 1     | 611  | CLA  | CMA-C3A-C4A | 2.71  | 119.06      | 111.77   |
| 22  | 9     | 604  | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | 3     | 608  | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | B     | 1239 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 22  | 2     | 608  | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 22  | 4     | 607  | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 25  | B     | 4001 | BCR  | C37-C22-C23 | 2.71  | 122.23      | 118.09   |
| 22  | A     | 1123 | CLA  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 22  | A     | 1130 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | A     | 1130 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 40  | 2     | 613  | CHL  | C1A-CHA-C4D | 2.71  | 123.50      | 118.98   |
| 22  | B     | 1225 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | B     | 1239 | CLA  | O2A-CGA-CBA | 2.71  | 120.09      | 111.83   |
| 22  | B     | 1022 | CLA  | OBD-CAD-C3D | -2.71 | 122.09      | 128.42   |
| 22  | 2     | 606  | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | B     | 1217 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | B     | 1213 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | 5     | 613  | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 39  | 2     | 501  | LUT  | C18-C5-C6   | -2.71 | 121.53      | 124.48   |
| 22  | 1     | 601  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | G     | 1602 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 8     | 609  | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | 8     | 608  | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 1     | 606  | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 22  | Z     | 602  | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 3     | 603  | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | A     | 1113 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | 6     | 601  | CLA  | C1-O2A-CGA  | 2.70  | 123.19      | 116.65   |
| 39  | 8     | 501  | LUT  | C38-C25-C24 | -2.70 | 116.97      | 123.36   |
| 25  | 4     | 503  | BCR  | C38-C26-C25 | -2.70 | 121.54      | 124.48   |
| 22  | B     | 1210 | CLA  | C4B-CHC-C1C | 2.70  | 132.60      | 126.25   |
| 22  | B     | 1201 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 25  | 3     | 503  | BCR  | C35-C13-C12 | 2.70  | 122.21      | 118.09   |
| 22  | A     | 1116 | CLA  | C1-C2-C3    | -2.70 | 121.77      | 126.20   |
| 22  | 4     | 603  | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 25  | A     | 4003 | BCR  | C4-C5-C6    | -2.70 | 119.06      | 122.70   |
| 22  | K     | 1401 | CLA  | C2C-C1C-NC  | 2.70  | 112.81      | 109.98   |
| 22  | 5     | 602  | CLA  | C2C-C1C-NC  | 2.70  | 112.81      | 109.98   |
| 25  | 4     | 503  | BCR  | C33-C5-C4   | 2.70  | 119.35      | 113.60   |
| 22  | 7     | 609  | CLA  | O2A-CGA-CBA | 2.70  | 120.05      | 111.83   |
| 22  | Z     | 611  | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 22  | 9     | 609  | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 22  | 6     | 618  | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | 2     | 603  | CLA  | CMA-C3A-C4A | 2.69  | 119.01      | 111.77   |
| 22  | 8     | 603  | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | A     | 1107 | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | B     | 1231 | CLA  | CHD-C1D-ND  | -2.69 | 121.02      | 124.80   |
| 22  | 5     | 612  | CLA  | CHD-C1D-ND  | -2.69 | 121.02      | 124.80   |
| 22  | B     | 1235 | CLA  | CHD-C1D-ND  | -2.69 | 121.02      | 124.80   |
| 22  | F     | 1301 | CLA  | CAA-C2A-C3A | -2.69 | 105.73      | 113.00   |
| 39  | 7     | 501  | LUT  | C15-C14-C13 | -2.69 | 123.51      | 127.28   |
| 39  | 4     | 502  | LUT  | C15-C14-C13 | -2.69 | 123.51      | 127.28   |
| 22  | 7     | 606  | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | 6     | 604  | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | A     | 1124 | CLA  | O2A-CGA-CBA | 2.69  | 120.03      | 111.83   |
| 22  | B     | 1211 | CLA  | C4B-CHC-C1C | 2.69  | 132.57      | 126.25   |
| 25  | J     | 4001 | BCR  | C36-C18-C17 | -2.69 | 118.46      | 122.82   |
| 22  | K     | 1402 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | 5     | 605  | CLA  | CHD-C1D-ND  | -2.69 | 121.02      | 124.80   |
| 22  | 8     | 604  | CLA  | C1-O2A-CGA  | 2.69  | 123.15      | 116.65   |
| 22  | 3     | 602  | CLA  | C2C-C1C-NC  | 2.69  | 112.80      | 109.98   |
| 23  | B     | 2002 | PQN  | C14-C13-C15 | 2.69  | 119.89      | 115.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 618  | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 40  | 2     | 609  | CHL  | C1A-CHA-C4D | 2.69  | 123.46      | 118.98   |
| 22  | J     | 1901 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | 4     | 603  | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | B     | 1218 | CLA  | C1-O2A-CGA  | 2.68  | 123.15      | 116.65   |
| 40  | 5     | 617  | CHL  | C1A-CHA-C4D | 2.68  | 123.46      | 118.98   |
| 22  | B     | 1229 | CLA  | CMA-C3A-C4A | 2.68  | 118.98      | 111.77   |
| 25  | B     | 4005 | BCR  | C12-C13-C14 | -2.68 | 114.79      | 119.01   |
| 22  | 5     | 605  | CLA  | CMD-C2D-C3D | -2.68 | 121.54      | 127.69   |
| 22  | 7     | 613  | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | A     | 1115 | CLA  | CMA-C3A-C4A | 2.68  | 118.98      | 111.77   |
| 22  | 1     | 608  | CLA  | CHD-C1D-ND  | -2.68 | 121.03      | 124.80   |
| 22  | Z     | 606  | CLA  | C2C-C1C-NC  | 2.68  | 112.80      | 109.98   |
| 22  | A     | 1121 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 22  | 9     | 605  | CLA  | CHA-C4D-ND  | 2.68  | 138.08      | 132.55   |
| 22  | 1     | 603  | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 40  | 2     | 613  | CHL  | C3C-C4C-NC  | -2.68 | 108.11      | 114.65   |
| 25  | L     | 4001 | BCR  | C27-C26-C25 | -2.68 | 119.09      | 122.70   |
| 22  | 8     | 609  | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | K     | 1403 | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 22  | Z     | 606  | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 22  | 4     | 609  | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 25  | K     | 4002 | BCR  | C31-C1-C6   | -2.68 | 106.05      | 110.24   |
| 22  | 8     | 607  | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 22  | A     | 1112 | CLA  | C2C-C1C-NC  | 2.68  | 112.79      | 109.98   |
| 22  | A     | 1133 | CLA  | C2C-C1C-NC  | 2.68  | 112.79      | 109.98   |
| 22  | B     | 1022 | CLA  | CAA-C2A-C3A | -2.67 | 105.77      | 113.00   |
| 40  | 2     | 610  | CHL  | CMA-C3A-C4A | 2.67  | 120.37      | 114.61   |
| 22  | A     | 1104 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 6     | 606  | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 1     | 613  | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 22  | B     | 1229 | CLA  | C1D-ND-C4D  | -2.67 | 104.44      | 106.31   |
| 22  | B     | 1240 | CLA  | O2A-CGA-CBA | 2.67  | 119.99      | 111.83   |
| 22  | 6     | 607  | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 26  | 4     | 802  | LHG  | O8-C23-C24  | 2.67  | 119.98      | 111.83   |
| 39  | 1     | 502  | LUT  | C35-C15-C14 | -2.67 | 118.05      | 123.52   |
| 36  | F     | 4001 | RRX  | C20-C19-C18 | -2.67 | 119.04      | 126.36   |
| 22  | B     | 1202 | CLA  | C6-C5-C3    | -2.67 | 106.96      | 113.47   |
| 22  | 2     | 607  | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | B     | 1207 | CLA  | O2D-CGD-O1D | -2.67 | 118.65      | 123.85   |
| 22  | 6     | 601  | CLA  | CAA-C2A-C3A | -2.67 | 105.78      | 113.00   |
| 26  | 9     | 801  | LHG  | O8-C23-C24  | 2.67  | 119.97      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 1     | 612  | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | B     | 1217 | CLA  | C2C-C1C-NC  | 2.67  | 112.78      | 109.98   |
| 22  | J     | 1901 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 21  | A     | 1011 | CL0  | C1-C2-C3    | -2.67 | 121.83      | 126.20   |
| 22  | 4     | 612  | CLA  | CHD-C1D-ND  | -2.67 | 121.05      | 124.80   |
| 25  | 7     | 503  | BCR  | C19-C18-C17 | 2.67  | 123.20      | 119.01   |
| 22  | 5     | 608  | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | A     | 1130 | CLA  | CMA-C3A-C4A | 2.67  | 118.94      | 111.77   |
| 22  | 7     | 611  | CLA  | C1D-ND-C4D  | -2.67 | 104.44      | 106.31   |
| 22  | B     | 1214 | CLA  | C1-O2A-CGA  | 2.67  | 123.10      | 116.65   |
| 22  | B     | 1231 | CLA  | O2D-CGD-O1D | -2.66 | 118.66      | 123.85   |
| 22  | 3     | 605  | CLA  | CHA-C4D-ND  | 2.66  | 138.05      | 132.55   |
| 22  | 6     | 605  | CLA  | C1-O2A-CGA  | 2.66  | 123.10      | 116.65   |
| 22  | 7     | 612  | CLA  | C2C-C1C-NC  | 2.66  | 112.78      | 109.98   |
| 22  | A     | 1133 | CLA  | O2A-CGA-CBA | 2.66  | 119.96      | 111.83   |
| 22  | B     | 1212 | CLA  | O2D-CGD-O1D | -2.66 | 118.66      | 123.85   |
| 22  | 5     | 605  | CLA  | C1-O2A-CGA  | 2.66  | 123.10      | 116.65   |
| 40  | 5     | 610  | CHL  | C1A-CHA-C4D | 2.66  | 123.42      | 118.98   |
| 22  | B     | 1226 | CLA  | C1-C2-C3    | -2.66 | 121.83      | 126.20   |
| 22  | A     | 1137 | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 22  | 4     | 609  | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 39  | 6     | 501  | LUT  | C10-C11-C12 | -2.66 | 115.49      | 123.20   |
| 22  | 9     | 604  | CLA  | C1-O2A-CGA  | 2.66  | 123.09      | 116.65   |
| 22  | A     | 1118 | CLA  | C1D-ND-C4D  | -2.66 | 104.44      | 106.31   |
| 22  | B     | 1223 | CLA  | CHA-C4D-ND  | 2.66  | 138.04      | 132.55   |
| 22  | 5     | 607  | CLA  | O2A-CGA-CBA | 2.66  | 119.95      | 111.83   |
| 22  | 3     | 604  | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 22  | 3     | 610  | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | 5     | 602  | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 26  | 1     | 801  | LHG  | C5-O7-C7    | -2.66 | 111.43      | 117.80   |
| 22  | 1     | 602  | CLA  | O2D-CGD-O1D | -2.66 | 118.67      | 123.85   |
| 22  | A     | 1129 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 39  | 1     | 501  | LUT  | C35-C15-C14 | -2.66 | 118.08      | 123.52   |
| 25  | A     | 4002 | BCR  | C33-C5-C6   | -2.66 | 121.58      | 124.48   |
| 22  | A     | 1101 | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 22  | B     | 1208 | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 22  | L     | 1502 | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 39  | 6     | 501  | LUT  | C39-C29-C28 | 2.66  | 122.15      | 118.09   |
| 22  | B     | 1234 | CLA  | O2D-CGD-O1D | -2.66 | 118.68      | 123.85   |
| 22  | B     | 1021 | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 22  | 8     | 603  | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 22  | 7     | 611  | CLA  | CMA-C3A-C4A | 2.66  | 118.91      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 8     | 601  | CLA  | CHA-C4D-ND  | 2.66  | 138.03      | 132.55   |
| 43  | 8     | 806  | 3PH  | O21-C21-C22 | 2.65  | 120.68      | 110.93   |
| 25  | 5     | 504  | BCR  | C33-C5-C4   | 2.65  | 119.25      | 113.60   |
| 22  | 8     | 602  | CLA  | O2D-CGD-O1D | -2.65 | 118.68      | 123.85   |
| 40  | 2     | 609  | CHL  | C4D-CHA-CBD | -2.65 | 106.29      | 108.97   |
| 42  | Z     | 504  | QTB  | C11-C10-C09 | 2.65  | 130.92      | 125.25   |
| 22  | A     | 1124 | CLA  | CAA-C2A-C1A | -2.65 | 103.28      | 111.97   |
| 22  | B     | 1231 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | 3     | 612  | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | 5     | 607  | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 26  | 5     | 801  | LHG  | O8-C23-C24  | 2.65  | 119.92      | 111.83   |
| 39  | 8     | 501  | LUT  | C18-C5-C6   | -2.65 | 121.59      | 124.48   |
| 36  | F     | 4001 | RRX  | C15-C16-C17 | -2.65 | 118.09      | 123.52   |
| 22  | A     | 1103 | CLA  | C1-C2-C3    | -2.65 | 121.85      | 126.20   |
| 43  | 5     | 802  | 3PH  | O31-C31-C32 | 2.65  | 119.92      | 111.83   |
| 22  | 2     | 605  | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | A     | 1118 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | 7     | 607  | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | Z     | 608  | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | 2     | 608  | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | Z     | 601  | CLA  | CAA-C2A-C3A | -2.65 | 105.84      | 113.00   |
| 22  | B     | 1221 | CLA  | O2D-CGD-O1D | -2.65 | 118.69      | 123.85   |
| 22  | A     | 1120 | CLA  | C1D-ND-C4D  | -2.65 | 104.45      | 106.31   |
| 22  | 3     | 604  | CLA  | C4B-CHC-C1C | 2.65  | 132.47      | 126.25   |
| 40  | 5     | 611  | CHL  | C1-C2-C3    | -2.65 | 122.48      | 126.76   |
| 22  | B     | 1222 | CLA  | CMA-C3A-C4A | 2.65  | 118.89      | 111.77   |
| 22  | A     | 1105 | CLA  | C1C-C2C-C3C | -2.65 | 104.20      | 106.98   |
| 39  | 3     | 501  | LUT  | C35-C15-C14 | -2.65 | 118.10      | 123.52   |
| 22  | 7     | 601  | CLA  | CHA-C4D-ND  | 2.65  | 138.01      | 132.55   |
| 22  | 9     | 601  | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | B     | 1206 | CLA  | O2A-CGA-CBA | 2.65  | 119.90      | 111.83   |
| 22  | 7     | 604  | CLA  | CMA-C3A-C4A | 2.65  | 118.89      | 111.77   |
| 22  | A     | 1118 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 25  | 7     | 503  | BCR  | C33-C5-C6   | -2.65 | 121.60      | 124.48   |
| 25  | A     | 4001 | BCR  | C23-C24-C25 | -2.65 | 119.93      | 127.00   |
| 22  | B     | 1202 | CLA  | CHD-C1D-ND  | -2.65 | 121.08      | 124.80   |
| 22  | L     | 1503 | CLA  | CMA-C3A-C4A | 2.65  | 118.88      | 111.77   |
| 22  | 1     | 605  | CLA  | C2C-C1C-NC  | 2.64  | 112.76      | 109.98   |
| 39  | 5     | 502  | LUT  | C35-C34-C33 | -2.64 | 123.57      | 127.28   |
| 22  | 2     | 615  | CLA  | C2C-C1C-NC  | 2.64  | 112.76      | 109.98   |
| 25  | 6     | 504  | BCR  | C28-C27-C26 | -2.64 | 109.34      | 114.06   |
| 22  | A     | 1105 | CLA  | O2D-CGD-O1D | -2.64 | 118.70      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1118 | CLA  | O2D-CGD-O1D | -2.64 | 118.70      | 123.85   |
| 39  | 4     | 502  | LUT  | C7-C8-C9    | -2.64 | 122.32      | 126.23   |
| 22  | A     | 1101 | CLA  | C2C-C1C-NC  | 2.64  | 112.76      | 109.98   |
| 22  | B     | 1221 | CLA  | CHA-C4D-ND  | 2.64  | 138.00      | 132.55   |
| 22  | 7     | 604  | CLA  | CAA-C2A-C1A | 2.64  | 120.63      | 111.97   |
| 22  | Z     | 601  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | B     | 1234 | CLA  | CMA-C3A-C4A | 2.64  | 118.87      | 111.77   |
| 40  | 9     | 610  | CHL  | C4D-CHA-CBD | -2.64 | 106.30      | 108.97   |
| 22  | F     | 1301 | CLA  | C2C-C1C-NC  | 2.64  | 112.76      | 109.98   |
| 22  | 6     | 602  | CLA  | C1C-C2C-C3C | -2.64 | 104.20      | 106.98   |
| 22  | A     | 1109 | CLA  | CHD-C1D-ND  | -2.64 | 121.09      | 124.80   |
| 22  | 3     | 604  | CLA  | CHD-C1D-ND  | -2.64 | 121.09      | 124.80   |
| 22  | 5     | 622  | CLA  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 22  | 7     | 606  | CLA  | CMD-C2D-C3D | -2.64 | 121.64      | 127.69   |
| 22  | 1     | 606  | CLA  | C1C-C2C-C3C | -2.64 | 104.20      | 106.98   |
| 22  | 7     | 613  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | A     | 1141 | CLA  | C1-C2-C3    | -2.64 | 121.87      | 126.20   |
| 22  | F     | 1301 | CLA  | C1C-C2C-C3C | -2.64 | 104.20      | 106.98   |
| 22  | A     | 1128 | CLA  | CMB-C2B-C1B | -2.64 | 121.40      | 125.42   |
| 22  | Z     | 602  | CLA  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 22  | 9     | 604  | CLA  | O1D-CGD-CBD | -2.64 | 119.31      | 124.52   |
| 22  | B     | 1209 | CLA  | C1-C2-C3    | -2.64 | 121.88      | 126.20   |
| 22  | 1     | 613  | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 22  | A     | 1130 | CLA  | C4B-CHC-C1C | 2.64  | 132.45      | 126.25   |
| 22  | B     | 1230 | CLA  | O2D-CGD-O1D | -2.64 | 118.72      | 123.85   |
| 22  | 5     | 609  | CLA  | C1C-C2C-C3C | -2.64 | 104.21      | 106.98   |
| 22  | 8     | 608  | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 40  | 6     | 613  | CHL  | C1-O2A-CGA  | 2.64  | 123.03      | 116.65   |
| 22  | 8     | 601  | CLA  | C4B-CHC-C1C | 2.64  | 132.44      | 126.25   |
| 28  | F     | 5001 | LMT  | C1'-O5'-C5' | -2.64 | 108.57      | 113.72   |
| 22  | 3     | 602  | CLA  | O2D-CGD-O1D | -2.64 | 118.72      | 123.85   |
| 25  | 7     | 503  | BCR  | C15-C14-C13 | -2.63 | 123.58      | 127.28   |
| 22  | 6     | 605  | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | A     | 1108 | CLA  | C1-C2-C3    | -2.63 | 121.88      | 126.20   |
| 22  | K     | 1402 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | 9     | 607  | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | B     | 1224 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 25  | I     | 4001 | BCR  | C35-C13-C12 | 2.63  | 122.11      | 118.09   |
| 22  | 5     | 605  | CLA  | O2A-CGA-CBA | 2.63  | 119.86      | 111.83   |
| 22  | 5     | 615  | CLA  | C4B-CHC-C1C | 2.63  | 132.44      | 126.25   |
| 22  | 1     | 605  | CLA  | CMA-C3A-C4A | 2.63  | 118.85      | 111.77   |
| 22  | B     | 1219 | CLA  | O2D-CGD-O1D | -2.63 | 118.72      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 7     | 503  | BCR  | C36-C18-C17 | -2.63 | 118.55      | 122.82   |
| 22  | 3     | 602  | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 22  | 7     | 615  | CLA  | C1-O2A-CGA  | 2.63  | 123.02      | 116.65   |
| 22  | B     | 1022 | CLA  | CHA-C4D-ND  | 2.63  | 137.98      | 132.55   |
| 22  | A     | 1124 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | 2     | 601  | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | 5     | 607  | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 25  | B     | 4003 | BCR  | C37-C22-C21 | -2.63 | 118.55      | 122.82   |
| 22  | F     | 1301 | CLA  | C4B-CHC-C1C | 2.63  | 132.43      | 126.25   |
| 39  | 9     | 501  | LUT  | C26-C27-C28 | -2.63 | 120.48      | 124.58   |
| 22  | A     | 1105 | CLA  | O2A-CGA-CBA | 2.63  | 119.85      | 111.83   |
| 22  | Z     | 606  | CLA  | CAA-C2A-C3A | -2.63 | 105.89      | 113.00   |
| 22  | B     | 1214 | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 22  | B     | 1240 | CLA  | CMA-C3A-C4A | 2.63  | 118.84      | 111.77   |
| 39  | 7     | 501  | LUT  | C38-C25-C24 | -2.63 | 117.14      | 123.36   |
| 22  | 6     | 602  | CLA  | O2A-CGA-CBA | 2.63  | 119.85      | 111.83   |
| 22  | 5     | 605  | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 22  | A     | 1120 | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 22  | 1     | 606  | CLA  | CMD-C2D-C3D | -2.63 | 121.66      | 127.69   |
| 25  | L     | 4001 | BCR  | C35-C13-C12 | 2.63  | 122.10      | 118.09   |
| 22  | 5     | 603  | CLA  | C2C-C1C-NC  | 2.63  | 112.74      | 109.98   |
| 22  | B     | 1222 | CLA  | CHD-C1D-ND  | -2.63 | 121.11      | 124.80   |
| 39  | 2     | 503  | LUT  | C38-C25-C24 | -2.63 | 117.15      | 123.36   |
| 22  | A     | 1116 | CLA  | O2D-CGD-O1D | -2.63 | 118.74      | 123.85   |
| 39  | 6     | 501  | LUT  | C26-C27-C28 | -2.63 | 120.49      | 124.58   |
| 22  | 7     | 611  | CLA  | C2D-C1D-ND  | 2.63  | 112.72      | 110.13   |
| 22  | K     | 1402 | CLA  | C2C-C1C-NC  | 2.62  | 112.74      | 109.98   |
| 39  | 5     | 502  | LUT  | C7-C8-C9    | -2.62 | 122.35      | 126.23   |
| 37  | J     | 4002 | C7Z  | C15-C35-C34 | -2.62 | 118.15      | 123.52   |
| 22  | 7     | 606  | CLA  | C2C-C1C-NC  | 2.62  | 112.74      | 109.98   |
| 22  | 8     | 603  | CLA  | CHD-C1D-ND  | -2.62 | 121.11      | 124.80   |
| 22  | 9     | 606  | CLA  | CHD-C1D-ND  | -2.62 | 121.11      | 124.80   |
| 22  | A     | 1135 | CLA  | O2D-CGD-O1D | -2.62 | 118.74      | 123.85   |
| 22  | 4     | 605  | CLA  | CHA-C4D-ND  | 2.62  | 137.96      | 132.55   |
| 22  | 8     | 608  | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 22  | B     | 1207 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | 8     | 606  | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | A     | 1109 | CLA  | O2D-CGD-O1D | -2.62 | 118.74      | 123.85   |
| 22  | 3     | 616  | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 22  | A     | 1126 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | 3     | 605  | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | 7     | 605  | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 2     | 601  | CLA  | O2D-CGD-O1D | -2.62 | 118.74      | 123.85   |
| 39  | 3     | 501  | LUT  | C38-C25-C24 | -2.62 | 117.16      | 123.36   |
| 22  | B     | 1227 | CLA  | C2C-C1C-NC  | 2.62  | 112.73      | 109.98   |
| 22  | 5     | 613  | CLA  | C2C-C1C-NC  | 2.62  | 112.73      | 109.98   |
| 22  | B     | 1236 | CLA  | C1D-ND-C4D  | -2.62 | 104.47      | 106.31   |
| 22  | B     | 1219 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | B     | 1236 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | 4     | 615  | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 40  | 8     | 613  | CHL  | C1A-CHA-C4D | 2.62  | 123.35      | 118.98   |
| 40  | 4     | 611  | CHL  | C1-C2-C3    | -2.62 | 122.53      | 126.76   |
| 22  | B     | 1230 | CLA  | C2D-C1D-ND  | 2.62  | 112.72      | 110.13   |
| 22  | A     | 1102 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 22  | A     | 1013 | CLA  | CMB-C2B-C1B | -2.62 | 121.43      | 125.42   |
| 22  | 7     | 615  | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 25  | 5     | 503  | BCR  | C36-C18-C17 | -2.62 | 118.58      | 122.82   |
| 22  | G     | 1601 | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 22  | B     | 1218 | CLA  | C1-C2-C3    | -2.61 | 121.91      | 126.20   |
| 22  | 7     | 609  | CLA  | C1-C2-C3    | -2.61 | 121.91      | 126.20   |
| 22  | 1     | 613  | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 22  | 5     | 608  | CLA  | O2D-CGD-O1D | -2.61 | 118.76      | 123.85   |
| 22  | 8     | 609  | CLA  | O2D-CGD-O1D | -2.61 | 118.76      | 123.85   |
| 22  | 4     | 605  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 39  | 4     | 502  | LUT  | C10-C11-C12 | -2.61 | 115.63      | 123.20   |
| 22  | 8     | 611  | CLA  | CMA-C3A-C4A | 2.61  | 118.80      | 111.77   |
| 39  | Z     | 501  | LUT  | C26-C27-C28 | -2.61 | 120.51      | 124.58   |
| 28  | 8     | 805  | LMT  | O5'-C1'-C2' | -2.61 | 105.00      | 110.37   |
| 22  | B     | 1235 | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 22  | 8     | 608  | CLA  | CHD-C1D-ND  | -2.61 | 121.13      | 124.80   |
| 22  | 5     | 608  | CLA  | CMA-C3A-C4A | 2.61  | 118.79      | 111.77   |
| 40  | 9     | 613  | CHL  | C4D-CHA-CBD | -2.61 | 106.33      | 108.97   |
| 22  | K     | 1404 | CLA  | O2D-CGD-O1D | -2.61 | 118.77      | 123.85   |
| 22  | A     | 1105 | CLA  | C1D-ND-C4D  | -2.61 | 104.48      | 106.31   |
| 26  | A     | 5001 | LHG  | O8-C23-C24  | 2.61  | 119.80      | 111.83   |
| 39  | 8     | 501  | LUT  | C22-C23-C24 | -2.61 | 107.31      | 111.18   |
| 22  | B     | 1214 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 22  | B     | 1216 | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 22  | 8     | 611  | CLA  | O2D-CGD-O1D | -2.61 | 118.77      | 123.85   |
| 39  | 9     | 502  | LUT  | C35-C34-C33 | -2.61 | 123.62      | 127.28   |
| 22  | 7     | 615  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 22  | A     | 1107 | CLA  | C1-C2-C3    | -2.61 | 121.92      | 126.20   |
| 22  | 6     | 619  | CLA  | O2A-CGA-CBA | 2.61  | 119.78      | 111.83   |
| 39  | Z     | 501  | LUT  | C22-C23-C24 | -2.61 | 107.31      | 111.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1231 | CLA  | CHA-C4D-ND  | 2.61  | 137.93      | 132.55   |
| 22  | B     | 1203 | CLA  | O2A-CGA-CBA | 2.60  | 119.78      | 111.83   |
| 22  | A     | 1112 | CLA  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 22  | A     | 1127 | CLA  | C4B-CHC-C1C | 2.60  | 132.37      | 126.25   |
| 22  | B     | 1226 | CLA  | CHD-C4C-C3C | 2.60  | 128.57      | 124.77   |
| 35  | B     | 5004 | T7X  | O18-C11-C31 | 2.60  | 119.78      | 111.83   |
| 40  | 5     | 611  | CHL  | CHA-C1A-C2A | -2.60 | 127.19      | 133.31   |
| 22  | 6     | 605  | CLA  | C2C-C1C-NC  | 2.60  | 112.72      | 109.98   |
| 22  | A     | 1126 | CLA  | C2C-C1C-NC  | 2.60  | 112.72      | 109.98   |
| 22  | 5     | 613  | CLA  | O2D-CGD-O1D | -2.60 | 118.78      | 123.85   |
| 39  | 3     | 502  | LUT  | C31-C30-C29 | -2.60 | 123.63      | 127.28   |
| 36  | F     | 4001 | RRX  | C8-C7-C6    | -2.60 | 120.05      | 127.00   |
| 39  | 7     | 502  | LUT  | C35-C15-C14 | -2.60 | 118.19      | 123.52   |
| 22  | B     | 1221 | CLA  | C1-C2-C3    | -2.60 | 121.94      | 126.20   |
| 22  | A     | 1012 | CLA  | CHA-C4D-ND  | 2.60  | 137.91      | 132.55   |
| 22  | B     | 1223 | CLA  | C2D-C1D-ND  | 2.60  | 112.70      | 110.13   |
| 22  | 3     | 602  | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | 8     | 601  | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | 2     | 603  | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | A     | 1106 | CLA  | O1D-CGD-CBD | -2.60 | 119.40      | 124.52   |
| 22  | 4     | 601  | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | B     | 1213 | CLA  | C2C-C1C-NC  | 2.60  | 112.71      | 109.98   |
| 22  | B     | 1021 | CLA  | CAA-C2A-C3A | -2.60 | 105.98      | 113.00   |
| 40  | 2     | 610  | CHL  | C3C-C4C-NC  | -2.60 | 108.31      | 114.65   |
| 22  | 2     | 615  | CLA  | CMA-C3A-C4A | 2.60  | 118.75      | 111.77   |
| 22  | 5     | 602  | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | K     | 1401 | CLA  | C4B-CHC-C1C | 2.59  | 132.35      | 126.25   |
| 22  | A     | 1106 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | 6     | 618  | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 25  | 8     | 503  | BCR  | C27-C26-C25 | -2.59 | 119.20      | 122.70   |
| 40  | Z     | 609  | CHL  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |
| 22  | 3     | 610  | CLA  | O1D-CGD-CBD | -2.59 | 119.40      | 124.52   |
| 22  | 3     | 601  | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | K     | 1401 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | 8     | 602  | CLA  | C2C-C1C-NC  | 2.59  | 112.70      | 109.98   |
| 22  | A     | 1108 | CLA  | C4B-CHC-C1C | 2.59  | 132.34      | 126.25   |
| 22  | B     | 1022 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | J     | 1901 | CLA  | C2C-C1C-NC  | 2.59  | 112.70      | 109.98   |
| 22  | 6     | 606  | CLA  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 22  | A     | 1124 | CLA  | C2C-C1C-NC  | 2.59  | 112.70      | 109.98   |
| 39  | 6     | 502  | LUT  | C31-C30-C29 | -2.59 | 123.64      | 127.28   |
| 22  | 5     | 607  | CLA  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1109 | CLA  | CMD-C2D-C3D | -2.59 | 121.75      | 127.69   |
| 42  | Z     | 504  | QTB  | C03-C04-C05 | -2.59 | 115.70      | 123.20   |
| 22  | 6     | 619  | CLA  | CHA-C4D-ND  | 2.59  | 137.89      | 132.55   |
| 22  | B     | 1209 | CLA  | CMA-C3A-C4A | 2.59  | 118.73      | 111.77   |
| 39  | 1     | 502  | LUT  | C38-C25-C24 | -2.59 | 117.23      | 123.36   |
| 22  | 7     | 616  | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 22  | 1     | 608  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | 7     | 609  | CLA  | C2D-C1D-ND  | 2.59  | 112.69      | 110.13   |
| 22  | A     | 1112 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 22  | A     | 1104 | CLA  | O2A-CGA-CBA | 2.59  | 119.73      | 111.83   |
| 40  | 6     | 613  | CHL  | C3C-C4C-NC  | -2.59 | 108.33      | 114.65   |
| 25  | B     | 4007 | BCR  | C35-C13-C12 | 2.59  | 122.04      | 118.09   |
| 39  | 7     | 501  | LUT  | C22-C23-C24 | -2.59 | 107.34      | 111.18   |
| 39  | 5     | 501  | LUT  | C10-C11-C12 | -2.59 | 115.70      | 123.20   |
| 22  | B     | 1237 | CLA  | C2C-C1C-NC  | 2.59  | 112.70      | 109.98   |
| 22  | 1     | 604  | CLA  | O2D-CGD-O1D | -2.59 | 118.81      | 123.85   |
| 22  | B     | 1209 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 22  | B     | 1223 | CLA  | C2C-C1C-NC  | 2.58  | 112.70      | 109.98   |
| 22  | B     | 1203 | CLA  | CHA-C4D-ND  | 2.58  | 137.88      | 132.55   |
| 22  | 1     | 611  | CLA  | C1-O2A-CGA  | 2.58  | 122.91      | 116.65   |
| 39  | 9     | 502  | LUT  | C18-C5-C6   | -2.58 | 121.66      | 124.48   |
| 22  | 6     | 603  | CLA  | C3B-C4B-NB  | -2.58 | 108.22      | 110.53   |
| 22  | A     | 1135 | CLA  | O1D-CGD-CBD | -2.58 | 119.42      | 124.52   |
| 22  | 7     | 607  | CLA  | CAA-C2A-C3A | -2.58 | 106.02      | 113.00   |
| 22  | 6     | 608  | CLA  | CHA-C4D-ND  | 2.58  | 137.88      | 132.55   |
| 22  | 8     | 606  | CLA  | O2D-CGD-O1D | -2.58 | 118.82      | 123.85   |
| 26  | 7     | 801  | LHG  | O8-C23-C24  | 2.58  | 119.70      | 111.83   |
| 22  | 5     | 609  | CLA  | CMA-C3A-C4A | 2.58  | 118.71      | 111.77   |
| 22  | 9     | 602  | CLA  | C1C-C2C-C3C | -2.58 | 104.27      | 106.98   |
| 22  | A     | 1134 | CLA  | O2D-CGD-O1D | -2.58 | 118.83      | 123.85   |
| 22  | 8     | 605  | CLA  | CHA-C4D-ND  | 2.58  | 137.87      | 132.55   |
| 25  | 3     | 506  | BCR  | C15-C14-C13 | -2.58 | 123.66      | 127.28   |
| 40  | 1     | 609  | CHL  | C4C-CHD-C1D | 2.58  | 125.30      | 116.07   |
| 22  | 4     | 602  | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 22  | B     | 1022 | CLA  | CHD-C1D-ND  | -2.58 | 121.17      | 124.80   |
| 22  | A     | 1119 | CLA  | CHA-C4D-ND  | 2.58  | 137.87      | 132.55   |
| 22  | A     | 1114 | CLA  | CMD-C2D-C3D | -2.58 | 121.78      | 127.69   |
| 22  | A     | 1111 | CLA  | O1D-CGD-CBD | -2.58 | 119.43      | 124.52   |
| 22  | A     | 1139 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 22  | F     | 1301 | CLA  | CHA-C4D-ND  | 2.58  | 137.87      | 132.55   |
| 22  | L     | 1502 | CLA  | C2D-C1D-ND  | 2.58  | 112.68      | 110.13   |
| 22  | B     | 1235 | CLA  | O2D-CGD-O1D | -2.58 | 118.83      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1125 | CLA  | C4B-CHC-C1C | 2.58  | 132.31      | 126.25   |
| 39  | 9     | 502  | LUT  | C7-C8-C9    | -2.58 | 122.42      | 126.23   |
| 22  | 1     | 604  | CLA  | C1C-C2C-C3C | -2.58 | 104.27      | 106.98   |
| 22  | 9     | 608  | CLA  | O2D-CGD-O1D | -2.58 | 118.83      | 123.85   |
| 22  | A     | 1125 | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 22  | 6     | 618  | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 22  | 8     | 603  | CLA  | CAA-C2A-C3A | -2.58 | 106.04      | 113.00   |
| 22  | 3     | 612  | CLA  | CHD-C1D-ND  | -2.58 | 121.18      | 124.80   |
| 22  | 1     | 611  | CLA  | CMD-C2D-C3D | -2.58 | 121.78      | 127.69   |
| 22  | A     | 1116 | CLA  | C1-O2A-CGA  | 2.58  | 122.89      | 116.65   |
| 22  | B     | 1229 | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 22  | 6     | 612  | CLA  | C1D-ND-C4D  | -2.58 | 104.50      | 106.31   |
| 22  | A     | 1101 | CLA  | C4B-CHC-C1C | 2.57  | 132.30      | 126.25   |
| 22  | K     | 1402 | CLA  | CMA-C3A-C4A | 2.57  | 118.69      | 111.77   |
| 22  | 5     | 607  | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 22  | A     | 1109 | CLA  | C1D-ND-C4D  | -2.57 | 104.51      | 106.31   |
| 22  | 3     | 608  | CLA  | O2D-CGD-O1D | -2.57 | 118.84      | 123.85   |
| 22  | Z     | 603  | CLA  | C1C-C2C-C3C | -2.57 | 104.27      | 106.98   |
| 22  | Z     | 605  | CLA  | CMD-C2D-C3D | -2.57 | 121.79      | 127.69   |
| 22  | 1     | 605  | CLA  | CHA-C4D-ND  | 2.57  | 137.86      | 132.55   |
| 22  | Z     | 608  | CLA  | CHD-C1D-ND  | -2.57 | 121.18      | 124.80   |
| 22  | A     | 1137 | CLA  | C1-O2A-CGA  | 2.57  | 122.88      | 116.65   |
| 22  | 3     | 603  | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 22  | A     | 1114 | CLA  | O2A-CGA-CBA | 2.57  | 119.68      | 111.83   |
| 22  | F     | 1302 | CLA  | C2C-C1C-NC  | 2.57  | 112.68      | 109.98   |
| 28  | A     | 5006 | LMT  | C1'-O5'-C5' | -2.57 | 108.70      | 113.72   |
| 22  | 9     | 609  | CLA  | O2D-CGD-O1D | -2.57 | 118.84      | 123.85   |
| 22  | A     | 1124 | CLA  | CMA-C3A-C4A | 2.57  | 118.68      | 111.77   |
| 22  | 1     | 613  | CLA  | CHA-C4D-ND  | 2.57  | 137.85      | 132.55   |
| 22  | A     | 1139 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 22  | 1     | 611  | CLA  | CHD-C1D-ND  | -2.57 | 121.19      | 124.80   |
| 22  | A     | 1111 | CLA  | C4B-CHC-C1C | 2.57  | 132.29      | 126.25   |
| 22  | 8     | 609  | CLA  | CHA-C4D-ND  | 2.57  | 137.85      | 132.55   |
| 22  | B     | 1230 | CLA  | O2A-CGA-CBA | 2.57  | 119.67      | 111.83   |
| 22  | A     | 1122 | CLA  | CHD-C1D-ND  | -2.57 | 121.19      | 124.80   |
| 22  | 5     | 618  | CLA  | C1D-ND-C4D  | -2.57 | 104.51      | 106.31   |
| 22  | 8     | 615  | CLA  | C4B-CHC-C1C | 2.57  | 132.28      | 126.25   |
| 22  | 7     | 602  | CLA  | C1C-C2C-C3C | -2.57 | 104.28      | 106.98   |
| 25  | A     | 4003 | BCR  | C35-C13-C12 | 2.57  | 122.01      | 118.09   |
| 22  | 7     | 616  | CLA  | C2C-C1C-NC  | 2.57  | 112.68      | 109.98   |
| 22  | 6     | 601  | CLA  | C2C-C1C-NC  | 2.57  | 112.68      | 109.98   |
| 22  | 3     | 612  | CLA  | O2D-CGD-O1D | -2.57 | 118.86      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 608  | CLA  | O2A-CGA-CBA | 2.56  | 119.66      | 111.83   |
| 22  | B     | 1237 | CLA  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 25  | 7     | 503  | BCR  | C38-C26-C25 | -2.56 | 121.69      | 124.48   |
| 22  | 3     | 606  | CLA  | C1D-ND-C4D  | -2.56 | 104.51      | 106.31   |
| 22  | A     | 1129 | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 22  | G     | 1601 | CLA  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 40  | 7     | 610  | CHL  | C1-O2A-CGA  | 2.56  | 122.86      | 116.65   |
| 41  | 2     | 803  | SQD  | O7-S-C6     | -2.56 | 102.93      | 106.76   |
| 40  | 8     | 613  | CHL  | C1-O2A-CGA  | 2.56  | 122.86      | 116.65   |
| 22  | A     | 1127 | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 22  | Z     | 603  | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 22  | 2     | 603  | CLA  | O1D-CGD-CBD | -2.56 | 119.46      | 124.52   |
| 22  | 5     | 622  | CLA  | CHA-C4D-ND  | 2.56  | 137.84      | 132.55   |
| 22  | 7     | 616  | CLA  | CHD-C1D-ND  | -2.56 | 121.20      | 124.80   |
| 39  | 4     | 501  | LUT  | C38-C25-C24 | -2.56 | 117.30      | 123.36   |
| 22  | Z     | 603  | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 25  | 5     | 503  | BCR  | C38-C26-C25 | -2.56 | 121.69      | 124.48   |
| 22  | 5     | 615  | CLA  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 22  | A     | 1134 | CLA  | CHA-C4D-ND  | 2.56  | 137.83      | 132.55   |
| 22  | 6     | 602  | CLA  | O2D-CGD-O1D | -2.56 | 118.87      | 123.85   |
| 22  | B     | 1204 | CLA  | O2D-CGD-O1D | -2.56 | 118.87      | 123.85   |
| 22  | 2     | 602  | CLA  | C1D-ND-C4D  | -2.56 | 104.52      | 106.31   |
| 39  | Z     | 502  | LUT  | C35-C15-C14 | -2.56 | 118.29      | 123.52   |
| 22  | Z     | 604  | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 22  | A     | 1126 | CLA  | O1D-CGD-CBD | -2.56 | 119.48      | 124.52   |
| 22  | 3     | 607  | CLA  | CHA-C4D-ND  | 2.56  | 137.82      | 132.55   |
| 22  | A     | 1121 | CLA  | CAA-C2A-C3A | -2.55 | 106.10      | 113.00   |
| 22  | Z     | 605  | CLA  | CHA-C4D-ND  | 2.55  | 137.82      | 132.55   |
| 22  | A     | 1137 | CLA  | CMA-C3A-C4A | 2.55  | 118.64      | 111.77   |
| 22  | 7     | 605  | CLA  | C1-O2A-CGA  | 2.55  | 122.83      | 116.65   |
| 22  | A     | 1125 | CLA  | C3D-C2D-C1D | -2.55 | 102.35      | 105.83   |
| 22  | A     | 1116 | CLA  | CHA-C4D-ND  | 2.55  | 137.82      | 132.55   |
| 22  | 8     | 605  | CLA  | O2D-CGD-O1D | -2.55 | 118.88      | 123.85   |
| 22  | A     | 1103 | CLA  | C1D-ND-C4D  | -2.55 | 104.52      | 106.31   |
| 39  | 8     | 501  | LUT  | C26-C27-C28 | -2.55 | 120.61      | 124.58   |
| 25  | K     | 4002 | BCR  | C35-C13-C12 | 2.55  | 121.99      | 118.09   |
| 40  | 8     | 613  | CHL  | C4C-CHD-C1D | 2.55  | 125.20      | 116.07   |
| 37  | J     | 4002 | C7Z  | C11-C10-C9  | -2.55 | 123.70      | 127.28   |
| 22  | L     | 1503 | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 22  | B     | 1021 | CLA  | O1D-CGD-CBD | -2.55 | 119.48      | 124.52   |
| 22  | B     | 1232 | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 25  | 5     | 503  | BCR  | C4-C5-C6    | -2.55 | 119.26      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1114 | CLA  | O2D-CGD-O1D | -2.55 | 118.88      | 123.85   |
| 22  | 3     | 616  | CLA  | O2D-CGD-O1D | -2.55 | 118.88      | 123.85   |
| 22  | 6     | 608  | CLA  | C1-C2-C3    | -2.55 | 122.02      | 126.20   |
| 22  | K     | 1404 | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 22  | 4     | 602  | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 22  | B     | 1241 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 22  | 7     | 612  | CLA  | CHD-C1D-ND  | -2.55 | 121.22      | 124.80   |
| 22  | A     | 1104 | CLA  | CHA-C4D-ND  | 2.55  | 137.81      | 132.55   |
| 22  | 7     | 609  | CLA  | C1D-ND-C4D  | -2.55 | 104.52      | 106.31   |
| 22  | B     | 1228 | CLA  | C2C-C1C-NC  | 2.55  | 112.66      | 109.98   |
| 22  | B     | 1215 | CLA  | CHD-C1D-ND  | -2.55 | 121.22      | 124.80   |
| 22  | 1     | 615  | CLA  | CHA-C4D-ND  | 2.55  | 137.81      | 132.55   |
| 22  | K     | 1404 | CLA  | CHA-C4D-ND  | 2.55  | 137.80      | 132.55   |
| 22  | 7     | 613  | CLA  | CMA-C3A-C4A | 2.55  | 118.62      | 111.77   |
| 22  | 3     | 616  | CLA  | O2A-CGA-CBA | 2.55  | 119.60      | 111.83   |
| 22  | 1     | 611  | CLA  | CAA-C2A-C3A | -2.55 | 106.12      | 113.00   |
| 39  | 3     | 502  | LUT  | C38-C25-C24 | -2.55 | 117.34      | 123.36   |
| 22  | 4     | 607  | CLA  | O2A-CGA-CBA | 2.55  | 119.59      | 111.83   |
| 22  | G     | 1602 | CLA  | CHA-C4D-ND  | 2.54  | 137.80      | 132.55   |
| 22  | 8     | 606  | CLA  | C2C-C1C-NC  | 2.54  | 112.65      | 109.98   |
| 22  | A     | 1132 | CLA  | CMA-C3A-C4A | 2.54  | 118.61      | 111.77   |
| 22  | 2     | 601  | CLA  | C4B-CHC-C1C | 2.54  | 132.23      | 126.25   |
| 22  | 3     | 601  | CLA  | C4B-CHC-C1C | 2.54  | 132.23      | 126.25   |
| 22  | B     | 1212 | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | 4     | 604  | CLA  | C2C-C1C-NC  | 2.54  | 112.65      | 109.98   |
| 39  | 1     | 501  | LUT  | C38-C25-C24 | -2.54 | 117.35      | 123.36   |
| 22  | 6     | 609  | CLA  | C3B-C4B-NB  | -2.54 | 108.26      | 110.53   |
| 22  | A     | 1135 | CLA  | C1C-C2C-C3C | -2.54 | 104.31      | 106.98   |
| 22  | B     | 1205 | CLA  | C1C-C2C-C3C | -2.54 | 104.31      | 106.98   |
| 22  | B     | 1211 | CLA  | CMD-C2D-C3D | -2.54 | 121.86      | 127.69   |
| 22  | B     | 1209 | CLA  | C2C-C1C-NC  | 2.54  | 112.65      | 109.98   |
| 22  | K     | 1401 | CLA  | CMA-C3A-C4A | 2.54  | 118.60      | 111.77   |
| 22  | 7     | 608  | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | B     | 1217 | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 39  | 7     | 501  | LUT  | C18-C5-C6   | -2.54 | 121.71      | 124.48   |
| 22  | 6     | 607  | CLA  | CAA-C2A-C3A | -2.54 | 106.14      | 113.00   |
| 22  | Z     | 601  | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | B     | 1216 | CLA  | O2D-CGD-O1D | -2.54 | 118.91      | 123.85   |
| 22  | A     | 1111 | CLA  | O2A-CGA-CBA | 2.54  | 119.58      | 111.83   |
| 22  | 6     | 601  | CLA  | CHA-C4D-ND  | 2.54  | 137.79      | 132.55   |
| 40  | 1     | 609  | CHL  | C1A-CHA-C4D | 2.54  | 123.22      | 118.98   |
| 22  | 2     | 602  | CLA  | CHD-C1D-ND  | -2.54 | 121.23      | 124.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 3     | 506  | BCR  | C38-C26-C25 | -2.54 | 121.72      | 124.48   |
| 22  | A     | 1108 | CLA  | CAA-C2A-C3A | -2.54 | 106.14      | 113.00   |
| 22  | 9     | 602  | CLA  | O2D-CGD-O1D | -2.54 | 118.91      | 123.85   |
| 22  | Z     | 606  | CLA  | CHA-C4D-ND  | 2.54  | 137.78      | 132.55   |
| 22  | A     | 1126 | CLA  | CHD-C1D-ND  | -2.54 | 121.23      | 124.80   |
| 22  | B     | 1226 | CLA  | CMB-C2B-C1B | -2.54 | 121.56      | 125.42   |
| 22  | A     | 1139 | CLA  | C1-O2A-CGA  | 2.54  | 122.79      | 116.65   |
| 22  | 8     | 608  | CLA  | O2A-CGA-CBA | 2.54  | 119.57      | 111.83   |
| 22  | 4     | 609  | CLA  | C1D-ND-C4D  | -2.53 | 104.53      | 106.31   |
| 22  | A     | 1130 | CLA  | CHA-C4D-ND  | 2.53  | 137.78      | 132.55   |
| 22  | 5     | 607  | CLA  | C1C-C2C-C3C | -2.53 | 104.31      | 106.98   |
| 22  | B     | 1219 | CLA  | CHA-C4D-ND  | 2.53  | 137.78      | 132.55   |
| 22  | 3     | 616  | CLA  | C1-O2A-CGA  | 2.53  | 122.78      | 116.65   |
| 22  | B     | 1223 | CLA  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 22  | B     | 1207 | CLA  | CAA-C2A-C3A | -2.53 | 106.15      | 113.00   |
| 22  | 4     | 601  | CLA  | CHD-C1D-ND  | -2.53 | 121.24      | 124.80   |
| 22  | 4     | 612  | CLA  | C2C-C1C-NC  | 2.53  | 112.64      | 109.98   |
| 22  | 6     | 608  | CLA  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 22  | B     | 1231 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 22  | 2     | 615  | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | 1     | 607  | CLA  | C2A-C1A-CHA | 2.53  | 128.26      | 123.87   |
| 22  | F     | 1302 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 39  | 8     | 501  | LUT  | C15-C14-C13 | -2.53 | 123.73      | 127.28   |
| 22  | 5     | 622  | CLA  | CMD-C2D-C3D | -2.53 | 121.89      | 127.69   |
| 22  | 5     | 601  | CLA  | CHD-C1D-ND  | -2.53 | 121.24      | 124.80   |
| 22  | A     | 1104 | CLA  | C2C-C1C-NC  | 2.53  | 112.64      | 109.98   |
| 22  | A     | 1134 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | 6     | 615  | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | A     | 1111 | CLA  | CHA-C4D-ND  | 2.53  | 137.77      | 132.55   |
| 22  | 3     | 601  | CLA  | O1D-CGD-CBD | -2.53 | 119.53      | 124.52   |
| 22  | 2     | 605  | CLA  | C1C-C2C-C3C | -2.53 | 104.32      | 106.98   |
| 22  | A     | 1120 | CLA  | C2D-C1D-ND  | 2.53  | 112.63      | 110.13   |
| 22  | B     | 1205 | CLA  | C2C-C1C-NC  | 2.53  | 112.64      | 109.98   |
| 22  | 1     | 603  | CLA  | C2C-C1C-NC  | 2.53  | 112.64      | 109.98   |
| 22  | F     | 1302 | CLA  | O2D-CGD-O1D | -2.53 | 118.93      | 123.85   |
| 22  | 1     | 603  | CLA  | CHD-C1D-ND  | -2.53 | 121.25      | 124.80   |
| 22  | B     | 1210 | CLA  | O2A-CGA-CBA | 2.53  | 119.54      | 111.83   |
| 22  | 6     | 619  | CLA  | CHD-C1D-ND  | -2.53 | 121.25      | 124.80   |
| 22  | A     | 1113 | CLA  | O2A-CGA-CBA | 2.53  | 119.54      | 111.83   |
| 22  | 7     | 605  | CLA  | CMA-C3A-C4A | 2.53  | 118.56      | 111.77   |
| 22  | 8     | 604  | CLA  | C1C-C2C-C3C | -2.53 | 104.32      | 106.98   |
| 25  | A     | 4001 | BCR  | C31-C1-C6   | -2.53 | 106.28      | 110.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1104 | CLA  | C4B-CHC-C1C | 2.53  | 132.19      | 126.25   |
| 22  | B     | 1235 | CLA  | C2C-C1C-NC  | 2.52  | 112.63      | 109.98   |
| 22  | 1     | 607  | CLA  | CHA-C4D-ND  | 2.52  | 137.76      | 132.55   |
| 22  | 2     | 607  | CLA  | C4B-CHC-C1C | 2.52  | 132.18      | 126.25   |
| 22  | B     | 1219 | CLA  | CMA-C3A-C4A | 2.52  | 118.56      | 111.77   |
| 39  | 1     | 501  | LUT  | C20-C13-C12 | 2.52  | 121.94      | 118.09   |
| 22  | B     | 1021 | CLA  | CHA-C4D-ND  | 2.52  | 137.75      | 132.55   |
| 22  | B     | 1224 | CLA  | O2A-CGA-CBA | 2.52  | 119.52      | 111.83   |
| 22  | G     | 1602 | CLA  | O2D-CGD-O1D | -2.52 | 118.94      | 123.85   |
| 22  | 7     | 609  | CLA  | C4B-CHC-C1C | 2.52  | 132.18      | 126.25   |
| 22  | 2     | 601  | CLA  | C1C-C2C-C3C | -2.52 | 104.33      | 106.98   |
| 22  | 2     | 601  | CLA  | O2A-CGA-CBA | 2.52  | 119.52      | 111.83   |
| 22  | 9     | 606  | CLA  | C1D-ND-C4D  | -2.52 | 104.54      | 106.31   |
| 22  | 9     | 601  | CLA  | C4B-CHC-C1C | 2.52  | 132.17      | 126.25   |
| 22  | B     | 1227 | CLA  | O2D-CGD-O1D | -2.52 | 118.94      | 123.85   |
| 22  | 3     | 613  | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | A     | 1106 | CLA  | C2C-C1C-NC  | 2.52  | 112.63      | 109.98   |
| 22  | 3     | 606  | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | Z     | 607  | CLA  | C1-C2-C3    | -2.52 | 122.07      | 126.20   |
| 22  | A     | 1130 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | K     | 1401 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | 9     | 609  | CLA  | C1C-C2C-C3C | -2.52 | 104.33      | 106.98   |
| 22  | 1     | 606  | CLA  | CHD-C1D-ND  | -2.52 | 121.26      | 124.80   |
| 22  | K     | 1403 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | 9     | 612  | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 22  | 9     | 609  | CLA  | C4B-CHC-C1C | 2.52  | 132.16      | 126.25   |
| 22  | 6     | 607  | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 22  | 7     | 612  | CLA  | C1C-C2C-C3C | -2.52 | 104.33      | 106.98   |
| 22  | 4     | 615  | CLA  | CHA-C4D-ND  | 2.52  | 137.74      | 132.55   |
| 22  | A     | 1125 | CLA  | CHA-C4D-ND  | 2.52  | 137.74      | 132.55   |
| 40  | 4     | 611  | CHL  | CMA-C3A-C4A | 2.52  | 120.03      | 114.61   |
| 22  | B     | 1202 | CLA  | C2C-C1C-NC  | 2.51  | 112.62      | 109.98   |
| 22  | 5     | 618  | CLA  | CMA-C3A-C4A | 2.51  | 118.53      | 111.77   |
| 22  | B     | 1241 | CLA  | OBD-CAD-C3D | -2.51 | 122.54      | 128.42   |
| 39  | 2     | 503  | LUT  | C32-C33-C34 | 2.51  | 122.96      | 119.01   |
| 22  | A     | 1124 | CLA  | C3B-C4B-NB  | -2.51 | 108.29      | 110.53   |
| 22  | B     | 1231 | CLA  | C1-C2-C3    | -2.51 | 122.08      | 126.20   |
| 22  | 8     | 612  | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | 2     | 612  | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | 3     | 610  | CLA  | CAA-C2A-C3A | -2.51 | 106.21      | 113.00   |
| 22  | 8     | 605  | CLA  | CMA-C3A-C4A | 2.51  | 118.53      | 111.77   |
| 22  | B     | 1234 | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 2     | 612  | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 22  | 1     | 604  | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | A     | 1138 | CLA  | CHD-C1D-ND  | -2.51 | 121.27      | 124.80   |
| 22  | 6     | 615  | CLA  | O1D-CGD-CBD | -2.51 | 119.56      | 124.52   |
| 22  | 1     | 605  | CLA  | CMD-C2D-C3D | -2.51 | 121.93      | 127.69   |
| 22  | A     | 1129 | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 6     | 619  | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 9     | 612  | CLA  | CAA-CBA-CGA | -2.51 | 106.08      | 113.21   |
| 22  | A     | 1121 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | K     | 1401 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | F     | 1301 | CLA  | O2D-CGD-O1D | -2.51 | 118.96      | 123.85   |
| 22  | 7     | 609  | CLA  | C2C-C1C-NC  | 2.51  | 112.62      | 109.98   |
| 22  | 8     | 609  | CLA  | C1-O2A-CGA  | 2.51  | 122.73      | 116.65   |
| 22  | A     | 1121 | CLA  | OBD-CAD-C3D | -2.51 | 122.55      | 128.42   |
| 22  | 3     | 606  | CLA  | C4B-CHC-C1C | 2.51  | 132.15      | 126.25   |
| 22  | B     | 1201 | CLA  | CHD-C1D-ND  | -2.51 | 121.27      | 124.80   |
| 22  | 5     | 605  | CLA  | C1D-ND-C4D  | -2.51 | 104.55      | 106.31   |
| 22  | 6     | 612  | CLA  | C2D-C1D-ND  | 2.51  | 112.61      | 110.13   |
| 22  | 2     | 605  | CLA  | C4B-CHC-C1C | 2.51  | 132.15      | 126.25   |
| 22  | 6     | 601  | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | A     | 1112 | CLA  | CMA-C3A-C4A | 2.51  | 118.52      | 111.77   |
| 22  | 8     | 604  | CLA  | C2C-C1C-NC  | 2.51  | 112.62      | 109.98   |
| 22  | 1     | 606  | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 25  | 7     | 504  | BCR  | C4-C5-C6    | -2.51 | 119.31      | 122.70   |
| 22  | A     | 1102 | CLA  | CHD-C1D-ND  | -2.51 | 121.27      | 124.80   |
| 22  | A     | 1103 | CLA  | CHD-C1D-ND  | -2.51 | 121.27      | 124.80   |
| 22  | B     | 1023 | CLA  | O2A-CGA-CBA | 2.51  | 119.48      | 111.83   |
| 22  | B     | 1218 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 28  | 1     | 803  | LMT  | C3'-C4'-C5' | -2.51 | 105.37      | 110.93   |
| 22  | G     | 1601 | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 22  | 6     | 605  | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 22  | 4     | 604  | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 2     | 602  | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 40  | 2     | 609  | CHL  | C4C-CHD-C1D | 2.51  | 125.04      | 116.07   |
| 22  | B     | 1214 | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 22  | 6     | 607  | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 22  | Z     | 604  | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 25  | 4     | 503  | BCR  | C35-C13-C12 | 2.51  | 121.92      | 118.09   |
| 22  | 7     | 606  | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 22  | A     | 1126 | CLA  | CMA-C3A-C4A | 2.51  | 118.51      | 111.77   |
| 22  | 5     | 603  | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 7     | 601  | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1216 | CLA  | C2C-C1C-NC  | 2.51  | 112.61      | 109.98   |
| 22  | 3     | 601  | CLA  | C2C-C1C-NC  | 2.51  | 112.61      | 109.98   |
| 25  | J     | 4001 | BCR  | C35-C13-C12 | 2.51  | 121.92      | 118.09   |
| 37  | J     | 4002 | C7Z  | C19-C9-C8   | 2.51  | 121.92      | 118.09   |
| 22  | B     | 1209 | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 22  | A     | 1122 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | A     | 1137 | CLA  | CHD-C1D-ND  | -2.51 | 121.28      | 124.80   |
| 22  | B     | 1241 | CLA  | CAA-CBA-CGA | -2.51 | 106.09      | 113.21   |
| 22  | A     | 1125 | CLA  | CAA-C2A-C3A | -2.50 | 106.23      | 113.00   |
| 22  | Z     | 603  | CLA  | CHD-C1D-ND  | -2.50 | 121.28      | 124.80   |
| 22  | B     | 1021 | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | A     | 1114 | CLA  | CHA-C4D-ND  | 2.50  | 137.72      | 132.55   |
| 25  | A     | 4001 | BCR  | C38-C26-C25 | -2.50 | 121.75      | 124.48   |
| 22  | 2     | 602  | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 22  | A     | 1129 | CLA  | CHA-C4D-ND  | 2.50  | 137.71      | 132.55   |
| 22  | 4     | 606  | CLA  | C1C-C2C-C3C | -2.50 | 104.35      | 106.98   |
| 22  | Z     | 608  | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | A     | 1121 | CLA  | C4B-CHC-C1C | 2.50  | 132.13      | 126.25   |
| 22  | 4     | 605  | CLA  | C1D-ND-C4D  | -2.50 | 104.56      | 106.31   |
| 22  | 1     | 605  | CLA  | O2A-CGA-CBA | 2.50  | 119.47      | 111.83   |
| 22  | 7     | 615  | CLA  | CMA-C3A-C4A | 2.50  | 118.50      | 111.77   |
| 22  | A     | 1120 | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | 3     | 613  | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | A     | 1141 | CLA  | CHA-C4D-ND  | 2.50  | 137.71      | 132.55   |
| 22  | 6     | 606  | CLA  | CAA-C2A-C3A | -2.50 | 106.24      | 113.00   |
| 22  | 9     | 606  | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |
| 22  | 8     | 611  | CLA  | CHD-C1D-ND  | -2.50 | 121.28      | 124.80   |
| 22  | B     | 1217 | CLA  | C1C-C2C-C3C | -2.50 | 104.35      | 106.98   |
| 22  | 7     | 604  | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | A     | 1110 | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | 5     | 606  | CLA  | CHA-C4D-ND  | 2.50  | 137.71      | 132.55   |
| 22  | A     | 1125 | CLA  | C2D-C1D-ND  | 2.50  | 112.60      | 110.13   |
| 40  | 2     | 613  | CHL  | CMA-C3A-C4A | 2.50  | 120.00      | 114.61   |
| 22  | B     | 1203 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | Z     | 604  | CLA  | C1-O2A-CGA  | 2.50  | 122.70      | 116.65   |
| 22  | B     | 1213 | CLA  | CHD-C1D-ND  | -2.50 | 121.29      | 124.80   |
| 22  | Z     | 601  | CLA  | CHD-C1D-ND  | -2.50 | 121.29      | 124.80   |
| 22  | 9     | 609  | CLA  | CHA-C4D-ND  | 2.50  | 137.70      | 132.55   |
| 22  | L     | 1502 | CLA  | C1D-ND-C4D  | -2.50 | 104.56      | 106.31   |
| 25  | 8     | 503  | BCR  | C23-C24-C25 | -2.50 | 120.32      | 127.00   |
| 25  | A     | 4001 | BCR  | C36-C18-C17 | -2.50 | 118.77      | 122.82   |
| 22  | B     | 1228 | CLA  | CMA-C3A-C4A | 2.50  | 118.49      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 1     | 602  | CLA  | CHA-C4D-ND  | 2.50  | 137.70      | 132.55   |
| 22  | B     | 1234 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | A     | 1118 | CLA  | C2D-C1D-ND  | 2.50  | 112.60      | 110.13   |
| 22  | A     | 1102 | CLA  | CHA-C4D-ND  | 2.50  | 137.70      | 132.55   |
| 22  | A     | 1119 | CLA  | C1-C2-C3    | -2.50 | 122.11      | 126.20   |
| 22  | B     | 1022 | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 22  | B     | 1212 | CLA  | O1D-CGD-CBD | -2.50 | 119.59      | 124.52   |
| 22  | 7     | 607  | CLA  | CHA-C4D-ND  | 2.50  | 137.70      | 132.55   |
| 22  | 5     | 607  | CLA  | CHA-C4D-ND  | 2.50  | 137.70      | 132.55   |
| 22  | 7     | 613  | CLA  | C2C-C1C-NC  | 2.50  | 112.60      | 109.98   |
| 22  | 3     | 605  | CLA  | O2D-CGD-O1D | -2.50 | 118.99      | 123.85   |
| 22  | F     | 1302 | CLA  | C1C-C2C-C3C | -2.49 | 104.36      | 106.98   |
| 22  | 7     | 604  | CLA  | C1C-C2C-C3C | -2.49 | 104.36      | 106.98   |
| 39  | 2     | 503  | LUT  | C36-C21-C26 | 2.49  | 113.32      | 109.55   |
| 22  | 8     | 608  | CLA  | CMA-C3A-C4A | 2.49  | 118.48      | 111.77   |
| 22  | 5     | 602  | CLA  | CHA-C4D-ND  | 2.49  | 137.70      | 132.55   |
| 22  | 9     | 606  | CLA  | CMD-C2D-C3D | -2.49 | 121.97      | 127.69   |
| 22  | 7     | 611  | CLA  | CHD-C1D-ND  | -2.49 | 121.29      | 124.80   |
| 22  | 5     | 622  | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | B     | 1239 | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | Z     | 608  | CLA  | CAA-C2A-C3A | -2.49 | 106.26      | 113.00   |
| 22  | 6     | 603  | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | A     | 1013 | CLA  | C2A-C1A-CHA | 2.49  | 128.19      | 123.87   |
| 22  | 7     | 601  | CLA  | C2C-C1C-NC  | 2.49  | 112.60      | 109.98   |
| 22  | B     | 1231 | CLA  | O2A-CGA-CBA | 2.49  | 119.44      | 111.83   |
| 22  | 5     | 601  | CLA  | C1-O2A-CGA  | 2.49  | 122.68      | 116.65   |
| 22  | Z     | 604  | CLA  | CHD-C1D-ND  | -2.49 | 121.30      | 124.80   |
| 40  | 9     | 613  | CHL  | CMA-C3A-C4A | 2.49  | 119.98      | 114.61   |
| 22  | G     | 1601 | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | 8     | 603  | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | B     | 1218 | CLA  | CHD-C1D-ND  | -2.49 | 121.30      | 124.80   |
| 22  | B     | 1209 | CLA  | CHD-C1D-ND  | -2.49 | 121.30      | 124.80   |
| 22  | A     | 1140 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | 9     | 603  | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | 7     | 607  | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 36  | F     | 4001 | RRX  | C11-C12-C13 | -2.49 | 119.53      | 126.36   |
| 22  | B     | 1232 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 40  | 1     | 610  | CHL  | CMA-C3A-C4A | 2.49  | 119.98      | 114.61   |
| 22  | 6     | 615  | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | 9     | 607  | CLA  | O2A-CGA-CBA | 2.49  | 119.42      | 111.83   |
| 22  | Z     | 604  | CLA  | CMD-C2D-C3D | -2.49 | 121.98      | 127.69   |
| 22  | 8     | 603  | CLA  | C2C-C1C-NC  | 2.49  | 112.60      | 109.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1102 | CLA  | CAA-CBA-CGA | -2.49 | 106.14      | 113.21   |
| 22  | A     | 1139 | CLA  | C1C-C2C-C3C | -2.49 | 104.36      | 106.98   |
| 25  | B     | 4007 | BCR  | C34-C9-C10  | -2.49 | 118.79      | 122.82   |
| 22  | B     | 1234 | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 22  | A     | 1012 | CLA  | O2D-CGD-O1D | -2.49 | 119.01      | 123.85   |
| 38  | 7     | 804  | SPH  | C3-C4-C5    | -2.49 | 119.54      | 124.69   |
| 22  | B     | 1207 | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 22  | 7     | 606  | CLA  | C4B-CHC-C1C | 2.49  | 132.09      | 126.25   |
| 22  | A     | 1132 | CLA  | C4B-CHC-C1C | 2.49  | 132.09      | 126.25   |
| 22  | B     | 1228 | CLA  | O2D-CGD-O1D | -2.49 | 119.01      | 123.85   |
| 22  | 5     | 618  | CLA  | O2D-CGD-O1D | -2.49 | 119.01      | 123.85   |
| 22  | 5     | 613  | CLA  | C1-C2-C3    | -2.49 | 122.12      | 126.20   |
| 39  | 3     | 501  | LUT  | C10-C11-C12 | -2.49 | 116.00      | 123.20   |
| 22  | 3     | 606  | CLA  | CHD-C1D-ND  | -2.49 | 121.31      | 124.80   |
| 39  | 9     | 501  | LUT  | C15-C14-C13 | -2.48 | 123.79      | 127.28   |
| 22  | B     | 1223 | CLA  | O2A-CGA-CBA | 2.48  | 119.41      | 111.83   |
| 22  | 3     | 613  | CLA  | CHA-C4D-ND  | 2.48  | 137.68      | 132.55   |
| 22  | A     | 1113 | CLA  | C1C-C2C-C3C | -2.48 | 104.37      | 106.98   |
| 22  | B     | 1203 | CLA  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 25  | A     | 4005 | BCR  | C37-C22-C23 | 2.48  | 121.88      | 118.09   |
| 22  | 3     | 607  | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |
| 22  | 7     | 603  | CLA  | C1C-C2C-C3C | -2.48 | 104.37      | 106.98   |
| 22  | Z     | 608  | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |
| 22  | 7     | 605  | CLA  | C2C-C1C-NC  | 2.48  | 112.59      | 109.98   |
| 22  | 6     | 602  | CLA  | CHA-C4D-ND  | 2.48  | 137.67      | 132.55   |
| 39  | 4     | 502  | LUT  | C1-C6-C5    | -2.48 | 119.24      | 122.64   |
| 22  | 6     | 612  | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 22  | 6     | 609  | CLA  | C1D-ND-C4D  | -2.48 | 104.57      | 106.31   |
| 22  | 3     | 608  | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |
| 22  | L     | 1503 | CLA  | CAA-C2A-C3A | -2.48 | 106.30      | 113.00   |
| 22  | 8     | 602  | CLA  | CHA-C4D-ND  | 2.48  | 137.67      | 132.55   |
| 22  | 3     | 616  | CLA  | C4B-CHC-C1C | 2.48  | 132.08      | 126.25   |
| 22  | 4     | 605  | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 22  | 3     | 612  | CLA  | CMA-C3A-C4A | 2.48  | 118.44      | 111.77   |
| 22  | B     | 1225 | CLA  | CMA-C3A-C4A | 2.48  | 118.44      | 111.77   |
| 25  | B     | 4007 | BCR  | C19-C18-C17 | 2.48  | 122.91      | 119.01   |
| 25  | B     | 4005 | BCR  | C33-C5-C4   | 2.48  | 118.88      | 113.60   |
| 22  | 3     | 618  | CLA  | CMA-C3A-C4A | 2.48  | 118.44      | 111.77   |
| 22  | 7     | 601  | CLA  | O1D-CGD-CBD | -2.48 | 119.63      | 124.52   |
| 22  | 5     | 602  | CLA  | C1D-ND-C4D  | -2.48 | 104.57      | 106.31   |
| 22  | 1     | 612  | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 22  | 4     | 602  | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 606  | CLA  | CMD-C2D-C3D | -2.48 | 122.01      | 127.69   |
| 22  | 4     | 606  | CLA  | CHD-C1D-ND  | -2.48 | 121.32      | 124.80   |
| 22  | A     | 1138 | CLA  | C2C-C1C-NC  | 2.48  | 112.58      | 109.98   |
| 22  | B     | 1224 | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 22  | 2     | 604  | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 22  | 6     | 615  | CLA  | O2A-CGA-CBA | 2.48  | 119.39      | 111.83   |
| 22  | B     | 1216 | CLA  | CHD-C1D-ND  | -2.48 | 121.32      | 124.80   |
| 22  | 2     | 603  | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 22  | 7     | 609  | CLA  | O1D-CGD-CBD | -2.48 | 119.64      | 124.52   |
| 25  | B     | 4003 | BCR  | C35-C13-C12 | 2.48  | 121.87      | 118.09   |
| 22  | A     | 1126 | CLA  | O2A-CGA-CBA | 2.47  | 119.38      | 111.83   |
| 22  | 9     | 607  | CLA  | CHA-C4D-ND  | 2.47  | 137.66      | 132.55   |
| 22  | A     | 1134 | CLA  | C1-O2A-CGA  | 2.47  | 122.64      | 116.65   |
| 22  | 7     | 605  | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | 5     | 605  | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | A     | 1102 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | 5     | 601  | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | Z     | 601  | CLA  | C1C-C2C-C3C | -2.47 | 104.38      | 106.98   |
| 22  | 8     | 602  | CLA  | C1C-C2C-C3C | -2.47 | 104.38      | 106.98   |
| 22  | 9     | 612  | CLA  | C1C-C2C-C3C | -2.47 | 104.38      | 106.98   |
| 22  | A     | 1119 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | B     | 1229 | CLA  | C1-O2A-CGA  | 2.47  | 122.64      | 116.65   |
| 22  | 9     | 604  | CLA  | CHD-C1D-ND  | -2.47 | 121.32      | 124.80   |
| 22  | B     | 1232 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | K     | 1402 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | A     | 1125 | CLA  | CMA-C3A-C4A | 2.47  | 118.42      | 111.77   |
| 22  | 5     | 615  | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 22  | 4     | 602  | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 39  | 9     | 502  | LUT  | C35-C15-C14 | -2.47 | 118.46      | 123.52   |
| 22  | B     | 1222 | CLA  | C1-C2-C3    | -2.47 | 122.15      | 126.20   |
| 22  | B     | 1218 | CLA  | C2D-C1D-ND  | 2.47  | 112.57      | 110.13   |
| 22  | B     | 1227 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | L     | 1502 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 25  | B     | 4001 | BCR  | C36-C18-C17 | -2.47 | 118.81      | 122.82   |
| 22  | B     | 1222 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | B     | 1204 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | A     | 1139 | CLA  | O2A-CGA-CBA | 2.47  | 119.37      | 111.83   |
| 22  | 7     | 608  | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 25  | A     | 4004 | BCR  | C34-C9-C8   | 2.47  | 121.86      | 118.09   |
| 22  | 3     | 613  | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 22  | A     | 1120 | CLA  | O1D-CGD-CBD | -2.47 | 119.65      | 124.52   |
| 22  | B     | 1208 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 612  | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | K     | 1401 | CLA  | C1C-C2C-C3C | -2.47 | 104.38      | 106.98   |
| 22  | A     | 1110 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | 1     | 615  | CLA  | CMD-C2D-C3D | -2.47 | 122.03      | 127.69   |
| 22  | B     | 1204 | CLA  | CHD-C1D-ND  | -2.47 | 121.33      | 124.80   |
| 22  | A     | 1140 | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 22  | B     | 1214 | CLA  | CMA-C3A-C4A | 2.47  | 118.40      | 111.77   |
| 22  | 7     | 606  | CLA  | C3B-C4B-NB  | -2.47 | 108.33      | 110.53   |
| 22  | 3     | 602  | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | B     | 1219 | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 25  | J     | 4001 | BCR  | C38-C26-C25 | -2.47 | 121.79      | 124.48   |
| 22  | B     | 1228 | CLA  | CHD-C1D-ND  | -2.47 | 121.33      | 124.80   |
| 22  | 4     | 606  | CLA  | CAA-C2A-C3A | -2.47 | 106.34      | 113.00   |
| 22  | B     | 1220 | CLA  | O2A-CGA-CBA | 2.47  | 119.35      | 111.83   |
| 22  | B     | 1221 | CLA  | C2C-C1C-NC  | 2.46  | 112.57      | 109.98   |
| 22  | 3     | 607  | CLA  | C1-C2-C3    | -2.46 | 122.16      | 126.20   |
| 22  | 5     | 605  | CLA  | O2D-CGD-O1D | -2.46 | 119.05      | 123.85   |
| 22  | B     | 1202 | CLA  | C1C-C2C-C3C | -2.46 | 104.39      | 106.98   |
| 22  | 1     | 607  | CLA  | CHA-C1A-NA  | -2.46 | 120.81      | 126.39   |
| 22  | Z     | 615  | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | Z     | 612  | CLA  | C3B-C4B-NB  | -2.46 | 108.33      | 110.53   |
| 22  | 6     | 602  | CLA  | CMA-C3A-C4A | 2.46  | 118.39      | 111.77   |
| 22  | B     | 1216 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | 1     | 601  | CLA  | C1C-C2C-C3C | -2.46 | 104.39      | 106.98   |
| 22  | 8     | 602  | CLA  | C4B-CHC-C1C | 2.46  | 132.03      | 126.25   |
| 22  | A     | 1139 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | 5     | 612  | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 25  | B     | 4003 | BCR  | C8-C9-C10   | 2.46  | 122.88      | 119.01   |
| 22  | B     | 1212 | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | Z     | 608  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | A     | 1115 | CLA  | C1C-C2C-C3C | -2.46 | 104.39      | 106.98   |
| 22  | 4     | 602  | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 22  | 4     | 608  | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 22  | K     | 1403 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 36  | F     | 4001 | RRX  | C2-C1-C6    | 2.46  | 114.01      | 110.44   |
| 22  | A     | 1112 | CLA  | CHD-C1D-ND  | -2.46 | 121.34      | 124.80   |
| 22  | 6     | 606  | CLA  | CHD-C1D-ND  | -2.46 | 121.34      | 124.80   |
| 22  | A     | 1102 | CLA  | C1C-C2C-C3C | -2.46 | 104.39      | 106.98   |
| 22  | 7     | 605  | CLA  | C1D-ND-C4D  | -2.46 | 104.59      | 106.31   |
| 22  | 4     | 607  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | 2     | 615  | CLA  | C2D-C1D-ND  | 2.46  | 112.56      | 110.13   |
| 22  | 5     | 609  | CLA  | C4B-CHC-C1C | 2.46  | 132.03      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 2     | 606  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | A     | 1103 | CLA  | O2D-CGD-O1D | -2.46 | 119.06      | 123.85   |
| 22  | A     | 1131 | CLA  | C3B-C4B-NB  | -2.46 | 108.34      | 110.53   |
| 22  | B     | 1205 | CLA  | C3B-C4B-NB  | -2.46 | 108.34      | 110.53   |
| 22  | B     | 1238 | CLA  | C3B-C4B-NB  | -2.46 | 108.34      | 110.53   |
| 22  | 5     | 601  | CLA  | CMD-C2D-C3D | -2.46 | 122.05      | 127.69   |
| 22  | B     | 1207 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 22  | Z     | 607  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | B     | 1217 | CLA  | C1-O2A-CGA  | 2.46  | 122.60      | 116.65   |
| 22  | 1     | 608  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | Z     | 602  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | 8     | 607  | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | 8     | 604  | CLA  | C4B-CHC-C1C | 2.46  | 132.02      | 126.25   |
| 22  | K     | 1404 | CLA  | O1D-CGD-CBD | -2.46 | 119.67      | 124.52   |
| 22  | A     | 1115 | CLA  | C2C-C1C-NC  | 2.46  | 112.56      | 109.98   |
| 22  | Z     | 615  | CLA  | O2D-CGD-O1D | -2.46 | 119.07      | 123.85   |
| 22  | 6     | 612  | CLA  | CHD-C1D-ND  | -2.46 | 121.35      | 124.80   |
| 22  | A     | 1128 | CLA  | CMA-C3A-C4A | 2.46  | 118.37      | 111.77   |
| 22  | A     | 1129 | CLA  | O2A-CGA-CBA | 2.46  | 119.32      | 111.83   |
| 22  | 1     | 608  | CLA  | C2C-C1C-NC  | 2.46  | 112.56      | 109.98   |
| 25  | A     | 4003 | BCR  | C36-C18-C17 | -2.46 | 118.84      | 122.82   |
| 22  | 9     | 606  | CLA  | C4B-CHC-C1C | 2.45  | 132.02      | 126.25   |
| 22  | A     | 1113 | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | 4     | 601  | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | 6     | 607  | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | 7     | 606  | CLA  | O2D-CGD-O1D | -2.45 | 119.07      | 123.85   |
| 22  | A     | 1123 | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | B     | 1229 | CLA  | O2D-CGD-O1D | -2.45 | 119.07      | 123.85   |
| 22  | A     | 1139 | CLA  | CHD-C1D-ND  | -2.45 | 121.35      | 124.80   |
| 22  | 5     | 612  | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | A     | 1110 | CLA  | C1C-C2C-C3C | -2.45 | 104.40      | 106.98   |
| 22  | B     | 1221 | CLA  | CMD-C2D-C3D | -2.45 | 122.06      | 127.69   |
| 40  | 1     | 609  | CHL  | C1-C2-C3    | -2.45 | 122.18      | 126.20   |
| 22  | 5     | 613  | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | 4     | 601  | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 22  | B     | 1201 | CLA  | C4B-CHC-C1C | 2.45  | 132.01      | 126.25   |
| 22  | A     | 1133 | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | 6     | 601  | CLA  | CMD-C2D-C3D | -2.45 | 122.06      | 127.69   |
| 22  | 4     | 606  | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 22  | 4     | 615  | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 22  | 7     | 612  | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 40  | 5     | 611  | CHL  | CMA-C3A-C4A | 2.45  | 119.89      | 114.61   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 3     | 603  | CLA  | C4B-CHC-C1C | 2.45  | 132.01      | 126.25   |
| 22  | 7     | 605  | CLA  | C4B-CHC-C1C | 2.45  | 132.01      | 126.25   |
| 22  | 7     | 603  | CLA  | CHD-C1D-ND  | -2.45 | 121.35      | 124.80   |
| 22  | 3     | 606  | CLA  | CMD-C2D-C3D | -2.45 | 122.07      | 127.69   |
| 22  | B     | 1222 | CLA  | CAA-C2A-C1A | -2.45 | 103.95      | 111.97   |
| 22  | A     | 1133 | CLA  | CHD-C1D-ND  | -2.45 | 121.36      | 124.80   |
| 22  | 1     | 601  | CLA  | CHD-C1D-ND  | -2.45 | 121.36      | 124.80   |
| 22  | A     | 1101 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | B     | 1240 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | A     | 1115 | CLA  | CGD-CBD-CAD | 2.45  | 118.78      | 110.85   |
| 22  | B     | 1232 | CLA  | C4B-CHC-C1C | 2.45  | 132.01      | 126.25   |
| 22  | 6     | 604  | CLA  | CHD-C1D-ND  | -2.45 | 121.36      | 124.80   |
| 22  | 1     | 602  | CLA  | CAC-C3C-C4C | 2.45  | 127.98      | 124.79   |
| 22  | 1     | 608  | CLA  | O2A-CGA-CBA | 2.45  | 119.30      | 111.83   |
| 22  | A     | 1115 | CLA  | CHD-C1D-ND  | -2.45 | 121.36      | 124.80   |
| 22  | 3     | 613  | CLA  | CHD-C1D-ND  | -2.45 | 121.36      | 124.80   |
| 22  | B     | 1214 | CLA  | O2A-CGA-CBA | 2.45  | 119.30      | 111.83   |
| 22  | B     | 1232 | CLA  | C2C-C1C-NC  | 2.45  | 112.55      | 109.98   |
| 22  | A     | 1138 | CLA  | C4B-CHC-C1C | 2.45  | 132.00      | 126.25   |
| 22  | B     | 1206 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | B     | 1217 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | B     | 1236 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 39  | 6     | 502  | LUT  | C7-C8-C9    | -2.45 | 122.61      | 126.23   |
| 22  | 7     | 608  | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 25  | L     | 4002 | BCR  | C34-C9-C10  | -2.45 | 118.85      | 122.82   |
| 22  | A     | 1112 | CLA  | O1D-CGD-CBD | -2.45 | 119.69      | 124.52   |
| 22  | A     | 1140 | CLA  | CMA-C3A-C4A | 2.45  | 118.35      | 111.77   |
| 25  | 3     | 506  | BCR  | C23-C22-C21 | 2.45  | 122.86      | 119.01   |
| 22  | A     | 1119 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 22  | 5     | 609  | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 25  | I     | 4001 | BCR  | C38-C26-C27 | 2.45  | 118.81      | 113.60   |
| 22  | 4     | 607  | CLA  | C3B-C4B-NB  | -2.45 | 108.35      | 110.53   |
| 22  | A     | 1141 | CLA  | O2A-CGA-CBA | 2.45  | 119.29      | 111.83   |
| 22  | B     | 1236 | CLA  | C2D-C1D-ND  | 2.45  | 112.55      | 110.13   |
| 22  | 5     | 605  | CLA  | CAA-C2A-C3A | -2.45 | 106.39      | 113.00   |
| 22  | A     | 1106 | CLA  | CHA-C4D-ND  | 2.45  | 137.59      | 132.55   |
| 22  | B     | 1240 | CLA  | CHA-C1A-NA  | -2.45 | 120.85      | 126.39   |
| 22  | Z     | 604  | CLA  | C1C-C2C-C3C | -2.45 | 104.41      | 106.98   |
| 22  | A     | 1106 | CLA  | CMA-C3A-C4A | 2.45  | 118.34      | 111.77   |
| 22  | 7     | 601  | CLA  | C1C-C2C-C3C | -2.44 | 104.41      | 106.98   |
| 22  | 3     | 602  | CLA  | C4B-CHC-C1C | 2.44  | 132.00      | 126.25   |
| 25  | K     | 4002 | BCR  | C36-C18-C17 | -2.44 | 118.86      | 122.82   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 3     | 603  | CLA  | C1D-ND-C4D  | -2.44 | 104.60      | 106.31   |
| 22  | B     | 1229 | CLA  | C2D-C1D-ND  | 2.44  | 112.55      | 110.13   |
| 22  | Z     | 608  | CLA  | CMD-C2D-C3D | -2.44 | 122.08      | 127.69   |
| 22  | 4     | 601  | CLA  | C2C-C1C-NC  | 2.44  | 112.55      | 109.98   |
| 22  | A     | 1139 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | B     | 1220 | CLA  | CMA-C3A-C4A | 2.44  | 118.34      | 111.77   |
| 22  | 6     | 608  | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | 8     | 615  | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 40  | 8     | 610  | CHL  | C1C-C2C-CMC | -2.44 | 122.40      | 126.80   |
| 22  | G     | 1601 | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 22  | 9     | 607  | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 22  | 4     | 606  | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | 2     | 608  | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | 2     | 604  | CLA  | CMA-C3A-C4A | 2.44  | 118.34      | 111.77   |
| 22  | A     | 1131 | CLA  | O2A-CGA-CBA | 2.44  | 119.28      | 111.83   |
| 39  | 6     | 501  | LUT  | C20-C13-C12 | 2.44  | 121.82      | 118.09   |
| 22  | B     | 1208 | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 22  | B     | 1022 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 22  | B     | 1210 | CLA  | CHD-C1D-ND  | -2.44 | 121.37      | 124.80   |
| 22  | 9     | 601  | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | A     | 1102 | CLA  | CHA-C1A-NA  | -2.44 | 120.86      | 126.39   |
| 22  | B     | 1223 | CLA  | C3D-C2D-C1D | -2.44 | 102.50      | 105.83   |
| 22  | Z     | 603  | CLA  | C1-O2A-CGA  | 2.44  | 122.56      | 116.65   |
| 25  | A     | 4005 | BCR  | C34-C9-C10  | -2.44 | 118.86      | 122.82   |
| 22  | A     | 1136 | CLA  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |
| 22  | 1     | 611  | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | A     | 1102 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | 1     | 608  | CLA  | C1D-ND-C4D  | -2.44 | 104.60      | 106.31   |
| 22  | 8     | 606  | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 28  | B     | 6101 | LMT  | O1'-C1'-C2' | 2.44  | 111.98      | 108.27   |
| 22  | A     | 1135 | CLA  | O2A-CGA-CBA | 2.44  | 119.27      | 111.83   |
| 22  | 3     | 603  | CLA  | CHD-C1D-ND  | -2.44 | 121.37      | 124.80   |
| 22  | 6     | 609  | CLA  | CHD-C1D-ND  | -2.44 | 121.37      | 124.80   |
| 22  | 6     | 608  | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 39  | 3     | 502  | LUT  | C37-C21-C26 | 2.44  | 113.24      | 109.55   |
| 22  | B     | 1208 | CLA  | CMA-C3A-C4A | 2.44  | 118.33      | 111.77   |
| 22  | Z     | 611  | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | 6     | 609  | CLA  | O2A-CGA-CBA | 2.44  | 119.27      | 111.83   |
| 22  | A     | 1013 | CLA  | C1C-C2C-C3C | -2.44 | 104.42      | 106.98   |
| 22  | B     | 1208 | CLA  | CHD-C1D-ND  | -2.44 | 121.37      | 124.80   |
| 22  | B     | 1211 | CLA  | C1-O2A-CGA  | 2.44  | 122.55      | 116.65   |
| 22  | B     | 1241 | CLA  | C1C-C2C-C3C | -2.44 | 104.42      | 106.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 612  | CLA  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 22  | 1     | 601  | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | 3     | 612  | CLA  | C3B-C4B-NB  | -2.44 | 108.36      | 110.53   |
| 22  | 1     | 606  | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | 1     | 613  | CLA  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 25  | 6     | 503  | BCR  | C38-C26-C25 | -2.44 | 121.83      | 124.48   |
| 22  | 8     | 604  | CLA  | CHA-C4D-ND  | 2.44  | 137.57      | 132.55   |
| 39  | Z     | 501  | LUT  | C10-C11-C12 | -2.44 | 116.14      | 123.20   |
| 22  | 4     | 606  | CLA  | C4B-CHC-C1C | 2.44  | 131.97      | 126.25   |
| 22  | A     | 1122 | CLA  | C3B-C4B-NB  | -2.44 | 108.36      | 110.53   |
| 22  | 7     | 615  | CLA  | CHA-C4D-ND  | 2.44  | 137.57      | 132.55   |
| 22  | 5     | 605  | CLA  | C4B-CHC-C1C | 2.43  | 131.97      | 126.25   |
| 22  | 9     | 602  | CLA  | C4B-CHC-C1C | 2.43  | 131.97      | 126.25   |
| 22  | 9     | 612  | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | 5     | 604  | CLA  | C1D-ND-C4D  | -2.43 | 104.60      | 106.31   |
| 22  | 2     | 612  | CLA  | C4B-CHC-C1C | 2.43  | 131.97      | 126.25   |
| 22  | B     | 1238 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | 6     | 601  | CLA  | C1-C2-C3    | -2.43 | 122.21      | 126.20   |
| 22  | B     | 1221 | CLA  | CHA-C1A-NA  | -2.43 | 120.88      | 126.39   |
| 22  | B     | 1240 | CLA  | C4B-CHC-C1C | 2.43  | 131.97      | 126.25   |
| 22  | A     | 1139 | CLA  | C2C-C1C-NC  | 2.43  | 112.54      | 109.98   |
| 22  | A     | 1131 | CLA  | O2D-CGD-O1D | -2.43 | 119.11      | 123.85   |
| 22  | G     | 1601 | CLA  | O2A-CGA-CBA | 2.43  | 119.25      | 111.83   |
| 22  | 4     | 601  | CLA  | CMD-C2D-C3D | -2.43 | 122.11      | 127.69   |
| 22  | B     | 1239 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | 6     | 619  | CLA  | O1D-CGD-CBD | -2.43 | 119.72      | 124.52   |
| 22  | A     | 1141 | CLA  | O2D-CGD-O1D | -2.43 | 119.11      | 123.85   |
| 22  | 2     | 603  | CLA  | C2D-C1D-ND  | 2.43  | 112.53      | 110.13   |
| 22  | 1     | 605  | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 22  | 8     | 612  | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 22  | A     | 1123 | CLA  | CHA-C1A-NA  | -2.43 | 120.88      | 126.39   |
| 22  | 7     | 613  | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | 9     | 602  | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | 9     | 612  | CLA  | C2C-C1C-NC  | 2.43  | 112.54      | 109.98   |
| 40  | 4     | 610  | CHL  | C1-C2-C3    | -2.43 | 122.83      | 126.76   |
| 22  | Z     | 608  | CLA  | O2D-CGD-O1D | -2.43 | 119.11      | 123.85   |
| 22  | A     | 1116 | CLA  | CHA-C1A-NA  | -2.43 | 120.89      | 126.39   |
| 22  | L     | 1503 | CLA  | C4B-CHC-C1C | 2.43  | 131.96      | 126.25   |
| 22  | 1     | 604  | CLA  | CMA-C3A-C4A | 2.43  | 118.31      | 111.77   |
| 22  | B     | 1212 | CLA  | C2C-C1C-NC  | 2.43  | 112.53      | 109.98   |
| 22  | 9     | 608  | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 39  | 6     | 502  | LUT  | C22-C23-C24 | -2.43 | 107.58      | 111.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 9     | 604  | CLA  | C2D-C1D-ND  | 2.43  | 112.53      | 110.13   |
| 22  | 1     | 604  | CLA  | C4B-CHC-C1C | 2.43  | 131.96      | 126.25   |
| 22  | B     | 1214 | CLA  | C2C-C1C-NC  | 2.43  | 112.53      | 109.98   |
| 22  | 4     | 606  | CLA  | C2C-C1C-NC  | 2.43  | 112.53      | 109.98   |
| 22  | 3     | 610  | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | Z     | 607  | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 22  | 9     | 608  | CLA  | CMA-C3A-C4A | 2.43  | 118.30      | 111.77   |
| 39  | Z     | 502  | LUT  | C38-C25-C24 | -2.43 | 117.61      | 123.36   |
| 22  | B     | 1225 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | J     | 1901 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 2     | 607  | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | B     | 1229 | CLA  | CHD-C1D-ND  | -2.43 | 121.39      | 124.80   |
| 22  | 6     | 605  | CLA  | CHA-C1A-NA  | -2.43 | 120.89      | 126.39   |
| 22  | 1     | 601  | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 7     | 609  | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 5     | 608  | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 3     | 618  | CLA  | CHA-C1A-NA  | -2.43 | 120.90      | 126.39   |
| 22  | A     | 1122 | CLA  | C1-C2-C3    | -2.43 | 122.22      | 126.20   |
| 22  | 5     | 601  | CLA  | C4B-CHC-C1C | 2.43  | 131.95      | 126.25   |
| 22  | A     | 1107 | CLA  | C4B-CHC-C1C | 2.43  | 131.95      | 126.25   |
| 22  | 6     | 606  | CLA  | C4B-CHC-C1C | 2.43  | 131.95      | 126.25   |
| 40  | 6     | 611  | CHL  | CMA-C3A-C4A | 2.43  | 119.84      | 114.61   |
| 22  | 1     | 608  | CLA  | O2D-CGD-O1D | -2.43 | 119.13      | 123.85   |
| 22  | B     | 1237 | CLA  | CHA-C4D-ND  | 2.43  | 137.55      | 132.55   |
| 22  | A     | 1109 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 22  | 7     | 602  | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | 6     | 604  | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | 6     | 604  | CLA  | CBA-CAA-C2A | 2.42  | 121.01      | 113.79   |
| 40  | 2     | 613  | CHL  | C1-O2A-CGA  | 2.42  | 122.52      | 116.65   |
| 22  | 1     | 615  | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 22  | Z     | 615  | CLA  | C4B-CHC-C1C | 2.42  | 131.95      | 126.25   |
| 22  | 3     | 610  | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 22  | 7     | 615  | CLA  | CHD-C1D-ND  | -2.42 | 121.39      | 124.80   |
| 22  | Z     | 611  | CLA  | CMD-C2D-C3D | -2.42 | 122.13      | 127.69   |
| 22  | 9     | 603  | CLA  | CMD-C2D-C3D | -2.42 | 122.14      | 127.69   |
| 22  | A     | 1132 | CLA  | O2A-CGA-CBA | 2.42  | 119.22      | 111.83   |
| 22  | A     | 1132 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | L     | 1503 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 22  | B     | 1221 | CLA  | C1C-C2C-C3C | -2.42 | 104.43      | 106.98   |
| 39  | 1     | 501  | LUT  | C22-C23-C24 | -2.42 | 107.59      | 111.18   |
| 22  | 7     | 605  | CLA  | CMD-C2D-C3D | -2.42 | 122.14      | 127.69   |
| 22  | A     | 1013 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1241 | CLA  | C4B-CHC-C1C | 2.42  | 131.94      | 126.25   |
| 22  | 6     | 602  | CLA  | C4B-CHC-C1C | 2.42  | 131.94      | 126.25   |
| 22  | 4     | 604  | CLA  | C4B-CHC-C1C | 2.42  | 131.94      | 126.25   |
| 22  | B     | 1236 | CLA  | CHD-C1D-ND  | -2.42 | 121.40      | 124.80   |
| 22  | B     | 1237 | CLA  | C1C-C2C-C3C | -2.42 | 104.44      | 106.98   |
| 22  | 8     | 607  | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 22  | B     | 1208 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 2     | 601  | CLA  | CAA-C2A-C3A | -2.42 | 106.47      | 113.00   |
| 22  | A     | 1013 | CLA  | C2D-C1D-ND  | 2.42  | 112.52      | 110.13   |
| 22  | A     | 1131 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 8     | 608  | CLA  | C4B-CHC-C1C | 2.42  | 131.93      | 126.25   |
| 22  | A     | 1127 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 6     | 601  | CLA  | C4B-CHC-C1C | 2.42  | 131.93      | 126.25   |
| 22  | 7     | 604  | CLA  | CHA-C4D-ND  | 2.42  | 137.53      | 132.55   |
| 22  | Z     | 611  | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 22  | 4     | 603  | CLA  | O2A-CGA-CBA | 2.42  | 119.20      | 111.83   |
| 37  | 1     | 503  | C7Z  | C31-C32-C33 | -2.42 | 119.74      | 126.36   |
| 22  | B     | 1240 | CLA  | C2C-C1C-NC  | 2.42  | 112.52      | 109.98   |
| 22  | 9     | 605  | CLA  | CMD-C2D-C3D | -2.42 | 122.15      | 127.69   |
| 22  | 5     | 618  | CLA  | C3D-C2D-C1D | -2.42 | 102.53      | 105.83   |
| 22  | 8     | 611  | CLA  | CHA-C4D-ND  | 2.42  | 137.53      | 132.55   |
| 22  | 9     | 601  | CLA  | C1C-C2C-C3C | -2.41 | 104.44      | 106.98   |
| 40  | 4     | 617  | CHL  | C4C-CHD-C1D | 2.41  | 124.71      | 116.07   |
| 22  | A     | 1113 | CLA  | C4B-CHC-C1C | 2.41  | 131.93      | 126.25   |
| 22  | 1     | 608  | CLA  | C4B-CHC-C1C | 2.41  | 131.93      | 126.25   |
| 22  | 5     | 603  | CLA  | CHD-C1D-ND  | -2.41 | 121.41      | 124.80   |
| 22  | B     | 1203 | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 22  | A     | 1103 | CLA  | C2D-C1D-ND  | 2.41  | 112.52      | 110.13   |
| 22  | 5     | 604  | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | B     | 1210 | CLA  | C2C-C1C-NC  | 2.41  | 112.52      | 109.98   |
| 39  | 2     | 502  | LUT  | C22-C23-C24 | -2.41 | 107.60      | 111.18   |
| 22  | 7     | 601  | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 28  | B     | 6101 | LMT  | O5B-C5B-C4B | 2.41  | 114.05      | 109.70   |
| 22  | J     | 1901 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 22  | 5     | 618  | CLA  | CHD-C1D-ND  | -2.41 | 121.41      | 124.80   |
| 22  | 5     | 613  | CLA  | O2A-CGA-CBA | 2.41  | 119.19      | 111.83   |
| 22  | 6     | 606  | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | B     | 1226 | CLA  | CHD-C1D-ND  | -2.41 | 121.41      | 124.80   |
| 22  | 5     | 603  | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | B     | 1235 | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 22  | 6     | 606  | CLA  | CMA-C3A-C4A | 2.41  | 118.25      | 111.77   |
| 25  | 7     | 504  | BCR  | C33-C5-C4   | 2.41  | 118.73      | 113.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 3     | 610  | CLA  | CMD-C2D-C3D | -2.41 | 122.16      | 127.69   |
| 22  | B     | 1227 | CLA  | CAA-C2A-C3A | -2.41 | 106.49      | 113.00   |
| 37  | J     | 4002 | C7Z  | C38-C25-C24 | 2.41  | 118.85      | 114.42   |
| 40  | 8     | 613  | CHL  | CMA-C3A-C2A | 2.41  | 123.43      | 114.13   |
| 22  | 4     | 607  | CLA  | O2D-CGD-O1D | -2.41 | 119.16      | 123.85   |
| 22  | 9     | 605  | CLA  | O2D-CGD-O1D | -2.41 | 119.16      | 123.85   |
| 22  | B     | 1210 | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | 4     | 609  | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | B     | 1202 | CLA  | CAA-C2A-C1A | -2.41 | 104.08      | 111.97   |
| 39  | 1     | 501  | LUT  | C26-C27-C28 | -2.41 | 120.83      | 124.58   |
| 25  | J     | 4001 | BCR  | C19-C18-C17 | 2.41  | 122.80      | 119.01   |
| 22  | A     | 1013 | CLA  | C1-O2A-CGA  | 2.41  | 122.48      | 116.65   |
| 22  | B     | 1230 | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 22  | K     | 1403 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 37  | 5     | 505  | C7Z  | C30-C31-C32 | -2.41 | 116.23      | 123.20   |
| 22  | 5     | 609  | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | A     | 1128 | CLA  | O2A-CGA-CBA | 2.41  | 119.17      | 111.83   |
| 22  | 8     | 609  | CLA  | O2A-CGA-CBA | 2.41  | 119.17      | 111.83   |
| 22  | 3     | 606  | CLA  | C1-C2-C3    | -2.41 | 122.25      | 126.20   |
| 39  | 2     | 503  | LUT  | C15-C35-C34 | -2.41 | 118.60      | 123.52   |
| 37  | J     | 4002 | C7Z  | C18-C5-C4   | 2.41  | 118.84      | 114.42   |
| 22  | B     | 1230 | CLA  | CMA-C3A-C4A | 2.41  | 118.24      | 111.77   |
| 22  | Z     | 604  | CLA  | C4B-CHC-C1C | 2.41  | 131.90      | 126.25   |
| 22  | 3     | 601  | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | 6     | 604  | CLA  | C4B-CHC-C1C | 2.41  | 131.90      | 126.25   |
| 22  | A     | 1138 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | 6     | 618  | CLA  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 22  | A     | 1116 | CLA  | C4B-CHC-C1C | 2.40  | 131.90      | 126.25   |
| 22  | 8     | 601  | CLA  | O2A-CGA-CBA | 2.40  | 119.17      | 111.83   |
| 22  | B     | 1228 | CLA  | CHA-C4D-ND  | 2.40  | 137.51      | 132.55   |
| 22  | B     | 1204 | CLA  | CHA-C4D-ND  | 2.40  | 137.51      | 132.55   |
| 22  | Z     | 612  | CLA  | CHD-C1D-ND  | -2.40 | 121.42      | 124.80   |
| 22  | 3     | 601  | CLA  | CHD-C1D-ND  | -2.40 | 121.42      | 124.80   |
| 22  | 2     | 602  | CLA  | CHA-C4D-ND  | 2.40  | 137.51      | 132.55   |
| 22  | A     | 1135 | CLA  | CHA-C4D-ND  | 2.40  | 137.51      | 132.55   |
| 37  | 1     | 503  | C7Z  | C24-C25-C26 | -2.40 | 115.82      | 120.76   |
| 22  | 8     | 601  | CLA  | CMD-C2D-C3D | -2.40 | 122.18      | 127.69   |
| 40  | Z     | 609  | CHL  | C1A-CHA-C4D | 2.40  | 122.99      | 118.98   |
| 22  | B     | 1235 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | B     | 1226 | CLA  | O2A-CGA-CBA | 2.40  | 119.16      | 111.83   |
| 22  | B     | 1229 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 7     | 601  | CLA  | CHD-C1D-ND  | -2.40 | 121.42      | 124.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 3     | 618  | CLA  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 40  | 5     | 617  | CHL  | C4C-CHD-C1D | 2.40  | 124.66      | 116.07   |
| 22  | 5     | 606  | CLA  | O2A-CGA-CBA | 2.40  | 119.16      | 111.83   |
| 22  | A     | 1132 | CLA  | CHD-C1D-ND  | -2.40 | 121.42      | 124.80   |
| 22  | Z     | 611  | CLA  | CHD-C1D-ND  | -2.40 | 121.42      | 124.80   |
| 22  | B     | 1201 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 7     | 608  | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 39  | 7     | 501  | LUT  | C10-C11-C12 | -2.40 | 116.25      | 123.20   |
| 25  | L     | 4002 | BCR  | C36-C18-C17 | -2.40 | 118.93      | 122.82   |
| 22  | A     | 1108 | CLA  | CHD-C1D-ND  | -2.40 | 121.43      | 124.80   |
| 22  | 9     | 601  | CLA  | C3B-C4B-NB  | -2.40 | 108.39      | 110.53   |
| 22  | 3     | 606  | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 5     | 615  | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 39  | Z     | 502  | LUT  | C11-C10-C9  | -2.40 | 123.92      | 127.28   |
| 22  | 8     | 606  | CLA  | C4B-CHC-C1C | 2.40  | 131.88      | 126.25   |
| 22  | B     | 1205 | CLA  | C6-C5-C3    | -2.40 | 107.63      | 113.47   |
| 22  | A     | 1135 | CLA  | CHA-C1A-NA  | -2.40 | 120.96      | 126.39   |
| 22  | 8     | 601  | CLA  | C2A-C1A-CHA | 2.40  | 128.03      | 123.87   |
| 22  | 4     | 608  | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 22  | 4     | 606  | CLA  | CMA-C3A-C4A | 2.40  | 118.21      | 111.77   |
| 22  | B     | 1235 | CLA  | CMD-C2D-C3D | -2.40 | 122.19      | 127.69   |
| 22  | B     | 1213 | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 39  | 8     | 501  | LUT  | C20-C13-C12 | 2.40  | 121.75      | 118.09   |
| 22  | B     | 1241 | CLA  | C2C-C1C-NC  | 2.39  | 112.50      | 109.98   |
| 39  | 4     | 501  | LUT  | C22-C23-C24 | -2.39 | 107.63      | 111.18   |
| 22  | L     | 1503 | CLA  | CHD-C1D-ND  | -2.39 | 121.43      | 124.80   |
| 22  | 5     | 601  | CLA  | C1C-C2C-C3C | -2.39 | 104.46      | 106.98   |
| 22  | A     | 1101 | CLA  | CHD-C1D-ND  | -2.39 | 121.43      | 124.80   |
| 22  | 1     | 613  | CLA  | CHA-C1A-NA  | -2.39 | 120.97      | 126.39   |
| 22  | B     | 1230 | CLA  | C4B-CHC-C1C | 2.39  | 131.88      | 126.25   |
| 22  | 5     | 601  | CLA  | O1D-CGD-CBD | -2.39 | 119.80      | 124.52   |
| 22  | 8     | 601  | CLA  | C3B-C4B-NB  | -2.39 | 108.39      | 110.53   |
| 22  | A     | 1112 | CLA  | CHA-C4D-ND  | 2.39  | 137.49      | 132.55   |
| 22  | B     | 1228 | CLA  | C1C-C2C-C3C | -2.39 | 104.46      | 106.98   |
| 26  | 6     | 801  | LHG  | C5-O7-C7    | -2.39 | 112.07      | 117.80   |
| 22  | 4     | 604  | CLA  | CHA-C4D-ND  | 2.39  | 137.48      | 132.55   |
| 22  | 6     | 612  | CLA  | CHA-C4D-ND  | 2.39  | 137.48      | 132.55   |
| 22  | 4     | 609  | CLA  | O2A-CGA-CBA | 2.39  | 119.12      | 111.83   |
| 22  | 8     | 615  | CLA  | C3B-C4B-NB  | -2.39 | 108.40      | 110.53   |
| 22  | 3     | 616  | CLA  | CHA-C4D-ND  | 2.39  | 137.48      | 132.55   |
| 22  | A     | 1137 | CLA  | CHA-C4D-ND  | 2.39  | 137.48      | 132.55   |
| 22  | Z     | 602  | CLA  | C4B-CHC-C1C | 2.39  | 131.87      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 5     | 612  | CLA  | C2C-C1C-NC  | 2.39  | 112.49      | 109.98   |
| 22  | A     | 1125 | CLA  | C1C-C2C-C3C | -2.39 | 104.47      | 106.98   |
| 25  | 6     | 504  | BCR  | C37-C22-C23 | 2.39  | 121.74      | 118.09   |
| 22  | 6     | 607  | CLA  | O2A-CGA-CBA | 2.39  | 119.12      | 111.83   |
| 22  | 9     | 608  | CLA  | C4B-CHC-C1C | 2.39  | 131.86      | 126.25   |
| 39  | 8     | 502  | LUT  | C31-C32-C33 | -2.39 | 119.81      | 126.36   |
| 22  | A     | 1105 | CLA  | CHD-C1D-ND  | -2.39 | 121.44      | 124.80   |
| 22  | 1     | 604  | CLA  | CMD-C2D-C3D | -2.39 | 122.21      | 127.69   |
| 26  | 2     | 801  | LHG  | C5-O7-C7    | -2.39 | 112.08      | 117.80   |
| 22  | J     | 1901 | CLA  | CHD-C1D-ND  | -2.39 | 121.44      | 124.80   |
| 22  | 8     | 609  | CLA  | CMA-C3A-C4A | 2.39  | 118.19      | 111.77   |
| 22  | 6     | 619  | CLA  | C3B-C4B-NB  | -2.39 | 108.40      | 110.53   |
| 22  | A     | 1107 | CLA  | CHA-C4D-ND  | 2.39  | 137.47      | 132.55   |
| 22  | Z     | 601  | CLA  | CHA-C4D-ND  | 2.39  | 137.47      | 132.55   |
| 22  | B     | 1223 | CLA  | OBD-CAD-C3D | -2.39 | 122.84      | 128.42   |
| 22  | 6     | 608  | CLA  | CHD-C1D-ND  | -2.39 | 121.44      | 124.80   |
| 22  | B     | 1213 | CLA  | CMA-C3A-C4A | 2.39  | 118.19      | 111.77   |
| 40  | 8     | 613  | CHL  | C4D-CHA-CBD | -2.39 | 106.56      | 108.97   |
| 22  | 5     | 612  | CLA  | C4B-CHC-C1C | 2.39  | 131.86      | 126.25   |
| 22  | 7     | 605  | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 22  | 9     | 606  | CLA  | CHA-C4D-ND  | 2.38  | 137.47      | 132.55   |
| 22  | B     | 1211 | CLA  | C1C-C2C-C3C | -2.38 | 104.47      | 106.98   |
| 22  | 6     | 601  | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 40  | 5     | 617  | CHL  | CMA-C3A-C4A | 2.38  | 119.75      | 114.61   |
| 22  | A     | 1118 | CLA  | C4B-CHC-C1C | 2.38  | 131.85      | 126.25   |
| 22  | 5     | 607  | CLA  | C4B-CHC-C1C | 2.38  | 131.85      | 126.25   |
| 22  | 7     | 604  | CLA  | CHA-C1A-NA  | -2.38 | 120.99      | 126.39   |
| 22  | B     | 1215 | CLA  | CHA-C4D-ND  | 2.38  | 137.47      | 132.55   |
| 22  | 4     | 608  | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 22  | B     | 1236 | CLA  | O2A-CGA-CBA | 2.38  | 119.10      | 111.83   |
| 22  | A     | 1117 | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 22  | B     | 1208 | CLA  | C4B-CHC-C1C | 2.38  | 131.85      | 126.25   |
| 39  | 9     | 501  | LUT  | C11-C10-C9  | -2.38 | 123.94      | 127.28   |
| 25  | B     | 4003 | BCR  | C4-C5-C6    | -2.38 | 119.48      | 122.70   |
| 22  | 1     | 603  | CLA  | CHA-C4D-ND  | 2.38  | 137.47      | 132.55   |
| 22  | 4     | 601  | CLA  | C1-O2A-CGA  | 2.38  | 122.42      | 116.65   |
| 22  | B     | 1226 | CLA  | CHA-C1A-NA  | -2.38 | 121.00      | 126.39   |
| 22  | 3     | 603  | CLA  | CHA-C4D-ND  | 2.38  | 137.46      | 132.55   |
| 22  | 6     | 619  | CLA  | C2C-C1C-NC  | 2.38  | 112.48      | 109.98   |
| 39  | 9     | 501  | LUT  | C39-C29-C28 | 2.38  | 121.73      | 118.09   |
| 22  | 7     | 603  | CLA  | C4B-CHC-C1C | 2.38  | 131.85      | 126.25   |
| 22  | B     | 1231 | CLA  | C2C-C1C-NC  | 2.38  | 112.48      | 109.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 605  | CLA  | CMA-C3A-C4A | 2.38  | 118.17      | 111.77   |
| 22  | 2     | 602  | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.79   |
| 22  | 5     | 601  | CLA  | C1D-ND-C4D  | -2.38 | 104.64      | 106.31   |
| 22  | 6     | 603  | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 22  | A     | 1122 | CLA  | CMD-C2D-C3D | -2.38 | 122.23      | 127.69   |
| 22  | 3     | 612  | CLA  | CHA-C4D-ND  | 2.38  | 137.46      | 132.55   |
| 22  | 6     | 603  | CLA  | CHA-C4D-ND  | 2.38  | 137.46      | 132.55   |
| 22  | A     | 1101 | CLA  | CMA-C3A-C4A | 2.38  | 118.17      | 111.77   |
| 22  | 7     | 616  | CLA  | CHA-C4D-ND  | 2.38  | 137.46      | 132.55   |
| 22  | 5     | 622  | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 22  | Z     | 615  | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 22  | 1     | 603  | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 22  | 1     | 612  | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 22  | 5     | 612  | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 39  | 5     | 501  | LUT  | C11-C10-C9  | -2.38 | 123.94      | 127.28   |
| 22  | Z     | 608  | CLA  | C4B-CHC-C1C | 2.38  | 131.84      | 126.25   |
| 22  | 9     | 605  | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 22  | A     | 1119 | CLA  | CMD-C2D-C3D | -2.38 | 122.24      | 127.69   |
| 22  | B     | 1239 | CLA  | CMA-C3A-C4A | 2.38  | 118.16      | 111.77   |
| 21  | A     | 1011 | CL0  | CAA-CBA-CGA | -2.38 | 106.46      | 113.21   |
| 39  | 8     | 502  | LUT  | C20-C13-C12 | 2.38  | 121.72      | 118.09   |
| 22  | 7     | 604  | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 22  | A     | 1117 | CLA  | CHD-C1D-ND  | -2.38 | 121.46      | 124.80   |
| 22  | A     | 1118 | CLA  | CHD-C1D-ND  | -2.38 | 121.46      | 124.80   |
| 22  | A     | 1109 | CLA  | CHA-C4D-ND  | 2.38  | 137.45      | 132.55   |
| 22  | B     | 1208 | CLA  | C2D-C1D-ND  | 2.38  | 112.48      | 110.13   |
| 25  | 3     | 504  | BCR  | C27-C26-C25 | -2.37 | 119.50      | 122.70   |
| 22  | 1     | 615  | CLA  | C4B-CHC-C1C | 2.37  | 131.83      | 126.25   |
| 22  | A     | 1012 | CLA  | C1C-C2C-C3C | -2.37 | 104.48      | 106.98   |
| 22  | A     | 1122 | CLA  | CHA-C4D-ND  | 2.37  | 137.45      | 132.55   |
| 22  | Z     | 601  | CLA  | O1D-CGD-CBD | -2.37 | 119.84      | 124.52   |
| 22  | B     | 1207 | CLA  | CHA-C4D-ND  | 2.37  | 137.45      | 132.55   |
| 22  | 1     | 615  | CLA  | O2A-CGA-CBA | 2.37  | 119.07      | 111.83   |
| 22  | 2     | 604  | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 22  | 6     | 605  | CLA  | C4B-CHC-C1C | 2.37  | 131.83      | 126.25   |
| 22  | 9     | 603  | CLA  | C4B-CHC-C1C | 2.37  | 131.83      | 126.25   |
| 22  | 8     | 612  | CLA  | CHD-C1D-ND  | -2.37 | 121.46      | 124.80   |
| 22  | A     | 1105 | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 22  | 3     | 608  | CLA  | CHA-C4D-ND  | 2.37  | 137.44      | 132.55   |
| 39  | 9     | 501  | LUT  | C37-C21-C22 | -2.37 | 104.98      | 109.41   |
| 22  | B     | 1213 | CLA  | C4B-CHC-C1C | 2.37  | 131.82      | 126.25   |
| 22  | 1     | 606  | CLA  | C3B-C4B-NB  | -2.37 | 108.41      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 618  | CLA  | C4B-CHC-C1C | 2.37  | 131.82      | 126.25   |
| 39  | 3     | 502  | LUT  | C18-C5-C6   | -2.37 | 121.90      | 124.48   |
| 22  | 8     | 601  | CLA  | C2C-C1C-NC  | 2.37  | 112.47      | 109.98   |
| 25  | 5     | 504  | BCR  | C12-C13-C14 | 2.37  | 122.74      | 119.01   |
| 22  | 6     | 612  | CLA  | C3B-C4B-NB  | -2.37 | 108.41      | 110.53   |
| 22  | B     | 1225 | CLA  | C1C-C2C-C3C | -2.37 | 104.49      | 106.98   |
| 22  | B     | 1221 | CLA  | O2A-CGA-O1A | -2.37 | 117.70      | 123.63   |
| 25  | B     | 4003 | BCR  | C36-C18-C17 | -2.37 | 118.98      | 122.82   |
| 22  | A     | 1130 | CLA  | CHD-C1D-ND  | -2.37 | 121.47      | 124.80   |
| 22  | A     | 1128 | CLA  | CHA-C4D-ND  | 2.37  | 137.44      | 132.55   |
| 37  | 5     | 505  | C7Z  | C15-C35-C34 | -2.37 | 118.67      | 123.52   |
| 40  | 1     | 609  | CHL  | C1-O2A-CGA  | 2.37  | 122.39      | 116.65   |
| 22  | 9     | 604  | CLA  | O1A-CGA-CBA | -2.37 | 114.51      | 123.78   |
| 22  | 2     | 603  | CLA  | O2A-CGA-CBA | 2.37  | 119.06      | 111.83   |
| 22  | 5     | 612  | CLA  | CMD-C2D-C3D | -2.37 | 122.25      | 127.69   |
| 22  | 1     | 604  | CLA  | C6-C5-C3    | -2.37 | 107.70      | 113.47   |
| 39  | 5     | 501  | LUT  | C20-C13-C12 | 2.37  | 121.71      | 118.09   |
| 22  | 9     | 604  | CLA  | CMC-C2C-C1C | 2.37  | 128.74      | 125.03   |
| 22  | 1     | 611  | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 22  | 7     | 613  | CLA  | CHD-C1D-ND  | -2.37 | 121.47      | 124.80   |
| 25  | I     | 4001 | BCR  | C37-C22-C23 | 2.37  | 121.71      | 118.09   |
| 22  | 1     | 605  | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 25  | 3     | 503  | BCR  | C38-C26-C25 | -2.37 | 121.90      | 124.48   |
| 25  | A     | 4002 | BCR  | C38-C26-C27 | 2.37  | 118.64      | 113.60   |
| 22  | G     | 1602 | CLA  | C4B-CHC-C1C | 2.37  | 131.81      | 126.25   |
| 22  | 3     | 613  | CLA  | CMD-C2D-C3D | -2.37 | 122.26      | 127.69   |
| 22  | 8     | 605  | CLA  | O2A-CGA-CBA | 2.37  | 119.05      | 111.83   |
| 22  | 1     | 606  | CLA  | C2C-C1C-NC  | 2.37  | 112.47      | 109.98   |
| 22  | F     | 1301 | CLA  | O2A-C1-C2   | 2.37  | 117.22      | 108.11   |
| 22  | B     | 1023 | CLA  | CHA-C4D-ND  | 2.37  | 137.43      | 132.55   |
| 22  | 2     | 612  | CLA  | O2A-CGA-CBA | 2.37  | 119.05      | 111.83   |
| 22  | 7     | 615  | CLA  | C4B-CHC-C1C | 2.37  | 131.81      | 126.25   |
| 22  | 7     | 613  | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 25  | J     | 4001 | BCR  | C12-C13-C14 | -2.37 | 115.29      | 119.01   |
| 21  | A     | 1011 | CL0  | C4C-CHD-C1D | 2.37  | 124.53      | 116.07   |
| 22  | 9     | 607  | CLA  | CAA-C2A-C3A | -2.37 | 106.61      | 113.00   |
| 22  | A     | 1104 | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 22  | 7     | 606  | CLA  | CHD-C1D-ND  | -2.37 | 121.47      | 124.80   |
| 22  | A     | 1117 | CLA  | CHA-C4D-ND  | 2.36  | 137.43      | 132.55   |
| 22  | Z     | 603  | CLA  | C1D-ND-C4D  | -2.36 | 104.65      | 106.31   |
| 22  | 5     | 606  | CLA  | CHD-C1D-ND  | -2.36 | 121.47      | 124.80   |
| 22  | 2     | 608  | CLA  | CHD-C1D-ND  | -2.36 | 121.47      | 124.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1234 | CLA  | O2A-CGA-CBA | 2.36  | 119.04      | 111.83   |
| 22  | A     | 1013 | CLA  | O2A-CGA-CBA | 2.36  | 119.04      | 111.83   |
| 22  | A     | 1126 | CLA  | CHA-C4D-ND  | 2.36  | 137.43      | 132.55   |
| 22  | 4     | 603  | CLA  | CHA-C4D-ND  | 2.36  | 137.43      | 132.55   |
| 22  | 1     | 612  | CLA  | CHD-C1D-ND  | -2.36 | 121.48      | 124.80   |
| 22  | L     | 1503 | CLA  | O2A-CGA-CBA | 2.36  | 119.04      | 111.83   |
| 22  | 3     | 607  | CLA  | C4B-CHC-C1C | 2.36  | 131.80      | 126.25   |
| 22  | 5     | 608  | CLA  | C4B-CHC-C1C | 2.36  | 131.80      | 126.25   |
| 22  | B     | 1022 | CLA  | CHA-C1A-NA  | -2.36 | 121.04      | 126.39   |
| 22  | 6     | 606  | CLA  | CMD-C2D-C3D | -2.36 | 122.27      | 127.69   |
| 22  | 4     | 612  | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 22  | 7     | 609  | CLA  | C1C-C2C-C3C | -2.36 | 104.50      | 106.98   |
| 22  | 2     | 602  | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | A     | 1112 | CLA  | CHA-C1A-NA  | -2.36 | 121.04      | 126.39   |
| 22  | A     | 1110 | CLA  | C1D-ND-C4D  | -2.36 | 104.66      | 106.31   |
| 22  | A     | 1120 | CLA  | C4B-CHC-C1C | 2.36  | 131.80      | 126.25   |
| 22  | 1     | 605  | CLA  | C4B-CHC-C1C | 2.36  | 131.80      | 126.25   |
| 22  | L     | 1503 | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 22  | 6     | 601  | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |
| 22  | B     | 1219 | CLA  | CMD-C2D-C3D | -2.36 | 122.27      | 127.69   |
| 25  | 7     | 504  | BCR  | C29-C28-C27 | 2.36  | 116.47      | 111.28   |
| 22  | 7     | 604  | CLA  | C4B-CHC-C1C | 2.36  | 131.80      | 126.25   |
| 22  | 9     | 604  | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 37  | J     | 4002 | C7Z  | C20-C13-C12 | 2.36  | 121.69      | 118.09   |
| 22  | 8     | 601  | CLA  | CHD-C1D-ND  | -2.36 | 121.48      | 124.80   |
| 22  | 5     | 605  | CLA  | C2C-C1C-NC  | 2.36  | 112.46      | 109.98   |
| 22  | 7     | 615  | CLA  | C2D-C1D-ND  | 2.36  | 112.46      | 110.13   |
| 39  | 8     | 501  | LUT  | C30-C31-C32 | -2.36 | 116.36      | 123.20   |
| 22  | A     | 1108 | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 39  | Z     | 502  | LUT  | C18-C5-C6   | -2.36 | 121.91      | 124.48   |
| 22  | A     | 1104 | CLA  | CAA-C2A-C3A | -2.36 | 106.62      | 113.00   |
| 22  | A     | 1012 | CLA  | C4B-CHC-C1C | 2.36  | 131.79      | 126.25   |
| 22  | J     | 1901 | CLA  | C4B-CHC-C1C | 2.36  | 131.79      | 126.25   |
| 22  | A     | 1107 | CLA  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 22  | 3     | 610  | CLA  | CHD-C1D-ND  | -2.36 | 121.48      | 124.80   |
| 22  | Z     | 604  | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |
| 22  | 4     | 606  | CLA  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 22  | 1     | 607  | CLA  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 22  | L     | 1502 | CLA  | C3B-C4B-NB  | -2.36 | 108.43      | 110.53   |
| 22  | 2     | 607  | CLA  | C3B-C4B-NB  | -2.36 | 108.43      | 110.53   |
| 37  | J     | 4002 | C7Z  | C28-C27-C26 | -2.36 | 120.70      | 127.00   |
| 22  | 7     | 611  | CLA  | CHA-C4D-ND  | 2.36  | 137.41      | 132.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1117 | CLA  | C1-O2A-CGA  | 2.36  | 122.36      | 116.65   |
| 22  | 8     | 605  | CLA  | C4B-CHC-C1C | 2.36  | 131.79      | 126.25   |
| 22  | B     | 1216 | CLA  | CMD-C2D-C3D | -2.36 | 122.29      | 127.69   |
| 22  | A     | 1114 | CLA  | C1-C2-C3    | -2.36 | 122.34      | 126.20   |
| 22  | B     | 1241 | CLA  | CHD-C1D-ND  | -2.36 | 121.49      | 124.80   |
| 22  | A     | 1109 | CLA  | C1C-C2C-C3C | -2.36 | 104.50      | 106.98   |
| 25  | K     | 4002 | BCR  | C19-C18-C17 | 2.35  | 122.71      | 119.01   |
| 22  | Z     | 615  | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 22  | A     | 1105 | CLA  | CHA-C4D-ND  | 2.35  | 137.41      | 132.55   |
| 22  | B     | 1216 | CLA  | C1-O2A-CGA  | 2.35  | 122.35      | 116.65   |
| 40  | 2     | 610  | CHL  | C4C-CHD-C1D | 2.35  | 124.49      | 116.07   |
| 22  | 3     | 604  | CLA  | C2D-C1D-ND  | 2.35  | 112.46      | 110.13   |
| 22  | 8     | 606  | CLA  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 22  | 3     | 618  | CLA  | CHA-C4D-ND  | 2.35  | 137.41      | 132.55   |
| 22  | 3     | 601  | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 37  | 1     | 503  | C7Z  | C28-C27-C26 | -2.35 | 120.71      | 127.00   |
| 22  | B     | 1214 | CLA  | C2D-C1D-ND  | 2.35  | 112.45      | 110.13   |
| 22  | 8     | 604  | CLA  | CHD-C1D-ND  | -2.35 | 121.49      | 124.80   |
| 22  | 4     | 601  | CLA  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 22  | 7     | 615  | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 22  | Z     | 604  | CLA  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 22  | 5     | 604  | CLA  | CHD-C1D-ND  | -2.35 | 121.49      | 124.80   |
| 22  | 4     | 615  | CLA  | C4B-CHC-C1C | 2.35  | 131.78      | 126.25   |
| 22  | A     | 1114 | CLA  | CHA-C1A-NA  | -2.35 | 121.07      | 126.39   |
| 22  | 2     | 612  | CLA  | CMA-C3A-C4A | 2.35  | 118.09      | 111.77   |
| 40  | 6     | 611  | CHL  | C1-O2A-CGA  | 2.35  | 122.34      | 116.65   |
| 22  | Z     | 603  | CLA  | CAA-C2A-C3A | -2.35 | 106.65      | 113.00   |
| 22  | A     | 1103 | CLA  | CMA-C3A-C4A | 2.35  | 118.09      | 111.77   |
| 22  | Z     | 606  | CLA  | CHD-C1D-ND  | -2.35 | 121.50      | 124.80   |
| 22  | 6     | 601  | CLA  | C2A-C1A-CHA | 2.35  | 127.94      | 123.87   |
| 22  | A     | 1129 | CLA  | CHD-C1D-ND  | -2.35 | 121.50      | 124.80   |
| 22  | B     | 1206 | CLA  | C1-O2A-CGA  | 2.35  | 122.34      | 116.65   |
| 22  | B     | 1239 | CLA  | CHD-C1D-ND  | -2.35 | 121.50      | 124.80   |
| 22  | 2     | 603  | CLA  | C4B-CHC-C1C | 2.35  | 131.77      | 126.25   |
| 22  | Z     | 607  | CLA  | CAA-C2A-C3A | -2.35 | 106.65      | 113.00   |
| 22  | 8     | 609  | CLA  | CMD-C2D-C3D | -2.35 | 122.30      | 127.69   |
| 22  | A     | 1136 | CLA  | CHA-C4D-ND  | 2.35  | 137.39      | 132.55   |
| 22  | 7     | 612  | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 22  | A     | 1012 | CLA  | CHA-C1A-NA  | -2.35 | 121.08      | 126.39   |
| 22  | 6     | 601  | CLA  | CHA-C1A-NA  | -2.35 | 121.08      | 126.39   |
| 22  | A     | 1119 | CLA  | C1C-C2C-C3C | -2.35 | 104.51      | 106.98   |
| 22  | 1     | 613  | CLA  | C4B-CHC-C1C | 2.35  | 131.77      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1104 | CLA  | C1-O2A-CGA  | 2.35  | 122.33      | 116.65   |
| 22  | 6     | 612  | CLA  | C4B-CHC-C1C | 2.35  | 131.77      | 126.25   |
| 22  | B     | 1237 | CLA  | C3B-C4B-NB  | -2.35 | 108.44      | 110.53   |
| 22  | 8     | 615  | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 22  | 3     | 605  | CLA  | O2A-CGA-CBA | 2.35  | 118.99      | 111.83   |
| 22  | 7     | 603  | CLA  | CHA-C4D-ND  | 2.35  | 137.39      | 132.55   |
| 22  | A     | 1124 | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 22  | A     | 1012 | CLA  | C2D-C1D-ND  | 2.35  | 112.45      | 110.13   |
| 22  | A     | 1136 | CLA  | CHD-C1D-ND  | -2.35 | 121.50      | 124.80   |
| 25  | K     | 4001 | BCR  | C3-C4-C5    | -2.35 | 109.87      | 114.06   |
| 22  | 2     | 601  | CLA  | CHA-C4D-ND  | 2.35  | 137.39      | 132.55   |
| 22  | 1     | 603  | CLA  | C2D-C1D-ND  | 2.35  | 112.45      | 110.13   |
| 22  | A     | 1013 | CLA  | CHA-C4D-ND  | 2.34  | 137.39      | 132.55   |
| 22  | 9     | 602  | CLA  | CHA-C1A-NA  | -2.34 | 121.08      | 126.39   |
| 22  | A     | 1129 | CLA  | C4B-CHC-C1C | 2.34  | 131.76      | 126.25   |
| 22  | A     | 1132 | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 22  | 6     | 609  | CLA  | CHA-C4D-ND  | 2.34  | 137.39      | 132.55   |
| 22  | Z     | 606  | CLA  | C4B-CHC-C1C | 2.34  | 131.76      | 126.25   |
| 22  | 6     | 619  | CLA  | C4B-CHC-C1C | 2.34  | 131.76      | 126.25   |
| 22  | 4     | 601  | CLA  | O1D-CGD-CBD | -2.34 | 119.90      | 124.52   |
| 22  | A     | 1141 | CLA  | CHD-C1D-ND  | -2.34 | 121.50      | 124.80   |
| 22  | 3     | 616  | CLA  | CHD-C1D-ND  | -2.34 | 121.50      | 124.80   |
| 22  | 6     | 615  | CLA  | C4B-CHC-C1C | 2.34  | 131.76      | 126.25   |
| 25  | A     | 4002 | BCR  | C36-C18-C17 | -2.34 | 119.02      | 122.82   |
| 22  | B     | 1217 | CLA  | CMA-C3A-C4A | 2.34  | 118.07      | 111.77   |
| 22  | 1     | 612  | CLA  | CHA-C1A-NA  | -2.34 | 121.09      | 126.39   |
| 22  | A     | 1119 | CLA  | O2A-CGA-CBA | 2.34  | 118.98      | 111.83   |
| 22  | 4     | 601  | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |
| 22  | B     | 1214 | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 22  | 2     | 605  | CLA  | CMD-C2D-C3D | -2.34 | 122.32      | 127.69   |
| 22  | B     | 1230 | CLA  | CHD-C1D-ND  | -2.34 | 121.51      | 124.80   |
| 22  | 7     | 613  | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |
| 40  | 7     | 610  | CHL  | CMA-C3A-C4A | 2.34  | 119.66      | 114.61   |
| 22  | B     | 1219 | CLA  | CAA-C2A-C3A | -2.34 | 106.67      | 113.00   |
| 28  | 9     | 803  | LMT  | C3'-C4'-C5' | -2.34 | 105.74      | 110.93   |
| 22  | 7     | 602  | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |
| 22  | 3     | 605  | CLA  | CMA-C3A-C4A | 2.34  | 118.06      | 111.77   |
| 22  | 7     | 613  | CLA  | CHA-C1A-NA  | -2.34 | 121.09      | 126.39   |
| 22  | 5     | 607  | CLA  | CAA-C2A-C3A | -2.34 | 106.68      | 113.00   |
| 22  | 6     | 609  | CLA  | O1D-CGD-CBD | -2.34 | 119.90      | 124.52   |
| 22  | B     | 1228 | CLA  | O2A-CGA-CBA | 2.34  | 118.97      | 111.83   |
| 22  | 7     | 616  | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 3     | 504  | BCR  | C23-C24-C25 | -2.34 | 120.75      | 127.00   |
| 22  | K     | 1401 | CLA  | CHA-C1A-NA  | -2.34 | 121.09      | 126.39   |
| 22  | B     | 1205 | CLA  | CHA-C4D-ND  | 2.34  | 137.38      | 132.55   |
| 22  | 4     | 603  | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 22  | Z     | 603  | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |
| 22  | 8     | 606  | CLA  | CHD-C1D-ND  | -2.34 | 121.51      | 124.80   |
| 22  | B     | 1218 | CLA  | C1D-ND-C4D  | -2.34 | 104.67      | 106.31   |
| 22  | B     | 1218 | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |
| 22  | 7     | 607  | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 22  | A     | 1115 | CLA  | C4B-CHC-C1C | 2.34  | 131.74      | 126.25   |
| 22  | 7     | 611  | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | 2     | 603  | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 36  | F     | 4001 | RRX  | C23-C24-C25 | -2.34 | 120.75      | 127.00   |
| 25  | 6     | 503  | BCR  | C4-C5-C6    | -2.34 | 119.55      | 122.70   |
| 22  | B     | 1228 | CLA  | C4B-CHC-C1C | 2.34  | 131.74      | 126.25   |
| 22  | B     | 1221 | CLA  | CHD-C1D-ND  | -2.34 | 121.52      | 124.80   |
| 22  | B     | 1236 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | 9     | 612  | CLA  | C4B-CHC-C1C | 2.34  | 131.74      | 126.25   |
| 22  | 5     | 603  | CLA  | C6-C5-C3    | -2.34 | 107.78      | 113.47   |
| 22  | A     | 1121 | CLA  | O2A-CGA-CBA | 2.34  | 118.96      | 111.83   |
| 22  | A     | 1133 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | 3     | 605  | CLA  | CMD-C2D-C3D | -2.34 | 122.33      | 127.69   |
| 22  | B     | 1238 | CLA  | C4B-CHC-C1C | 2.33  | 131.74      | 126.25   |
| 22  | A     | 1137 | CLA  | O2A-CGA-CBA | 2.33  | 118.95      | 111.83   |
| 22  | B     | 1202 | CLA  | CHA-C4D-ND  | 2.33  | 137.36      | 132.55   |
| 25  | G     | 4001 | BCR  | C35-C13-C12 | 2.33  | 121.65      | 118.09   |
| 22  | Z     | 611  | CLA  | C4B-CHC-C1C | 2.33  | 131.73      | 126.25   |
| 22  | 2     | 612  | CLA  | CHD-C1D-ND  | -2.33 | 121.52      | 124.80   |
| 22  | Z     | 605  | CLA  | C3B-C4B-NB  | -2.33 | 108.45      | 110.53   |
| 22  | 7     | 612  | CLA  | O2A-CGA-CBA | 2.33  | 118.95      | 111.83   |
| 22  | A     | 1136 | CLA  | C4B-CHC-C1C | 2.33  | 131.73      | 126.25   |
| 22  | 1     | 613  | CLA  | CMD-C2D-C3D | -2.33 | 122.34      | 127.69   |
| 22  | Z     | 607  | CLA  | O2A-CGA-CBA | 2.33  | 118.94      | 111.83   |
| 22  | 7     | 609  | CLA  | CHD-C1D-ND  | -2.33 | 121.52      | 124.80   |
| 22  | 1     | 601  | CLA  | O1D-CGD-CBD | -2.33 | 119.92      | 124.52   |
| 22  | A     | 1111 | CLA  | C2C-C1C-NC  | 2.33  | 112.43      | 109.98   |
| 22  | B     | 1241 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 22  | A     | 1137 | CLA  | C4B-CHC-C1C | 2.33  | 131.73      | 126.25   |
| 22  | K     | 1403 | CLA  | CHD-C1D-ND  | -2.33 | 121.52      | 124.80   |
| 22  | Z     | 604  | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 25  | A     | 4001 | BCR  | C33-C5-C6   | -2.33 | 121.94      | 124.48   |
| 22  | A     | 1101 | CLA  | O1D-CGD-CBD | -2.33 | 119.92      | 124.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | F     | 1302 | CLA  | C2D-C1D-ND  | 2.33  | 112.43      | 110.13   |
| 22  | B     | 1237 | CLA  | O2A-CGA-CBA | 2.33  | 118.94      | 111.83   |
| 22  | 9     | 604  | CLA  | CHA-C1A-NA  | -2.33 | 121.12      | 126.39   |
| 22  | B     | 1222 | CLA  | C1C-C2C-C3C | -2.33 | 104.53      | 106.98   |
| 22  | L     | 1502 | CLA  | O2A-CGA-CBA | 2.33  | 118.94      | 111.83   |
| 22  | 4     | 609  | CLA  | O1D-CGD-CBD | -2.33 | 119.92      | 124.52   |
| 25  | K     | 4001 | BCR  | C35-C13-C12 | 2.33  | 121.65      | 118.09   |
| 39  | 9     | 501  | LUT  | C20-C13-C12 | 2.33  | 121.65      | 118.09   |
| 22  | 3     | 608  | CLA  | C2D-C1D-ND  | 2.33  | 112.43      | 110.13   |
| 22  | 6     | 615  | CLA  | CHA-C1A-NA  | -2.33 | 121.12      | 126.39   |
| 22  | Z     | 603  | CLA  | CHA-C4D-ND  | 2.33  | 137.35      | 132.55   |
| 22  | B     | 1220 | CLA  | C2D-C1D-ND  | 2.33  | 112.43      | 110.13   |
| 22  | 8     | 603  | CLA  | C2D-C1D-ND  | 2.33  | 112.43      | 110.13   |
| 25  | 7     | 504  | BCR  | C33-C5-C6   | -2.33 | 121.94      | 124.48   |
| 22  | B     | 1216 | CLA  | O2A-CGA-CBA | 2.33  | 118.93      | 111.83   |
| 22  | 1     | 603  | CLA  | C4B-CHC-C1C | 2.33  | 131.72      | 126.25   |
| 22  | 5     | 603  | CLA  | C4B-CHC-C1C | 2.33  | 131.72      | 126.25   |
| 22  | 5     | 609  | CLA  | CHA-C1A-NA  | -2.33 | 121.12      | 126.39   |
| 40  | 3     | 611  | CHL  | C1-O2A-CGA  | 2.33  | 122.28      | 116.65   |
| 22  | 6     | 603  | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 22  | 4     | 604  | CLA  | O2A-CGA-CBA | 2.33  | 118.93      | 111.83   |
| 22  | A     | 1123 | CLA  | C4B-CHC-C1C | 2.33  | 131.72      | 126.25   |
| 22  | 3     | 603  | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 22  | 6     | 602  | CLA  | C3B-C4B-NB  | -2.33 | 108.45      | 110.53   |
| 22  | Z     | 615  | CLA  | CMA-C3A-C4A | 2.33  | 118.02      | 111.77   |
| 22  | 7     | 608  | CLA  | CHD-C1D-ND  | -2.33 | 121.53      | 124.80   |
| 22  | 1     | 612  | CLA  | C4B-CHC-C1C | 2.33  | 131.72      | 126.25   |
| 22  | 3     | 610  | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 22  | 6     | 607  | CLA  | C4B-CHC-C1C | 2.32  | 131.71      | 126.25   |
| 22  | B     | 1211 | CLA  | CMB-C2B-C3B | 2.32  | 132.02      | 126.55   |
| 22  | 1     | 602  | CLA  | C1C-C2C-C3C | -2.32 | 104.53      | 106.98   |
| 22  | B     | 1202 | CLA  | C4B-CHC-C1C | 2.32  | 131.71      | 126.25   |
| 25  | A     | 4004 | BCR  | C30-C25-C24 | 2.32  | 121.95      | 115.65   |
| 22  | 3     | 618  | CLA  | C3B-C4B-NB  | -2.32 | 108.45      | 110.53   |
| 22  | 4     | 607  | CLA  | C4B-CHC-C1C | 2.32  | 131.71      | 126.25   |
| 22  | 5     | 603  | CLA  | C3B-C4B-NB  | -2.32 | 108.46      | 110.53   |
| 22  | A     | 1013 | CLA  | CHA-C1A-NA  | -2.32 | 121.13      | 126.39   |
| 22  | A     | 1106 | CLA  | CHD-C1D-ND  | -2.32 | 121.53      | 124.80   |
| 22  | Z     | 605  | CLA  | C4B-CHC-C1C | 2.32  | 131.71      | 126.25   |
| 22  | 2     | 605  | CLA  | CMA-C3A-C4A | 2.32  | 118.02      | 111.77   |
| 39  | 7     | 502  | LUT  | C31-C30-C29 | -2.32 | 124.02      | 127.28   |
| 22  | 9     | 601  | CLA  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | 5     | 504  | BCR  | C28-C27-C26 | -2.32 | 109.92      | 114.06   |
| 22  | K     | 1402 | CLA  | C4B-CHC-C1C | 2.32  | 131.71      | 126.25   |
| 22  | A     | 1114 | CLA  | CHD-C1D-ND  | -2.32 | 121.53      | 124.80   |
| 22  | A     | 1135 | CLA  | CHD-C1D-ND  | -2.32 | 121.53      | 124.80   |
| 22  | 4     | 612  | CLA  | CMD-C2D-C3D | -2.32 | 122.36      | 127.69   |
| 22  | 7     | 615  | CLA  | CHA-C1A-NA  | -2.32 | 121.13      | 126.39   |
| 28  | 1     | 803  | LMT  | C1'-O5'-C5' | -2.32 | 109.19      | 113.72   |
| 22  | B     | 1238 | CLA  | CHD-C1D-ND  | -2.32 | 121.54      | 124.80   |
| 22  | B     | 1219 | CLA  | CHA-C1A-NA  | -2.32 | 121.14      | 126.39   |
| 39  | 7     | 502  | LUT  | C31-C32-C33 | -2.32 | 120.00      | 126.36   |
| 22  | A     | 1131 | CLA  | CMA-C3A-C4A | 2.32  | 118.01      | 111.77   |
| 22  | 1     | 603  | CLA  | C1-O2A-CGA  | 2.32  | 122.26      | 116.65   |
| 22  | 6     | 609  | CLA  | CMD-C2D-C3D | -2.32 | 122.37      | 127.69   |
| 22  | A     | 1119 | CLA  | CHD-C1D-ND  | -2.32 | 121.54      | 124.80   |
| 26  | Z     | 801  | LHG  | C6-C5-C4    | -2.32 | 106.38      | 111.78   |
| 22  | B     | 1211 | CLA  | CHA-C4D-ND  | 2.32  | 137.33      | 132.55   |
| 22  | B     | 1232 | CLA  | CHD-C1D-ND  | -2.32 | 121.54      | 124.80   |
| 25  | 3     | 506  | BCR  | C29-C28-C27 | 2.32  | 116.37      | 111.28   |
| 40  | Z     | 613  | CHL  | CMA-C3A-C4A | 2.32  | 119.60      | 114.61   |
| 40  | Z     | 613  | CHL  | C1C-C2C-CMC | 2.32  | 130.98      | 126.80   |
| 22  | 4     | 605  | CLA  | O2A-CGA-CBA | 2.32  | 118.90      | 111.83   |
| 22  | B     | 1241 | CLA  | CBA-CAA-C2A | 2.32  | 120.68      | 113.79   |
| 22  | 3     | 603  | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 40  | 9     | 613  | CHL  | C4C-CHD-C1D | 2.32  | 124.35      | 116.07   |
| 25  | J     | 4001 | BCR  | C31-C1-C6   | -2.32 | 106.61      | 110.24   |
| 22  | B     | 1220 | CLA  | C4B-CHC-C1C | 2.32  | 131.69      | 126.25   |
| 22  | 7     | 607  | CLA  | C4B-CHC-C1C | 2.32  | 131.69      | 126.25   |
| 25  | A     | 4005 | BCR  | C33-C5-C6   | -2.31 | 121.96      | 124.48   |
| 39  | 3     | 502  | LUT  | C22-C23-C24 | -2.31 | 107.75      | 111.18   |
| 22  | 1     | 601  | CLA  | C2D-C1D-ND  | 2.31  | 112.42      | 110.13   |
| 22  | 6     | 603  | CLA  | CMD-C2D-C3D | -2.31 | 122.38      | 127.69   |
| 22  | 9     | 605  | CLA  | C1D-ND-C4D  | -2.31 | 104.69      | 106.31   |
| 22  | 7     | 601  | CLA  | CMA-C3A-C4A | 2.31  | 117.99      | 111.77   |
| 22  | A     | 1118 | CLA  | CHA-C4D-ND  | 2.31  | 137.32      | 132.55   |
| 22  | A     | 1109 | CLA  | C4B-CHC-C1C | 2.31  | 131.69      | 126.25   |
| 25  | B     | 4006 | BCR  | C33-C5-C6   | -2.31 | 121.96      | 124.48   |
| 25  | J     | 4001 | BCR  | C30-C25-C26 | -2.31 | 119.47      | 122.64   |
| 22  | B     | 1218 | CLA  | CHA-C4D-ND  | 2.31  | 137.32      | 132.55   |
| 22  | 5     | 604  | CLA  | C2D-C1D-ND  | 2.31  | 112.42      | 110.13   |
| 40  | 1     | 609  | CHL  | CMA-C3A-C4A | 2.31  | 119.59      | 114.61   |
| 22  | 5     | 606  | CLA  | CMD-C2D-C3D | -2.31 | 122.39      | 127.69   |
| 22  | 3     | 618  | CLA  | C4B-CHC-C1C | 2.31  | 131.68      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 611  | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 22  | Z     | 601  | CLA  | CMA-C3A-C4A | 2.31  | 117.99      | 111.77   |
| 22  | L     | 1502 | CLA  | CHA-C4D-ND  | 2.31  | 137.32      | 132.55   |
| 25  | B     | 4007 | BCR  | C37-C22-C23 | 2.31  | 121.62      | 118.09   |
| 22  | 1     | 602  | CLA  | C3B-C4B-NB  | -2.31 | 108.47      | 110.53   |
| 40  | 6     | 613  | CHL  | C4C-CHD-C1D | 2.31  | 124.33      | 116.07   |
| 22  | 5     | 608  | CLA  | CHD-C1D-ND  | -2.31 | 121.55      | 124.80   |
| 22  | 8     | 604  | CLA  | CHA-C1A-NA  | -2.31 | 121.16      | 126.39   |
| 22  | 1     | 602  | CLA  | C4B-CHC-C1C | 2.31  | 131.68      | 126.25   |
| 22  | Z     | 607  | CLA  | C4B-CHC-C1C | 2.31  | 131.68      | 126.25   |
| 22  | 2     | 604  | CLA  | C4B-CHC-C1C | 2.31  | 131.68      | 126.25   |
| 22  | 8     | 608  | CLA  | CHA-C4D-ND  | 2.31  | 137.31      | 132.55   |
| 40  | 3     | 611  | CHL  | C4C-CHD-C1D | 2.31  | 124.33      | 116.07   |
| 22  | Z     | 605  | CLA  | C1D-ND-C4D  | -2.31 | 104.69      | 106.31   |
| 39  | 5     | 501  | LUT  | C39-C29-C28 | 2.31  | 121.61      | 118.09   |
| 22  | A     | 1012 | CLA  | C2C-C1C-NC  | 2.31  | 112.41      | 109.98   |
| 22  | A     | 1105 | CLA  | C2C-C1C-NC  | 2.31  | 112.41      | 109.98   |
| 22  | 7     | 611  | CLA  | C2C-C1C-NC  | 2.31  | 112.41      | 109.98   |
| 22  | B     | 1225 | CLA  | O2A-CGA-CBA | 2.31  | 118.87      | 111.83   |
| 22  | A     | 1111 | CLA  | CHD-C1D-ND  | -2.31 | 121.55      | 124.80   |
| 22  | B     | 1213 | CLA  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 39  | 9     | 502  | LUT  | C39-C29-C28 | 2.31  | 121.61      | 118.09   |
| 22  | F     | 1302 | CLA  | CMA-C3A-C4A | 2.31  | 117.98      | 111.77   |
| 22  | 8     | 607  | CLA  | C4B-CHC-C1C | 2.31  | 131.67      | 126.25   |
| 22  | 5     | 608  | CLA  | C2D-C1D-ND  | 2.31  | 112.41      | 110.13   |
| 22  | 9     | 608  | CLA  | CHD-C1D-ND  | -2.31 | 121.56      | 124.80   |
| 22  | A     | 1106 | CLA  | C1D-ND-C4D  | -2.31 | 104.69      | 106.31   |
| 22  | 8     | 606  | CLA  | C1D-ND-C4D  | -2.31 | 104.69      | 106.31   |
| 22  | A     | 1128 | CLA  | C1-O2A-CGA  | 2.31  | 122.24      | 116.65   |
| 22  | 9     | 608  | CLA  | CHA-C1A-NA  | -2.31 | 121.17      | 126.39   |
| 40  | 4     | 613  | CHL  | C4C-CHD-C1D | 2.31  | 124.32      | 116.07   |
| 22  | 4     | 606  | CLA  | CMD-C2D-C3D | -2.31 | 122.40      | 127.69   |
| 22  | A     | 1101 | CLA  | C1D-ND-C4D  | -2.31 | 104.69      | 106.31   |
| 22  | 6     | 601  | CLA  | O1D-CGD-CBD | -2.31 | 119.97      | 124.52   |
| 22  | A     | 1012 | CLA  | C1-C2-C3    | -2.31 | 122.42      | 126.20   |
| 22  | 8     | 604  | CLA  | O1A-CGA-CBA | -2.30 | 114.77      | 123.78   |
| 22  | 3     | 608  | CLA  | C4B-CHC-C1C | 2.30  | 131.67      | 126.25   |
| 22  | K     | 1404 | CLA  | C3B-C4B-NB  | -2.30 | 108.47      | 110.53   |
| 22  | 7     | 612  | CLA  | C4B-CHC-C1C | 2.30  | 131.66      | 126.25   |
| 22  | 5     | 606  | CLA  | C4B-CHC-C1C | 2.30  | 131.66      | 126.25   |
| 22  | A     | 1137 | CLA  | CHA-C1A-NA  | -2.30 | 121.17      | 126.39   |
| 22  | 9     | 605  | CLA  | CMA-C3A-C4A | 2.30  | 117.96      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1121 | CLA  | C1D-ND-C4D  | -2.30 | 104.70      | 106.31   |
| 33  | B     | 5003 | DGD  | C2G-O2G-C1B | -2.30 | 112.28      | 117.80   |
| 22  | 1     | 615  | CLA  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 22  | B     | 1201 | CLA  | CAA-C2A-C3A | -2.30 | 106.78      | 113.00   |
| 39  | 4     | 502  | LUT  | C38-C25-C24 | -2.30 | 117.91      | 123.36   |
| 39  | 1     | 501  | LUT  | C30-C31-C32 | -2.30 | 116.53      | 123.20   |
| 22  | 2     | 608  | CLA  | C4B-CHC-C1C | 2.30  | 131.66      | 126.25   |
| 39  | 4     | 501  | LUT  | C20-C13-C12 | 2.30  | 121.60      | 118.09   |
| 22  | A     | 1134 | CLA  | O1D-CGD-CBD | -2.30 | 119.98      | 124.52   |
| 25  | B     | 4001 | BCR  | C19-C18-C17 | 2.30  | 122.63      | 119.01   |
| 40  | 9     | 610  | CHL  | C4C-CHD-C1D | 2.30  | 124.30      | 116.07   |
| 22  | 9     | 607  | CLA  | CHD-C1D-ND  | -2.30 | 121.56      | 124.80   |
| 22  | 4     | 606  | CLA  | C1D-ND-C4D  | -2.30 | 104.70      | 106.31   |
| 22  | G     | 1602 | CLA  | CHA-C1A-NA  | -2.30 | 121.18      | 126.39   |
| 22  | 8     | 603  | CLA  | CHA-C4D-ND  | 2.30  | 137.29      | 132.55   |
| 38  | K     | 5001 | SPH  | C3-C4-C5    | -2.30 | 119.92      | 124.69   |
| 22  | 1     | 615  | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 25  | 7     | 504  | BCR  | C38-C26-C25 | -2.30 | 121.98      | 124.48   |
| 22  | 4     | 604  | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 40  | Z     | 613  | CHL  | C4C-CHD-C1D | 2.30  | 124.29      | 116.07   |
| 22  | 6     | 618  | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 40  | 5     | 611  | CHL  | C3D-C4D-ND  | -2.30 | 109.25      | 112.94   |
| 22  | 2     | 601  | CLA  | C3B-C4B-NB  | -2.30 | 108.48      | 110.53   |
| 22  | A     | 1128 | CLA  | CHA-C1A-NA  | -2.30 | 121.19      | 126.39   |
| 40  | 2     | 610  | CHL  | C1-O2A-CGA  | 2.30  | 123.20      | 116.67   |
| 22  | 7     | 605  | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 22  | 8     | 612  | CLA  | O2D-CGD-O1D | -2.30 | 119.38      | 123.85   |
| 39  | 7     | 501  | LUT  | C20-C13-C12 | 2.30  | 121.60      | 118.09   |
| 22  | A     | 1118 | CLA  | O1D-CGD-CBD | -2.30 | 119.99      | 124.52   |
| 22  | 2     | 615  | CLA  | CHA-C4D-ND  | 2.30  | 137.29      | 132.55   |
| 22  | B     | 1214 | CLA  | C3D-C2D-C1D | -2.30 | 102.70      | 105.83   |
| 22  | B     | 1235 | CLA  | C4B-CHC-C1C | 2.30  | 131.65      | 126.25   |
| 22  | B     | 1205 | CLA  | CMA-C3A-C4A | 2.30  | 117.94      | 111.77   |
| 22  | 4     | 605  | CLA  | CMD-C2D-C3D | -2.29 | 122.43      | 127.69   |
| 39  | 2     | 503  | LUT  | C10-C11-C12 | -2.29 | 116.55      | 123.20   |
| 22  | 2     | 603  | CLA  | C1D-ND-C4D  | -2.29 | 104.70      | 106.31   |
| 22  | B     | 1213 | CLA  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 22  | 9     | 608  | CLA  | C3B-C4B-NB  | -2.29 | 108.48      | 110.53   |
| 40  | 6     | 617  | CHL  | CMA-C3A-C4A | 2.29  | 119.55      | 114.61   |
| 40  | 3     | 611  | CHL  | CMA-C3A-C4A | 2.29  | 119.55      | 114.61   |
| 22  | B     | 1241 | CLA  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 39  | 3     | 502  | LUT  | C7-C8-C9    | -2.29 | 122.84      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | K     | 1402 | CLA  | C1-O2A-CGA  | 2.29  | 122.20      | 116.65   |
| 22  | B     | 1222 | CLA  | C1D-ND-C4D  | -2.29 | 104.70      | 106.31   |
| 22  | 2     | 602  | CLA  | O1D-CGD-CBD | -2.29 | 120.00      | 124.52   |
| 22  | 2     | 612  | CLA  | CHA-C1A-NA  | -2.29 | 121.20      | 126.39   |
| 22  | A     | 1112 | CLA  | C4B-CHC-C1C | 2.29  | 131.63      | 126.25   |
| 22  | B     | 1209 | CLA  | CMD-C2D-C3D | -2.29 | 122.44      | 127.69   |
| 22  | 1     | 603  | CLA  | CAA-C2A-C3A | -2.29 | 106.81      | 113.00   |
| 22  | 9     | 604  | CLA  | CAA-C2A-C3A | -2.29 | 106.81      | 113.00   |
| 22  | A     | 1012 | CLA  | CHD-C1D-ND  | -2.29 | 121.58      | 124.80   |
| 22  | 9     | 603  | CLA  | CHA-C1A-NA  | -2.29 | 121.21      | 126.39   |
| 22  | B     | 1210 | CLA  | CMA-C3A-C4A | 2.29  | 117.93      | 111.77   |
| 22  | 5     | 613  | CLA  | C4B-CHC-C1C | 2.29  | 131.63      | 126.25   |
| 22  | 2     | 615  | CLA  | C1D-ND-C4D  | -2.29 | 104.71      | 106.31   |
| 22  | Z     | 608  | CLA  | O2A-CGA-CBA | 2.29  | 118.81      | 111.83   |
| 22  | 5     | 604  | CLA  | C1C-C2C-C3C | -2.29 | 104.57      | 106.98   |
| 22  | B     | 1202 | CLA  | CMD-C2D-C3D | -2.29 | 122.44      | 127.69   |
| 22  | B     | 1236 | CLA  | CHA-C1A-NA  | -2.29 | 121.21      | 126.39   |
| 22  | A     | 1141 | CLA  | C4B-CHC-C1C | 2.29  | 131.63      | 126.25   |
| 22  | 5     | 613  | CLA  | CMA-C3A-C4A | 2.29  | 117.92      | 111.77   |
| 22  | 2     | 612  | CLA  | C1C-C2C-C3C | -2.29 | 104.57      | 106.98   |
| 22  | F     | 1302 | CLA  | CHA-C1A-NA  | -2.29 | 121.21      | 126.39   |
| 22  | B     | 1224 | CLA  | CMA-C3A-C4A | 2.29  | 117.92      | 111.77   |
| 25  | 5     | 504  | BCR  | C4-C5-C6    | -2.29 | 119.61      | 122.70   |
| 22  | Z     | 606  | CLA  | C1-O2A-CGA  | 2.29  | 122.19      | 116.65   |
| 22  | 9     | 607  | CLA  | C4B-CHC-C1C | 2.29  | 131.62      | 126.25   |
| 25  | 6     | 504  | BCR  | C36-C18-C17 | -2.29 | 119.11      | 122.82   |
| 22  | A     | 1113 | CLA  | CHD-C1D-ND  | -2.29 | 121.58      | 124.80   |
| 22  | 7     | 604  | CLA  | O1A-CGA-CBA | -2.29 | 114.84      | 123.78   |
| 22  | 5     | 604  | CLA  | CAA-C2A-C3A | -2.29 | 106.82      | 113.00   |
| 22  | A     | 1133 | CLA  | C3B-C4B-NB  | -2.29 | 108.49      | 110.53   |
| 25  | L     | 4002 | BCR  | C12-C13-C14 | -2.28 | 115.42      | 119.01   |
| 22  | K     | 1403 | CLA  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 25  | B     | 4003 | BCR  | C39-C30-C25 | -2.28 | 106.66      | 110.24   |
| 22  | 9     | 605  | CLA  | C4B-CHC-C1C | 2.28  | 131.62      | 126.25   |
| 22  | A     | 1130 | CLA  | O2A-CGA-CBA | 2.28  | 118.80      | 111.83   |
| 25  | 3     | 503  | BCR  | C12-C13-C14 | -2.28 | 115.42      | 119.01   |
| 22  | A     | 1134 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | Z     | 612  | CLA  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 22  | B     | 1201 | CLA  | C3B-C4B-NB  | -2.28 | 108.49      | 110.53   |
| 22  | B     | 1211 | CLA  | C3B-C4B-NB  | -2.28 | 108.49      | 110.53   |
| 22  | 2     | 606  | CLA  | C3B-C4B-NB  | -2.28 | 108.49      | 110.53   |
| 22  | B     | 1227 | CLA  | C4B-CHC-C1C | 2.28  | 131.62      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 5     | 615  | CLA  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 22  | A     | 1120 | CLA  | CHA-C4D-ND  | 2.28  | 137.26      | 132.55   |
| 39  | 2     | 502  | LUT  | C28-C29-C30 | -2.28 | 115.42      | 119.01   |
| 25  | B     | 4005 | BCR  | C4-C5-C6    | -2.28 | 119.62      | 122.70   |
| 22  | F     | 1302 | CLA  | CHA-C4D-ND  | 2.28  | 137.26      | 132.55   |
| 22  | 3     | 603  | CLA  | CMD-C2D-C3D | -2.28 | 122.46      | 127.69   |
| 22  | 6     | 618  | CLA  | C3D-C2D-C1D | -2.28 | 102.72      | 105.83   |
| 22  | 6     | 603  | CLA  | C1D-ND-C4D  | -2.28 | 104.71      | 106.31   |
| 22  | A     | 1105 | CLA  | CMD-C2D-C3D | -2.28 | 122.46      | 127.69   |
| 25  | L     | 4002 | BCR  | C35-C13-C12 | 2.28  | 121.57      | 118.09   |
| 37  | 1     | 503  | C7Z  | C19-C9-C8   | 2.28  | 121.57      | 118.09   |
| 22  | A     | 1122 | CLA  | CAA-C2A-C3A | -2.28 | 106.84      | 113.00   |
| 22  | 1     | 611  | CLA  | C4B-CHC-C1C | 2.28  | 131.61      | 126.25   |
| 39  | Z     | 501  | LUT  | C38-C25-C24 | -2.28 | 117.96      | 123.36   |
| 25  | B     | 4001 | BCR  | C12-C13-C14 | -2.28 | 115.42      | 119.01   |
| 22  | 1     | 603  | CLA  | O2A-CGA-CBA | 2.28  | 118.79      | 111.83   |
| 22  | 5     | 603  | CLA  | C1D-ND-C4D  | -2.28 | 104.71      | 106.31   |
| 25  | B     | 4004 | BCR  | C31-C1-C6   | -2.28 | 106.67      | 110.24   |
| 22  | A     | 1124 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | A     | 1114 | CLA  | C4B-CHC-C1C | 2.28  | 131.61      | 126.25   |
| 25  | B     | 4004 | BCR  | C38-C26-C25 | -2.28 | 122.00      | 124.48   |
| 22  | A     | 1131 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | F     | 1301 | CLA  | CHD-C1D-ND  | -2.28 | 121.60      | 124.80   |
| 22  | 9     | 607  | CLA  | CHA-C1A-NA  | -2.28 | 121.23      | 126.39   |
| 22  | 7     | 611  | CLA  | O2A-CGA-CBA | 2.28  | 118.78      | 111.83   |
| 25  | L     | 4001 | BCR  | C12-C13-C14 | -2.28 | 115.43      | 119.01   |
| 40  | 2     | 613  | CHL  | C3D-C4D-ND  | -2.28 | 109.28      | 112.94   |
| 22  | B     | 1204 | CLA  | C1D-ND-C4D  | -2.28 | 104.71      | 106.31   |
| 40  | 9     | 613  | CHL  | CAA-C2A-C3A | -2.28 | 111.01      | 116.23   |
| 22  | A     | 1125 | CLA  | OBD-CAD-C3D | -2.28 | 123.09      | 128.42   |
| 22  | B     | 1021 | CLA  | O2D-CGD-O1D | -2.28 | 119.42      | 123.85   |
| 22  | 3     | 602  | CLA  | CHA-C1A-NA  | -2.28 | 121.23      | 126.39   |
| 37  | 5     | 505  | C7Z  | C38-C25-C24 | 2.28  | 118.61      | 114.42   |
| 22  | B     | 1229 | CLA  | CHA-C1A-NA  | -2.28 | 121.24      | 126.39   |
| 22  | 7     | 601  | CLA  | CMD-C2D-C3D | -2.28 | 122.47      | 127.69   |
| 22  | A     | 1105 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | Z     | 603  | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | A     | 1106 | CLA  | C1-O2A-CGA  | 2.28  | 122.16      | 116.65   |
| 22  | 3     | 601  | CLA  | CMA-C3A-C4A | 2.27  | 117.89      | 111.77   |
| 22  | 5     | 608  | CLA  | C3B-C4B-NB  | -2.27 | 108.50      | 110.53   |
| 26  | 5     | 801  | LHG  | C6-C5-C4    | -2.27 | 106.48      | 111.78   |
| 22  | 6     | 604  | CLA  | C1-O2A-CGA  | 2.27  | 122.15      | 116.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | K     | 1403 | CLA  | C4B-CHC-C1C | 2.27  | 131.59      | 126.25   |
| 22  | 8     | 604  | CLA  | O2D-CGD-O1D | -2.27 | 119.42      | 123.85   |
| 22  | B     | 1240 | CLA  | C1C-C2C-C3C | -2.27 | 104.59      | 106.98   |
| 22  | A     | 1106 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | 6     | 619  | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | A     | 1118 | CLA  | O2A-CGA-CBA | 2.27  | 118.76      | 111.83   |
| 22  | Z     | 607  | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 22  | A     | 1141 | CLA  | C2D-C1D-ND  | 2.27  | 112.38      | 110.13   |
| 22  | 2     | 602  | CLA  | C2D-C1D-ND  | 2.27  | 112.38      | 110.13   |
| 22  | 7     | 601  | CLA  | C3D-C2D-C1D | -2.27 | 102.73      | 105.83   |
| 22  | B     | 1221 | CLA  | C4B-CHC-C1C | 2.27  | 131.59      | 126.25   |
| 22  | K     | 1402 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | A     | 1122 | CLA  | C1D-ND-C4D  | -2.27 | 104.72      | 106.31   |
| 22  | 8     | 607  | CLA  | C3B-C4B-NB  | -2.27 | 108.50      | 110.53   |
| 22  | 4     | 603  | CLA  | C4B-CHC-C1C | 2.27  | 131.59      | 126.25   |
| 22  | Z     | 612  | CLA  | O2A-CGA-CBA | 2.27  | 118.76      | 111.83   |
| 22  | A     | 1132 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | A     | 1127 | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 22  | 8     | 605  | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 22  | A     | 1130 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | A     | 1107 | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 22  | 8     | 601  | CLA  | OBD-CAD-C3D | -2.27 | 123.11      | 128.42   |
| 22  | B     | 1230 | CLA  | CAA-CBA-CGA | -2.27 | 106.76      | 113.21   |
| 22  | B     | 1222 | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 22  | A     | 1140 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | 9     | 609  | CLA  | CAA-C2A-C3A | -2.27 | 106.87      | 113.00   |
| 22  | 4     | 603  | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | 4     | 604  | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 22  | 1     | 602  | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 22  | 8     | 601  | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 22  | 7     | 616  | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 39  | Z     | 501  | LUT  | C39-C29-C28 | 2.27  | 121.55      | 118.09   |
| 22  | Z     | 601  | CLA  | C1D-ND-C4D  | -2.27 | 104.72      | 106.31   |
| 22  | A     | 1136 | CLA  | OBD-CAD-C3D | -2.27 | 123.12      | 128.42   |
| 22  | B     | 1216 | CLA  | C4B-CHC-C1C | 2.27  | 131.58      | 126.25   |
| 22  | B     | 1224 | CLA  | C4B-CHC-C1C | 2.27  | 131.58      | 126.25   |
| 22  | A     | 1138 | CLA  | C3B-C4B-NB  | -2.27 | 108.51      | 110.53   |
| 22  | L     | 1502 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | 1     | 615  | CLA  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |
| 22  | 1     | 615  | CLA  | CHA-C1A-NA  | -2.27 | 121.26      | 126.39   |
| 22  | 8     | 603  | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 25  | L     | 4002 | BCR  | C29-C28-C27 | 2.27  | 116.26      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | 1     | 502  | LUT  | C18-C5-C6   | -2.27 | 122.01      | 124.48   |
| 22  | A     | 1134 | CLA  | C4B-CHC-C1C | 2.27  | 131.57      | 126.25   |
| 22  | 6     | 605  | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 22  | B     | 1229 | CLA  | CMD-C2D-C3D | -2.26 | 122.50      | 127.69   |
| 22  | 1     | 611  | CLA  | C1D-ND-C4D  | -2.26 | 104.72      | 106.31   |
| 22  | 3     | 616  | CLA  | C1D-ND-C4D  | -2.26 | 104.72      | 106.31   |
| 22  | 6     | 615  | CLA  | CMA-C3A-C4A | 2.26  | 117.86      | 111.77   |
| 22  | 3     | 616  | CLA  | C2D-C1D-ND  | 2.26  | 112.37      | 110.13   |
| 22  | 2     | 601  | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 9     | 603  | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 33  | B     | 5003 | DGD  | O2G-C1B-O1B | -2.26 | 118.41      | 123.70   |
| 40  | 6     | 613  | CHL  | CMA-C3A-C4A | 2.26  | 119.49      | 114.61   |
| 22  | A     | 1130 | CLA  | CHA-C1A-NA  | -2.26 | 121.27      | 126.39   |
| 22  | B     | 1227 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 9     | 606  | CLA  | C1C-C2C-C3C | -2.26 | 104.60      | 106.98   |
| 22  | L     | 1503 | CLA  | CMD-C2D-C3D | -2.26 | 122.50      | 127.69   |
| 22  | 9     | 605  | CLA  | CHA-C1A-NA  | -2.26 | 121.27      | 126.39   |
| 39  | 9     | 502  | LUT  | C31-C32-C33 | -2.26 | 120.16      | 126.36   |
| 22  | B     | 1208 | CLA  | C2C-C1C-NC  | 2.26  | 112.36      | 109.98   |
| 22  | A     | 1013 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 9     | 609  | CLA  | CHA-C1A-NA  | -2.26 | 121.27      | 126.39   |
| 39  | 6     | 502  | LUT  | C18-C5-C6   | -2.26 | 122.02      | 124.48   |
| 22  | 8     | 605  | CLA  | C3B-C4B-NB  | -2.26 | 108.51      | 110.53   |
| 22  | 5     | 615  | CLA  | C2D-C1D-ND  | 2.26  | 112.36      | 110.13   |
| 22  | A     | 1131 | CLA  | C4B-CHC-C1C | 2.26  | 131.56      | 126.25   |
| 22  | L     | 1502 | CLA  | C4B-CHC-C1C | 2.26  | 131.56      | 126.25   |
| 22  | B     | 1023 | CLA  | C2A-C1A-CHA | 2.26  | 127.79      | 123.87   |
| 22  | B     | 1208 | CLA  | C1D-ND-C4D  | -2.26 | 104.73      | 106.31   |
| 22  | 4     | 612  | CLA  | O2A-CGA-CBA | 2.26  | 118.73      | 111.83   |
| 22  | A     | 1112 | CLA  | CMD-C2D-C3D | -2.26 | 122.51      | 127.69   |
| 22  | 3     | 612  | CLA  | O2A-CGA-CBA | 2.26  | 118.73      | 111.83   |
| 22  | 8     | 612  | CLA  | C4B-CHC-C1C | 2.26  | 131.56      | 126.25   |
| 22  | 3     | 613  | CLA  | CHA-C1A-NA  | -2.26 | 121.28      | 126.39   |
| 22  | 5     | 602  | CLA  | C2D-C1D-ND  | 2.26  | 112.36      | 110.13   |
| 22  | Z     | 611  | CLA  | CAA-C2A-C3A | -2.26 | 106.89      | 113.00   |
| 22  | Z     | 604  | CLA  | C1D-ND-C4D  | -2.26 | 104.73      | 106.31   |
| 22  | 2     | 615  | CLA  | C4B-CHC-C1C | 2.26  | 131.56      | 126.25   |
| 22  | 2     | 608  | CLA  | CHA-C1A-NA  | -2.26 | 121.28      | 126.39   |
| 22  | 9     | 606  | CLA  | CHA-C1A-NA  | -2.26 | 121.28      | 126.39   |
| 22  | 2     | 612  | CLA  | C2C-C1C-NC  | 2.26  | 112.35      | 109.98   |
| 22  | B     | 1234 | CLA  | C3B-C4B-NB  | -2.26 | 108.51      | 110.53   |
| 22  | 4     | 615  | CLA  | C3B-C4B-NB  | -2.26 | 108.51      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 618  | CLA  | CHA-C4D-ND  | 2.26  | 137.21      | 132.55   |
| 22  | 3     | 610  | CLA  | CMA-C3A-C4A | 2.26  | 117.84      | 111.77   |
| 22  | A     | 1117 | CLA  | C4B-CHC-C1C | 2.26  | 131.56      | 126.25   |
| 22  | 6     | 604  | CLA  | C3B-C4B-NB  | -2.26 | 108.52      | 110.53   |
| 22  | 8     | 607  | CLA  | CHD-C1D-ND  | -2.26 | 121.63      | 124.80   |
| 22  | Z     | 603  | CLA  | O2D-CGD-O1D | -2.26 | 119.46      | 123.85   |
| 22  | 1     | 603  | CLA  | CMD-C2D-C3D | -2.26 | 122.52      | 127.69   |
| 22  | 5     | 603  | CLA  | CMD-C2D-C3D | -2.26 | 122.52      | 127.69   |
| 22  | 1     | 607  | CLA  | C4B-CHC-C1C | 2.25  | 131.55      | 126.25   |
| 22  | Z     | 601  | CLA  | C2C-C1C-NC  | 2.25  | 112.35      | 109.98   |
| 22  | 2     | 602  | CLA  | C4B-CHC-C1C | 2.25  | 131.55      | 126.25   |
| 39  | 6     | 502  | LUT  | C31-C32-C33 | -2.25 | 120.18      | 126.36   |
| 36  | F     | 4001 | RRX  | C38-C26-C27 | 2.25  | 118.57      | 114.42   |
| 22  | F     | 1301 | CLA  | CMD-C2D-C3D | -2.25 | 122.52      | 127.69   |
| 22  | 8     | 602  | CLA  | CHA-C1A-NA  | -2.25 | 121.29      | 126.39   |
| 22  | 3     | 607  | CLA  | O2A-CGA-CBA | 2.25  | 118.71      | 111.83   |
| 22  | A     | 1119 | CLA  | C2C-C1C-NC  | 2.25  | 112.35      | 109.98   |
| 22  | A     | 1120 | CLA  | C3D-C2D-C1D | -2.25 | 102.76      | 105.83   |
| 22  | 3     | 608  | CLA  | CHD-C1D-ND  | -2.25 | 121.63      | 124.80   |
| 22  | 7     | 604  | CLA  | CHD-C1D-ND  | -2.25 | 121.63      | 124.80   |
| 22  | 2     | 602  | CLA  | CMA-C3A-C4A | 2.25  | 117.83      | 111.77   |
| 22  | 5     | 612  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 7     | 603  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | A     | 1103 | CLA  | C4B-CHC-C1C | 2.25  | 131.54      | 126.25   |
| 22  | 2     | 606  | CLA  | CHA-C1A-NA  | -2.25 | 121.29      | 126.39   |
| 22  | 1     | 612  | CLA  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 22  | 1     | 602  | CLA  | CMA-C3A-C4A | 2.25  | 117.82      | 111.77   |
| 22  | B     | 1224 | CLA  | CHA-C1A-NA  | -2.25 | 121.29      | 126.39   |
| 22  | Z     | 604  | CLA  | CHA-C1A-NA  | -2.25 | 121.29      | 126.39   |
| 22  | A     | 1133 | CLA  | C4B-CHC-C1C | 2.25  | 131.54      | 126.25   |
| 22  | Z     | 605  | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | B     | 1213 | CLA  | C1D-ND-C4D  | -2.25 | 104.73      | 106.31   |
| 22  | 4     | 603  | CLA  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 22  | 3     | 602  | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 36  | F     | 4001 | RRX  | C2-C3-C4    | 2.25  | 116.22      | 111.28   |
| 22  | 4     | 605  | CLA  | C2D-C1D-ND  | 2.25  | 112.35      | 110.13   |
| 22  | 7     | 602  | CLA  | CHA-C1A-NA  | -2.25 | 121.30      | 126.39   |
| 22  | 1     | 605  | CLA  | C1D-ND-C4D  | -2.25 | 104.73      | 106.31   |
| 22  | Z     | 601  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | 7     | 604  | CLA  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 25  | 7     | 504  | BCR  | C1-C6-C5    | -2.25 | 119.56      | 122.64   |
| 22  | 4     | 607  | CLA  | CAA-C2A-C3A | -2.25 | 106.92      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1023 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | B     | 1217 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | 1     | 603  | CLA  | C1D-ND-C4D  | -2.25 | 104.73      | 106.31   |
| 22  | 7     | 603  | CLA  | C1D-ND-C4D  | -2.25 | 104.73      | 106.31   |
| 26  | 5     | 801  | LHG  | C5-O7-C7    | -2.25 | 112.42      | 117.80   |
| 22  | K     | 1404 | CLA  | C4B-CHC-C1C | 2.25  | 131.53      | 126.25   |
| 22  | 7     | 611  | CLA  | C3D-C2D-C1D | -2.25 | 102.76      | 105.83   |
| 22  | 6     | 615  | CLA  | C2D-C1D-ND  | 2.25  | 112.35      | 110.13   |
| 22  | A     | 1103 | CLA  | CHA-C4D-ND  | 2.25  | 137.19      | 132.55   |
| 22  | 5     | 604  | CLA  | CHA-C1A-NA  | -2.25 | 121.30      | 126.39   |
| 22  | 6     | 606  | CLA  | CHA-C1A-NA  | -2.25 | 121.31      | 126.39   |
| 22  | F     | 1302 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | B     | 1215 | CLA  | C4B-CHC-C1C | 2.25  | 131.53      | 126.25   |
| 22  | B     | 1201 | CLA  | C1C-C2C-C3C | -2.25 | 104.62      | 106.98   |
| 25  | 8     | 503  | BCR  | C15-C14-C13 | -2.25 | 124.13      | 127.28   |
| 22  | Z     | 603  | CLA  | CMD-C2D-C3D | -2.25 | 122.54      | 127.69   |
| 39  | 3     | 502  | LUT  | C30-C31-C32 | -2.25 | 116.69      | 123.20   |
| 39  | 6     | 502  | LUT  | C27-C28-C29 | -2.24 | 121.50      | 126.32   |
| 22  | 3     | 612  | CLA  | C4B-CHC-C1C | 2.24  | 131.53      | 126.25   |
| 22  | B     | 1022 | CLA  | C1-O2A-CGA  | 2.24  | 122.08      | 116.65   |
| 22  | 7     | 603  | CLA  | C2C-C1C-NC  | 2.24  | 112.34      | 109.98   |
| 22  | A     | 1108 | CLA  | CMD-C2D-C3D | -2.24 | 122.54      | 127.69   |
| 40  | 5     | 610  | CHL  | C4C-CHD-C1D | 2.24  | 124.10      | 116.07   |
| 22  | A     | 1103 | CLA  | CAC-C3C-C4C | 2.24  | 127.71      | 124.79   |
| 22  | K     | 1401 | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 41  | 1     | 802  | SQD  | O3-C3-C2    | -2.24 | 105.09      | 110.38   |
| 22  | B     | 1205 | CLA  | C4B-CHC-C1C | 2.24  | 131.52      | 126.25   |
| 22  | 6     | 605  | CLA  | O2D-CGD-O1D | -2.24 | 119.48      | 123.85   |
| 22  | B     | 1230 | CLA  | O1D-CGD-CBD | -2.24 | 120.09      | 124.52   |
| 22  | 8     | 609  | CLA  | CHD-C1D-ND  | -2.24 | 121.65      | 124.80   |
| 22  | 6     | 605  | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 25  | K     | 4002 | BCR  | C2-C1-C6    | 2.24  | 113.70      | 110.44   |
| 22  | A     | 1116 | CLA  | CHD-C1D-ND  | -2.24 | 121.65      | 124.80   |
| 22  | L     | 1502 | CLA  | C1-O2A-CGA  | 2.24  | 122.08      | 116.65   |
| 22  | 2     | 607  | CLA  | CHA-C1A-NA  | -2.24 | 121.32      | 126.39   |
| 22  | 2     | 608  | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | Z     | 615  | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 22  | 7     | 604  | CLA  | O1D-CGD-CBD | -2.24 | 120.10      | 124.52   |
| 22  | 3     | 604  | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 22  | A     | 1129 | CLA  | CMD-C2D-C3D | -2.24 | 122.56      | 127.69   |
| 22  | 4     | 608  | CLA  | C4B-CHC-C1C | 2.24  | 131.51      | 126.25   |
| 40  | Z     | 609  | CHL  | C4C-CHD-C1D | 2.24  | 124.08      | 116.07   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1232 | CLA  | CHA-C1A-NA  | -2.24 | 121.32      | 126.39   |
| 25  | B     | 4004 | BCR  | C33-C5-C4   | 2.24  | 118.37      | 113.60   |
| 22  | A     | 1129 | CLA  | CHA-C1A-NA  | -2.24 | 121.33      | 126.39   |
| 22  | 1     | 606  | CLA  | C1D-ND-C4D  | -2.24 | 104.74      | 106.31   |
| 22  | 8     | 602  | CLA  | C1D-ND-C4D  | -2.24 | 104.74      | 106.31   |
| 22  | 4     | 603  | CLA  | C1D-ND-C4D  | -2.24 | 104.74      | 106.31   |
| 22  | 2     | 602  | CLA  | CMD-C2D-C3D | -2.24 | 122.56      | 127.69   |
| 22  | 9     | 612  | CLA  | O1D-CGD-CBD | -2.24 | 120.11      | 124.52   |
| 39  | 6     | 501  | LUT  | C38-C25-C24 | -2.24 | 118.07      | 123.36   |
| 22  | A     | 1101 | CLA  | CHA-C1A-NA  | -2.24 | 121.33      | 126.39   |
| 22  | B     | 1212 | CLA  | CHA-C1A-NA  | -2.24 | 121.33      | 126.39   |
| 22  | B     | 1240 | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 22  | 2     | 615  | CLA  | O2D-CGD-O1D | -2.23 | 119.50      | 123.85   |
| 22  | A     | 1109 | CLA  | C2C-C1C-NC  | 2.23  | 112.33      | 109.98   |
| 22  | Z     | 607  | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | 9     | 601  | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | B     | 1207 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | A     | 1115 | CLA  | CHA-C4D-ND  | 2.23  | 137.16      | 132.55   |
| 22  | B     | 1220 | CLA  | CHA-C4D-ND  | 2.23  | 137.16      | 132.55   |
| 22  | B     | 1022 | CLA  | O2A-CGA-CBA | 2.23  | 118.64      | 111.83   |
| 22  | 5     | 622  | CLA  | CHA-C1A-NA  | -2.23 | 121.34      | 126.39   |
| 22  | B     | 1232 | CLA  | CAA-C2A-C3A | -2.23 | 106.97      | 113.00   |
| 22  | 3     | 612  | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | A     | 1102 | CLA  | C2A-C1A-CHA | 2.23  | 127.74      | 123.87   |
| 22  | B     | 1023 | CLA  | C2C-C1C-NC  | 2.23  | 112.33      | 109.98   |
| 22  | 7     | 602  | CLA  | C3B-C4B-NB  | -2.23 | 108.54      | 110.53   |
| 22  | 5     | 618  | CLA  | C4B-CHC-C1C | 2.23  | 131.49      | 126.25   |
| 40  | Z     | 610  | CHL  | CMA-C3A-C4A | 2.23  | 119.42      | 114.61   |
| 22  | A     | 1102 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | 6     | 612  | CLA  | O2A-CGA-CBA | 2.23  | 118.64      | 111.83   |
| 26  | 4     | 801  | LHG  | C5-O7-C7    | -2.23 | 112.46      | 117.80   |
| 22  | 7     | 616  | CLA  | C1D-ND-C4D  | -2.23 | 104.75      | 106.31   |
| 22  | B     | 1237 | CLA  | C4B-CHC-C1C | 2.23  | 131.49      | 126.25   |
| 22  | B     | 1204 | CLA  | C3B-C4B-NB  | -2.23 | 108.54      | 110.53   |
| 22  | 8     | 604  | CLA  | C3B-C4B-NB  | -2.23 | 108.54      | 110.53   |
| 39  | 3     | 501  | LUT  | C30-C31-C32 | -2.23 | 116.74      | 123.20   |
| 22  | 7     | 602  | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | B     | 1203 | CLA  | CHD-C1D-ND  | -2.23 | 121.67      | 124.80   |
| 22  | B     | 1241 | CLA  | CHA-C4D-ND  | 2.23  | 137.15      | 132.55   |
| 22  | B     | 1220 | CLA  | C2C-C1C-NC  | 2.23  | 112.32      | 109.98   |
| 22  | 6     | 604  | CLA  | CHA-C1A-NA  | -2.23 | 121.34      | 126.39   |
| 22  | B     | 1212 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 5     | 613  | CLA  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 22  | 6     | 605  | CLA  | C1D-ND-C4D  | -2.23 | 104.75      | 106.31   |
| 22  | Z     | 602  | CLA  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 39  | Z     | 501  | LUT  | C20-C13-C12 | 2.23  | 121.49      | 118.09   |
| 22  | 4     | 612  | CLA  | C3B-C4B-NB  | -2.23 | 108.54      | 110.53   |
| 22  | 7     | 609  | CLA  | C3D-C2D-C1D | -2.23 | 102.79      | 105.83   |
| 39  | 5     | 502  | LUT  | C31-C30-C29 | -2.23 | 124.16      | 127.28   |
| 22  | 6     | 608  | CLA  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 22  | 5     | 601  | CLA  | C2A-C1A-CHA | 2.23  | 127.73      | 123.87   |
| 22  | B     | 1215 | CLA  | O2A-CGA-CBA | 2.23  | 118.62      | 111.83   |
| 22  | A     | 1012 | CLA  | O1D-CGD-CBD | -2.23 | 120.13      | 124.52   |
| 22  | B     | 1021 | CLA  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 22  | B     | 1223 | CLA  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 21  | A     | 1011 | CL0  | O1D-CGD-CBD | -2.23 | 121.35      | 124.72   |
| 22  | Z     | 612  | CLA  | CAA-C2A-C3A | -2.23 | 106.99      | 113.00   |
| 22  | 9     | 604  | CLA  | CBA-CAA-C2A | 2.22  | 120.41      | 113.79   |
| 22  | B     | 1203 | CLA  | C2D-C1D-ND  | 2.22  | 112.33      | 110.13   |
| 22  | Z     | 601  | CLA  | C2D-C1D-ND  | 2.22  | 112.33      | 110.13   |
| 25  | 7     | 503  | BCR  | C30-C25-C24 | 2.22  | 121.68      | 115.65   |
| 22  | A     | 1111 | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 22  | 6     | 618  | CLA  | CAA-C2A-C3A | -2.22 | 106.99      | 113.00   |
| 22  | 3     | 608  | CLA  | CHA-C1A-NA  | -2.22 | 121.36      | 126.39   |
| 22  | 5     | 603  | CLA  | CAC-C3C-C4C | 2.22  | 127.68      | 124.79   |
| 22  | 2     | 606  | CLA  | C4B-CHC-C1C | 2.22  | 131.48      | 126.25   |
| 25  | K     | 4002 | BCR  | C38-C26-C25 | -2.22 | 122.06      | 124.48   |
| 40  | 6     | 617  | CHL  | C4C-CHD-C1D | 2.22  | 124.02      | 116.07   |
| 22  | 8     | 604  | CLA  | CAA-C2A-C1A | 2.22  | 119.26      | 111.97   |
| 22  | 5     | 618  | CLA  | CHA-C1A-NA  | -2.22 | 121.36      | 126.39   |
| 25  | K     | 4002 | BCR  | C12-C13-C14 | -2.22 | 115.51      | 119.01   |
| 22  | 3     | 604  | CLA  | C3A-C2A-C1A | 2.22  | 104.67      | 101.34   |
| 22  | 8     | 601  | CLA  | C3D-C2D-C1D | -2.22 | 102.80      | 105.83   |
| 22  | 1     | 612  | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 22  | A     | 1140 | CLA  | CAA-C2A-C3A | -2.22 | 107.00      | 113.00   |
| 39  | 1     | 501  | LUT  | C39-C29-C28 | 2.22  | 121.48      | 118.09   |
| 22  | 5     | 618  | CLA  | O2A-CGA-CBA | 2.22  | 118.61      | 111.83   |
| 22  | A     | 1101 | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 28  | B     | 5005 | LMT  | O1'-C1'-C2' | 2.22  | 111.65      | 108.27   |
| 22  | 4     | 603  | CLA  | CHA-C1A-NA  | -2.22 | 121.36      | 126.39   |
| 22  | A     | 1123 | CLA  | O2A-CGA-CBA | 2.22  | 118.61      | 111.83   |
| 22  | B     | 1202 | CLA  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 22  | B     | 1230 | CLA  | CHA-C4D-ND  | 2.22  | 137.13      | 132.55   |
| 22  | J     | 1901 | CLA  | CHA-C1A-NA  | -2.22 | 121.36      | 126.39   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 8     | 606  | CLA  | C2D-C1D-ND  | 2.22  | 112.32      | 110.13   |
| 22  | 7     | 615  | CLA  | C3D-C2D-C1D | -2.22 | 102.80      | 105.83   |
| 22  | B     | 1205 | CLA  | CMD-C2D-C3D | -2.22 | 122.60      | 127.69   |
| 40  | 6     | 611  | CHL  | C4C-CHD-C1D | 2.22  | 124.01      | 116.07   |
| 22  | A     | 1124 | CLA  | CHA-C4D-ND  | 2.22  | 137.12      | 132.55   |
| 22  | Z     | 612  | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 22  | B     | 1220 | CLA  | C1D-ND-C4D  | -2.22 | 104.76      | 106.31   |
| 31  | A     | 5003 | LMG  | C8-O7-C10   | -2.22 | 112.49      | 117.80   |
| 22  | B     | 1212 | CLA  | CHD-C1D-ND  | -2.22 | 121.68      | 124.80   |
| 22  | 4     | 602  | CLA  | CHA-C1A-NA  | -2.22 | 121.37      | 126.39   |
| 22  | L     | 1503 | CLA  | CHA-C1A-NA  | -2.22 | 121.37      | 126.39   |
| 22  | K     | 1403 | CLA  | CMD-C2D-C3D | -2.22 | 122.61      | 127.69   |
| 22  | 7     | 612  | CLA  | CMD-C2D-C3D | -2.22 | 122.61      | 127.69   |
| 22  | 5     | 602  | CLA  | O2A-CGA-CBA | 2.22  | 118.59      | 111.83   |
| 40  | 1     | 610  | CHL  | C1-O2A-CGA  | 2.22  | 122.97      | 116.67   |
| 22  | B     | 1238 | CLA  | CMD-C2D-C3D | -2.22 | 122.61      | 127.69   |
| 22  | 5     | 607  | CLA  | CHA-C1A-NA  | -2.22 | 121.37      | 126.39   |
| 22  | 1     | 604  | CLA  | CHD-C1D-ND  | -2.22 | 121.69      | 124.80   |
| 39  | 1     | 501  | LUT  | C18-C5-C6   | -2.22 | 122.07      | 124.48   |
| 22  | 1     | 601  | CLA  | C1D-ND-C4D  | -2.21 | 104.76      | 106.31   |
| 22  | 3     | 605  | CLA  | C1D-ND-C4D  | -2.21 | 104.76      | 106.31   |
| 22  | B     | 1021 | CLA  | O2A-CGA-CBA | 2.21  | 118.59      | 111.83   |
| 22  | 1     | 603  | CLA  | O2D-CGD-O1D | -2.21 | 119.54      | 123.85   |
| 22  | 8     | 611  | CLA  | CHA-C1A-NA  | -2.21 | 121.38      | 126.39   |
| 22  | B     | 1222 | CLA  | C2C-C1C-NC  | 2.21  | 112.31      | 109.98   |
| 22  | 1     | 605  | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 9     | 603  | CLA  | O1D-CGD-CBD | -2.21 | 120.15      | 124.52   |
| 25  | 3     | 503  | BCR  | C29-C28-C27 | 2.21  | 116.14      | 111.28   |
| 25  | 5     | 504  | BCR  | C37-C22-C21 | -2.21 | 119.23      | 122.82   |
| 36  | F     | 4001 | RRX  | C36-C18-C19 | 2.21  | 121.47      | 118.09   |
| 22  | 7     | 606  | CLA  | O2A-CGA-CBA | 2.21  | 118.58      | 111.83   |
| 22  | J     | 1901 | CLA  | C2D-C1D-ND  | 2.21  | 112.32      | 110.13   |
| 22  | 2     | 605  | CLA  | CHA-C1A-NA  | -2.21 | 121.38      | 126.39   |
| 22  | 8     | 608  | CLA  | C1D-ND-C4D  | -2.21 | 104.76      | 106.31   |
| 22  | A     | 1124 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 4     | 602  | CLA  | C2D-C1D-ND  | 2.21  | 112.32      | 110.13   |
| 22  | B     | 1240 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 4     | 604  | CLA  | C1-O2A-CGA  | 2.21  | 122.00      | 116.65   |
| 39  | 2     | 501  | LUT  | C37-C21-C26 | 2.21  | 112.89      | 109.55   |
| 22  | 2     | 607  | CLA  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 22  | K     | 1404 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | A     | 1127 | CLA  | O2D-CGD-O1D | -2.21 | 119.55      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 8     | 609  | CLA  | O1D-CGD-CBD | -2.21 | 120.16      | 124.52   |
| 39  | 8     | 501  | LUT  | C39-C29-C28 | 2.21  | 121.46      | 118.09   |
| 22  | 3     | 607  | CLA  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 39  | 6     | 501  | LUT  | C22-C23-C24 | -2.21 | 107.90      | 111.18   |
| 22  | 5     | 602  | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 39  | Z     | 503  | LUT  | C35-C15-C14 | -2.21 | 119.00      | 123.52   |
| 22  | B     | 1228 | CLA  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 22  | G     | 1601 | CLA  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 22  | Z     | 602  | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | A     | 1116 | CLA  | OBD-CAD-C3D | -2.21 | 123.25      | 128.42   |
| 22  | 5     | 608  | CLA  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 25  | B     | 4001 | BCR  | C35-C13-C12 | 2.21  | 121.46      | 118.09   |
| 22  | 4     | 608  | CLA  | C3B-C4B-NB  | -2.21 | 108.56      | 110.53   |
| 22  | 7     | 613  | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | A     | 1104 | CLA  | C1D-ND-C4D  | -2.21 | 104.76      | 106.31   |
| 22  | 2     | 603  | CLA  | CHD-C1D-ND  | -2.21 | 121.70      | 124.80   |
| 22  | 4     | 609  | CLA  | CMA-C3A-C4A | 2.21  | 117.70      | 111.77   |
| 22  | 3     | 610  | CLA  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 26  | B     | 5006 | LHG  | O7-C7-O9    | -2.21 | 118.55      | 123.70   |
| 22  | 5     | 604  | CLA  | O1A-CGA-CBA | -2.21 | 115.15      | 123.78   |
| 22  | B     | 1218 | CLA  | C3D-C2D-C1D | -2.21 | 102.82      | 105.83   |
| 22  | B     | 1214 | CLA  | C4B-CHC-C1C | 2.21  | 131.44      | 126.25   |
| 22  | K     | 1401 | CLA  | CHD-C1D-ND  | -2.21 | 121.70      | 124.80   |
| 22  | 4     | 615  | CLA  | CHD-C1D-ND  | -2.21 | 121.70      | 124.80   |
| 22  | 8     | 615  | CLA  | CHA-C1A-NA  | -2.21 | 121.40      | 126.39   |
| 22  | B     | 1219 | CLA  | C4B-CHC-C1C | 2.21  | 131.43      | 126.25   |
| 22  | A     | 1110 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | 4     | 615  | CLA  | CHA-C1A-NA  | -2.21 | 121.40      | 126.39   |
| 22  | 3     | 606  | CLA  | O2A-CGA-CBA | 2.21  | 118.56      | 111.83   |
| 22  | B     | 1210 | CLA  | C1D-ND-C4D  | -2.20 | 104.77      | 106.31   |
| 22  | 6     | 615  | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | Z     | 606  | CLA  | C3B-C4B-NB  | -2.20 | 108.56      | 110.53   |
| 39  | 9     | 501  | LUT  | C30-C31-C32 | -2.20 | 116.81      | 123.20   |
| 22  | G     | 1602 | CLA  | O1D-CGD-CBD | -2.20 | 120.17      | 124.52   |
| 22  | B     | 1222 | CLA  | CHA-C4D-ND  | 2.20  | 137.10      | 132.55   |
| 40  | Z     | 610  | CHL  | C4C-CHD-C1D | 2.20  | 123.95      | 116.07   |
| 39  | 4     | 501  | LUT  | C39-C29-C28 | 2.20  | 121.45      | 118.09   |
| 39  | 6     | 501  | LUT  | C11-C10-C9  | -2.20 | 124.19      | 127.28   |
| 22  | 2     | 615  | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | 2     | 603  | CLA  | C2A-C1A-CHA | 2.20  | 127.69      | 123.87   |
| 22  | B     | 1223 | CLA  | CAA-C2A-C3A | -2.20 | 107.05      | 113.00   |
| 22  | 2     | 604  | CLA  | C1D-ND-C4D  | -2.20 | 104.77      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 39  | 8     | 502  | LUT  | C31-C30-C29 | -2.20 | 124.19      | 127.28   |
| 22  | K     | 1404 | CLA  | O2A-CGA-CBA | 2.20  | 118.55      | 111.83   |
| 22  | 1     | 602  | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | 4     | 608  | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | 7     | 602  | CLA  | C1D-ND-C4D  | -2.20 | 104.77      | 106.31   |
| 22  | 4     | 601  | CLA  | O2D-CGD-O1D | -2.20 | 119.56      | 123.85   |
| 22  | B     | 1213 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | A     | 1139 | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | B     | 1239 | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | 4     | 605  | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | 1     | 612  | CLA  | O2A-CGA-CBA | 2.20  | 118.54      | 111.83   |
| 39  | 7     | 502  | LUT  | C20-C13-C12 | 2.20  | 121.45      | 118.09   |
| 22  | 9     | 608  | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | 1     | 604  | CLA  | O2A-CGA-CBA | 2.20  | 118.54      | 111.83   |
| 22  | 3     | 607  | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | 7     | 611  | CLA  | C4B-CHC-C1C | 2.20  | 131.42      | 126.25   |
| 22  | 7     | 612  | CLA  | C3B-C4B-NB  | -2.20 | 108.57      | 110.53   |
| 22  | 8     | 611  | CLA  | C3B-C4B-NB  | -2.20 | 108.57      | 110.53   |
| 22  | 6     | 605  | CLA  | C3B-C4B-NB  | -2.20 | 108.57      | 110.53   |
| 22  | 5     | 622  | CLA  | CHD-C1D-ND  | -2.20 | 121.71      | 124.80   |
| 22  | A     | 1104 | CLA  | CMA-C3A-C4A | 2.20  | 117.68      | 111.77   |
| 22  | B     | 1204 | CLA  | CMD-C2D-C3D | -2.20 | 122.65      | 127.69   |
| 22  | 1     | 607  | CLA  | CHD-C1D-ND  | -2.20 | 121.71      | 124.80   |
| 22  | 3     | 612  | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | F     | 1302 | CLA  | C1D-ND-C4D  | -2.20 | 104.77      | 106.31   |
| 22  | 4     | 602  | CLA  | C1D-ND-C4D  | -2.20 | 104.77      | 106.31   |
| 22  | F     | 1301 | CLA  | C2D-C1D-ND  | 2.20  | 112.30      | 110.13   |
| 41  | 2     | 803  | SQD  | O3-C3-C2    | -2.20 | 105.20      | 110.38   |
| 22  | A     | 1102 | CLA  | C2C-C1C-NC  | 2.20  | 112.29      | 109.98   |
| 22  | 9     | 607  | CLA  | CMD-C2D-C3D | -2.20 | 122.65      | 127.69   |
| 22  | A     | 1120 | CLA  | O2A-CGA-CBA | 2.20  | 118.53      | 111.83   |
| 35  | B     | 5004 | T7X  | C12-C13-C14 | -2.20 | 108.55      | 113.35   |
| 22  | 5     | 608  | CLA  | C3D-C2D-C1D | -2.20 | 102.83      | 105.83   |
| 22  | A     | 1137 | CLA  | CMD-C2D-C3D | -2.20 | 122.65      | 127.69   |
| 22  | 3     | 605  | CLA  | CAA-C2A-C3A | -2.20 | 107.06      | 113.00   |
| 22  | 5     | 606  | CLA  | CHA-C1A-NA  | -2.20 | 121.42      | 126.39   |
| 22  | A     | 1136 | CLA  | CMD-C2D-C3D | -2.20 | 122.65      | 127.69   |
| 22  | B     | 1210 | CLA  | CMD-C2D-C3D | -2.20 | 122.65      | 127.69   |
| 22  | 3     | 613  | CLA  | C4B-CHC-C1C | 2.20  | 131.41      | 126.25   |
| 25  | L     | 4001 | BCR  | C38-C26-C27 | 2.19  | 118.28      | 113.60   |
| 22  | Z     | 605  | CLA  | O2A-CGA-CBA | 2.19  | 118.53      | 111.83   |
| 22  | 4     | 607  | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1239 | CLA  | C3B-C4B-NB  | -2.19 | 108.57      | 110.53   |
| 22  | 7     | 607  | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | A     | 1111 | CLA  | CHA-C1A-NA  | -2.19 | 121.42      | 126.39   |
| 22  | 6     | 607  | CLA  | CHA-C1A-NA  | -2.19 | 121.42      | 126.39   |
| 22  | B     | 1023 | CLA  | CAC-C3C-C4C | 2.19  | 127.64      | 124.79   |
| 25  | G     | 4001 | BCR  | C23-C24-C25 | -2.19 | 121.14      | 127.00   |
| 22  | 5     | 601  | CLA  | C2D-C1D-ND  | 2.19  | 112.30      | 110.13   |
| 22  | 8     | 604  | CLA  | CMD-C2D-C3D | -2.19 | 122.66      | 127.69   |
| 22  | 5     | 603  | CLA  | C2D-C1D-ND  | 2.19  | 112.30      | 110.13   |
| 22  | B     | 1236 | CLA  | CMA-C3A-C4A | 2.19  | 117.66      | 111.77   |
| 25  | K     | 4002 | BCR  | C33-C5-C6   | -2.19 | 122.09      | 124.48   |
| 22  | 1     | 607  | CLA  | C3B-C4B-NB  | -2.19 | 108.57      | 110.53   |
| 22  | 9     | 609  | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | B     | 1227 | CLA  | CMA-C3A-C4A | 2.19  | 117.66      | 111.77   |
| 22  | A     | 1137 | CLA  | CAA-CBA-CGA | -2.19 | 106.99      | 113.21   |
| 22  | 9     | 604  | CLA  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 22  | 3     | 613  | CLA  | C3B-C4B-NB  | -2.19 | 108.58      | 110.53   |
| 22  | 6     | 602  | CLA  | CHA-C1A-NA  | -2.19 | 121.43      | 126.39   |
| 22  | 7     | 602  | CLA  | O2A-CGA-CBA | 2.19  | 118.51      | 111.83   |
| 22  | A     | 1117 | CLA  | CAA-C2A-C1A | -2.19 | 104.80      | 111.97   |
| 22  | B     | 1214 | CLA  | O1D-CGD-CBD | -2.19 | 120.20      | 124.52   |
| 22  | 3     | 608  | CLA  | C3D-C2D-C1D | -2.19 | 102.84      | 105.83   |
| 37  | 1     | 503  | C7Z  | C18-C5-C4   | 2.19  | 118.45      | 114.42   |
| 39  | 9     | 501  | LUT  | C38-C25-C24 | -2.19 | 118.18      | 123.36   |
| 22  | 5     | 618  | CLA  | CHA-C4D-ND  | 2.19  | 137.06      | 132.55   |
| 22  | 5     | 615  | CLA  | C2A-C1A-CHA | 2.19  | 127.67      | 123.87   |
| 22  | 6     | 605  | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | 1     | 607  | CLA  | O2A-CGA-CBA | 2.19  | 118.51      | 111.83   |
| 22  | Z     | 612  | CLA  | CMD-C2D-C3D | -2.19 | 122.67      | 127.69   |
| 22  | 4     | 615  | CLA  | CMD-C2D-C3D | -2.19 | 122.67      | 127.69   |
| 22  | 6     | 606  | CLA  | C1D-ND-C4D  | -2.19 | 104.78      | 106.31   |
| 37  | 5     | 505  | C7Z  | C24-C25-C26 | -2.19 | 116.26      | 120.76   |
| 22  | 3     | 618  | CLA  | C2D-C1D-ND  | 2.19  | 112.29      | 110.13   |
| 22  | 2     | 603  | CLA  | C3D-C2D-C1D | -2.19 | 102.85      | 105.83   |
| 22  | 4     | 607  | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |
| 22  | A     | 1125 | CLA  | O2D-CGD-O1D | -2.19 | 119.59      | 123.85   |
| 22  | 6     | 604  | CLA  | O2D-CGD-O1D | -2.19 | 119.59      | 123.85   |
| 22  | Z     | 606  | CLA  | O1D-CGD-CBD | -2.19 | 120.21      | 124.52   |
| 40  | 4     | 613  | CHL  | CMA-C3A-C4A | 2.19  | 119.32      | 114.61   |
| 22  | G     | 1602 | CLA  | CMD-C2D-C3D | -2.19 | 122.68      | 127.69   |
| 22  | 8     | 601  | CLA  | O1D-CGD-CBD | -2.19 | 120.21      | 124.52   |
| 22  | 8     | 609  | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 2     | 612  | CLA  | C2D-C1D-ND  | 2.19  | 112.29      | 110.13   |
| 22  | 8     | 607  | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |
| 22  | 2     | 603  | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 22  | B     | 1211 | CLA  | C3B-C2B-C1B | -2.18 | 104.60      | 107.17   |
| 25  | 7     | 504  | BCR  | C23-C24-C25 | -2.18 | 121.17      | 127.00   |
| 22  | Z     | 608  | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 22  | 3     | 602  | CLA  | C1D-ND-C4D  | -2.18 | 104.78      | 106.31   |
| 22  | 9     | 608  | CLA  | CAA-C2A-C3A | -2.18 | 107.10      | 113.00   |
| 22  | A     | 1133 | CLA  | CMD-C2D-C3D | -2.18 | 122.69      | 127.69   |
| 22  | 6     | 604  | CLA  | CMD-C2D-C3D | -2.18 | 122.69      | 127.69   |
| 22  | 4     | 612  | CLA  | C4B-CHC-C1C | 2.18  | 131.38      | 126.25   |
| 22  | 4     | 604  | CLA  | O2D-CGD-O1D | -2.18 | 119.60      | 123.85   |
| 39  | 6     | 501  | LUT  | C28-C29-C30 | -2.18 | 115.58      | 119.01   |
| 22  | 4     | 609  | CLA  | C2D-C1D-ND  | 2.18  | 112.28      | 110.13   |
| 22  | A     | 1109 | CLA  | OBD-CAD-C3D | -2.18 | 123.32      | 128.42   |
| 22  | A     | 1136 | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 22  | B     | 1225 | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 22  | A     | 1104 | CLA  | CHD-C1D-ND  | -2.18 | 121.73      | 124.80   |
| 22  | B     | 1206 | CLA  | CHA-C1A-NA  | -2.18 | 121.46      | 126.39   |
| 22  | A     | 1120 | CLA  | CMD-C2D-C3D | -2.18 | 122.69      | 127.69   |
| 40  | Z     | 610  | CHL  | C3D-C4D-ND  | -2.18 | 109.44      | 112.94   |
| 22  | B     | 1207 | CLA  | CMD-C2D-C3D | -2.18 | 122.69      | 127.69   |
| 22  | 7     | 611  | CLA  | CAA-C2A-C3A | -2.18 | 107.11      | 113.00   |
| 22  | 9     | 602  | CLA  | C2D-C1D-ND  | 2.18  | 112.28      | 110.13   |
| 22  | B     | 1219 | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | 8     | 602  | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | A     | 1117 | CLA  | CBA-CAA-C2A | 2.18  | 120.27      | 113.79   |
| 22  | Z     | 608  | CLA  | C1D-ND-C4D  | -2.18 | 104.78      | 106.31   |
| 22  | 8     | 608  | CLA  | CMD-C2D-C3D | -2.18 | 122.70      | 127.69   |
| 22  | 5     | 604  | CLA  | CMC-C2C-C1C | 2.18  | 128.44      | 125.03   |
| 22  | Z     | 606  | CLA  | C1D-ND-C4D  | -2.18 | 104.78      | 106.31   |
| 26  | 6     | 801  | LHG  | O7-C7-O9    | -2.18 | 118.62      | 123.70   |
| 22  | A     | 1103 | CLA  | C1-O2A-CGA  | 2.18  | 121.92      | 116.65   |
| 22  | A     | 1135 | CLA  | CBB-CAB-C3B | -2.18 | 116.66      | 127.53   |
| 22  | 5     | 607  | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | Z     | 615  | CLA  | CHA-C1A-NA  | -2.18 | 121.47      | 126.39   |
| 22  | Z     | 602  | CLA  | CMA-C3A-C4A | 2.18  | 117.62      | 111.77   |
| 22  | B     | 1232 | CLA  | CMD-C2D-C3D | -2.17 | 122.70      | 127.69   |
| 22  | B     | 1220 | CLA  | C3B-C4B-NB  | -2.17 | 108.59      | 110.53   |
| 22  | 5     | 615  | CLA  | C3D-C2D-C1D | -2.17 | 102.86      | 105.83   |
| 22  | Z     | 611  | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | A     | 1118 | CLA  | CAA-C2A-C3A | -2.17 | 107.12      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 9     | 612  | CLA  | CAA-C2A-C3A | -2.17 | 107.12      | 113.00   |
| 22  | 8     | 605  | CLA  | C1-O2A-CGA  | 2.17  | 121.91      | 116.65   |
| 25  | 3     | 503  | BCR  | C37-C22-C23 | 2.17  | 121.41      | 118.09   |
| 39  | Z     | 501  | LUT  | C11-C10-C9  | -2.17 | 124.23      | 127.28   |
| 22  | G     | 1602 | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 22  | 3     | 601  | CLA  | C2D-C1D-ND  | 2.17  | 112.28      | 110.13   |
| 22  | B     | 1237 | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 22  | 7     | 605  | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | 5     | 602  | CLA  | CMD-C2D-C3D | -2.17 | 122.71      | 127.69   |
| 22  | 3     | 604  | CLA  | O2D-CGD-O1D | -2.17 | 119.62      | 123.85   |
| 25  | 3     | 504  | BCR  | C3-C4-C5    | -2.17 | 110.19      | 114.06   |
| 22  | 8     | 605  | CLA  | CMD-C2D-C3D | -2.17 | 122.71      | 127.69   |
| 22  | 1     | 605  | CLA  | O1D-CGD-CBD | -2.17 | 120.24      | 124.52   |
| 22  | B     | 1215 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 22  | 8     | 615  | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 25  | 8     | 503  | BCR  | C29-C28-C27 | 2.17  | 116.05      | 111.28   |
| 22  | 1     | 601  | CLA  | C2C-C1C-NC  | 2.17  | 112.26      | 109.98   |
| 22  | 8     | 612  | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 40  | 2     | 613  | CHL  | C4C-CHD-C1D | 2.17  | 123.83      | 116.07   |
| 22  | 4     | 602  | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 39  | 9     | 502  | LUT  | C22-C23-C24 | -2.17 | 107.96      | 111.18   |
| 40  | 3     | 611  | CHL  | C1C-C2C-CMC | 2.17  | 130.71      | 126.80   |
| 40  | 4     | 611  | CHL  | C4C-CHD-C1D | 2.17  | 123.83      | 116.07   |
| 22  | 4     | 603  | CLA  | CMD-C2D-C3D | -2.17 | 122.72      | 127.69   |
| 22  | 4     | 604  | CLA  | CMD-C2D-C3D | -2.17 | 122.72      | 127.69   |
| 22  | L     | 1503 | CLA  | C1D-ND-C4D  | -2.17 | 104.79      | 106.31   |
| 22  | 4     | 601  | CLA  | C1D-ND-C4D  | -2.17 | 104.79      | 106.31   |
| 22  | 5     | 615  | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 22  | J     | 1901 | CLA  | CMD-C2D-C3D | -2.17 | 122.72      | 127.69   |
| 22  | A     | 1125 | CLA  | C3B-C4B-NB  | -2.17 | 108.59      | 110.53   |
| 22  | 4     | 603  | CLA  | C2D-C1D-ND  | 2.17  | 112.27      | 110.13   |
| 22  | 5     | 612  | CLA  | CMA-C3A-C4A | 2.17  | 117.60      | 111.77   |
| 22  | 6     | 609  | CLA  | CMA-C3A-C4A | 2.17  | 117.59      | 111.77   |
| 22  | 9     | 612  | CLA  | CHA-C1A-NA  | -2.17 | 121.49      | 126.39   |
| 22  | A     | 1110 | CLA  | CMD-C2D-C3D | -2.17 | 122.72      | 127.69   |
| 22  | 5     | 605  | CLA  | CHA-C1A-NA  | -2.17 | 121.49      | 126.39   |
| 22  | A     | 1125 | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 22  | 8     | 607  | CLA  | CMD-C2D-C3D | -2.17 | 122.72      | 127.69   |
| 22  | F     | 1302 | CLA  | C3D-C2D-C1D | -2.17 | 102.88      | 105.83   |
| 28  | 9     | 803  | LMT  | O1B-C1B-C2B | 2.17  | 113.42      | 108.09   |
| 25  | 4     | 503  | BCR  | C1-C6-C7    | 2.16  | 121.52      | 115.65   |
| 27  | 3     | 802  | NKP  | OAB-PAC-OAF | -2.16 | 101.03      | 106.67   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1140 | CLA  | O2D-CGD-O1D | -2.16 | 119.64      | 123.85   |
| 22  | 8     | 611  | CLA  | CMD-C2D-C3D | -2.16 | 122.73      | 127.69   |
| 22  | B     | 1224 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | A     | 1140 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 22  | B     | 1234 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 27  | A     | 5004 | NKP  | OAB-PAC-OAF | -2.16 | 101.03      | 106.67   |
| 22  | A     | 1141 | CLA  | C3D-C2D-C1D | -2.16 | 102.88      | 105.83   |
| 22  | B     | 1234 | CLA  | CAA-C2A-C3A | -2.16 | 107.15      | 113.00   |
| 22  | B     | 1220 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | F     | 1301 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 27  | 8     | 802  | NKP  | OAB-PAC-OAF | -2.16 | 101.03      | 106.67   |
| 22  | 5     | 604  | CLA  | C2C-C1C-NC  | 2.16  | 112.25      | 109.98   |
| 22  | B     | 1228 | CLA  | C1-O2A-CGA  | 2.16  | 121.88      | 116.65   |
| 22  | A     | 1120 | CLA  | C3B-C4B-NB  | -2.16 | 108.60      | 110.53   |
| 22  | 1     | 606  | CLA  | O2A-CGA-CBA | 2.16  | 118.43      | 111.83   |
| 22  | 7     | 608  | CLA  | C3D-C2D-C1D | -2.16 | 102.88      | 105.83   |
| 22  | K     | 1404 | CLA  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 22  | 3     | 616  | CLA  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 22  | 8     | 604  | CLA  | CBA-CAA-C2A | 2.16  | 120.22      | 113.79   |
| 22  | 9     | 601  | CLA  | CMD-C2D-C3D | -2.16 | 122.73      | 127.69   |
| 22  | A     | 1115 | CLA  | C3B-C4B-NB  | -2.16 | 108.60      | 110.53   |
| 40  | Z     | 609  | CHL  | CMD-C2D-C3D | 2.16  | 129.00      | 124.68   |
| 22  | 2     | 601  | CLA  | C1D-ND-C4D  | -2.16 | 104.80      | 106.31   |
| 22  | B     | 1240 | CLA  | CMD-C2D-C3D | -2.16 | 122.73      | 127.69   |
| 22  | B     | 1236 | CLA  | C3D-C2D-C1D | -2.16 | 102.88      | 105.83   |
| 39  | 3     | 502  | LUT  | C35-C15-C14 | -2.16 | 119.10      | 123.52   |
| 22  | 3     | 603  | CLA  | C1-C2-C3    | -2.16 | 122.66      | 126.20   |
| 22  | A     | 1108 | CLA  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 22  | 3     | 616  | CLA  | CMD-C2D-C3D | -2.16 | 122.74      | 127.69   |
| 40  | 6     | 610  | CHL  | C3D-C4D-ND  | -2.16 | 109.47      | 112.94   |
| 22  | 8     | 602  | CLA  | C2D-C1D-ND  | 2.16  | 112.26      | 110.13   |
| 22  | A     | 1140 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | 3     | 601  | CLA  | CMD-C2D-C3D | -2.16 | 122.74      | 127.69   |
| 22  | 7     | 605  | CLA  | C2D-C1D-ND  | 2.16  | 112.26      | 110.13   |
| 22  | 2     | 602  | CLA  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 40  | 6     | 610  | CHL  | C4C-CHD-C1D | 2.16  | 123.79      | 116.07   |
| 22  | 6     | 604  | CLA  | CAA-C2A-C3A | -2.16 | 107.17      | 113.00   |
| 39  | 1     | 502  | LUT  | C22-C23-C24 | -2.16 | 107.98      | 111.18   |
| 39  | 3     | 502  | LUT  | O23-C23-C22 | 2.16  | 113.88      | 110.06   |
| 39  | 9     | 502  | LUT  | C18-C5-C4   | 2.16  | 118.39      | 114.42   |
| 22  | B     | 1230 | CLA  | C1C-C2C-C3C | -2.16 | 104.71      | 106.98   |
| 22  | A     | 1102 | CLA  | CMB-C2B-C3B | 2.16  | 131.62      | 126.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1110 | CLA  | CHD-C1D-ND  | -2.16 | 121.77      | 124.80   |
| 22  | 1     | 612  | CLA  | C2A-C1A-CHA | 2.16  | 127.61      | 123.87   |
| 22  | 7     | 612  | CLA  | CAC-C3C-C4C | 2.16  | 127.59      | 124.79   |
| 22  | 3     | 605  | CLA  | CHA-C1A-NA  | -2.16 | 121.51      | 126.39   |
| 22  | Z     | 611  | CLA  | O2A-CGA-CBA | 2.16  | 118.41      | 111.83   |
| 25  | 5     | 504  | BCR  | C30-C25-C24 | 2.15  | 121.50      | 115.65   |
| 22  | A     | 1126 | CLA  | C4B-CHC-C1C | 2.15  | 131.31      | 126.25   |
| 25  | B     | 4004 | BCR  | C12-C13-C14 | -2.15 | 115.62      | 119.01   |
| 25  | 7     | 503  | BCR  | C33-C5-C4   | 2.15  | 118.19      | 113.60   |
| 22  | B     | 1205 | CLA  | CHD-C1D-ND  | -2.15 | 121.77      | 124.80   |
| 40  | 1     | 610  | CHL  | C4C-CHD-C1D | 2.15  | 123.78      | 116.07   |
| 22  | 7     | 608  | CLA  | CHA-C1A-NA  | -2.15 | 121.51      | 126.39   |
| 22  | 8     | 604  | CLA  | C1D-ND-C4D  | -2.15 | 104.80      | 106.31   |
| 22  | B     | 1023 | CLA  | C1-C2-C3    | -2.15 | 122.67      | 126.20   |
| 22  | A     | 1139 | CLA  | CMD-C2D-C3D | -2.15 | 122.75      | 127.69   |
| 22  | 8     | 604  | CLA  | O1D-CGD-CBD | -2.15 | 120.27      | 124.52   |
| 22  | K     | 1402 | CLA  | C2D-C1D-ND  | 2.15  | 112.26      | 110.13   |
| 39  | 2     | 501  | LUT  | C40-C33-C32 | 2.15  | 121.38      | 118.09   |
| 22  | 6     | 605  | CLA  | C3D-C2D-C1D | -2.15 | 102.89      | 105.83   |
| 22  | 1     | 605  | CLA  | CHA-C1A-NA  | -2.15 | 121.52      | 126.39   |
| 22  | 7     | 609  | CLA  | CHA-C1A-NA  | -2.15 | 121.52      | 126.39   |
| 25  | I     | 4001 | BCR  | C12-C13-C14 | -2.15 | 115.62      | 119.01   |
| 22  | A     | 1116 | CLA  | C3D-C2D-C1D | -2.15 | 102.89      | 105.83   |
| 39  | Z     | 503  | LUT  | C11-C12-C13 | -2.15 | 120.46      | 126.36   |
| 22  | Z     | 612  | CLA  | C4B-CHC-C1C | 2.15  | 131.31      | 126.25   |
| 25  | 8     | 503  | BCR  | C36-C18-C17 | -2.15 | 119.33      | 122.82   |
| 28  | 9     | 803  | LMT  | C1'-O5'-C5' | -2.15 | 109.52      | 113.72   |
| 22  | 7     | 616  | CLA  | C2D-C1D-ND  | 2.15  | 112.25      | 110.13   |
| 22  | B     | 1212 | CLA  | CMD-C2D-C3D | -2.15 | 122.76      | 127.69   |
| 22  | 7     | 605  | CLA  | CAA-C2A-C3A | -2.15 | 107.19      | 113.00   |
| 39  | 2     | 503  | LUT  | C11-C10-C9  | -2.15 | 124.26      | 127.28   |
| 22  | B     | 1222 | CLA  | CMD-C2D-C3D | -2.15 | 122.76      | 127.69   |
| 22  | B     | 1208 | CLA  | CMD-C2D-C3D | -2.15 | 122.76      | 127.69   |
| 22  | A     | 1141 | CLA  | CHA-C1A-NA  | -2.15 | 121.52      | 126.39   |
| 22  | B     | 1217 | CLA  | C2D-C1D-ND  | 2.15  | 112.25      | 110.13   |
| 22  | 8     | 606  | CLA  | CMD-C2D-C3D | -2.15 | 122.76      | 127.69   |
| 22  | A     | 1122 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | 3     | 610  | CLA  | O2A-CGA-CBA | 2.15  | 118.39      | 111.83   |
| 22  | 3     | 610  | CLA  | C2A-C1A-CHA | 2.15  | 127.59      | 123.87   |
| 22  | A     | 1127 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | 1     | 613  | CLA  | CAA-C2A-C3A | -2.15 | 107.19      | 113.00   |
| 22  | J     | 1901 | CLA  | O1D-CGD-CBD | -2.15 | 120.28      | 124.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1227 | CLA  | O2A-CGA-CBA | 2.15  | 118.38      | 111.83   |
| 22  | 2     | 608  | CLA  | C3D-C2D-C1D | -2.15 | 102.90      | 105.83   |
| 22  | 6     | 619  | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 25  | 3     | 505  | BCR  | C36-C18-C17 | -2.15 | 119.34      | 122.82   |
| 22  | A     | 1132 | CLA  | O1D-CGD-CBD | -2.15 | 120.28      | 124.52   |
| 22  | A     | 1115 | CLA  | C1-O2A-CGA  | 2.15  | 121.84      | 116.65   |
| 22  | 4     | 605  | CLA  | CMA-C3A-C4A | 2.15  | 117.54      | 111.77   |
| 39  | 2     | 502  | LUT  | C10-C11-C12 | -2.15 | 116.98      | 123.20   |
| 25  | L     | 4002 | BCR  | C19-C18-C17 | 2.15  | 122.38      | 119.01   |
| 22  | A     | 1140 | CLA  | C1D-ND-C4D  | -2.14 | 104.81      | 106.31   |
| 22  | 3     | 601  | CLA  | C1D-ND-C4D  | -2.14 | 104.81      | 106.31   |
| 22  | A     | 1127 | CLA  | C1C-C2C-C3C | -2.14 | 104.72      | 106.98   |
| 22  | Z     | 601  | CLA  | C3D-C2D-C1D | -2.14 | 102.90      | 105.83   |
| 40  | 2     | 609  | CHL  | C1-O2A-CGA  | 2.14  | 121.84      | 116.65   |
| 22  | 2     | 612  | CLA  | CAA-C2A-C3A | -2.14 | 107.20      | 113.00   |
| 22  | 5     | 603  | CLA  | O2D-CGD-O1D | -2.14 | 119.67      | 123.85   |
| 22  | K     | 1402 | CLA  | C1D-ND-C4D  | -2.14 | 104.81      | 106.31   |
| 22  | 6     | 609  | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 22  | B     | 1227 | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 22  | G     | 1601 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 39  | 2     | 503  | LUT  | C8-C7-C6    | 2.14  | 132.72      | 127.00   |
| 22  | A     | 1131 | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 22  | B     | 1230 | CLA  | C1-O2A-CGA  | 2.14  | 121.84      | 116.65   |
| 26  | 1     | 801  | LHG  | O7-C7-O9    | -2.14 | 118.70      | 123.70   |
| 39  | 5     | 502  | LUT  | C27-C28-C29 | -2.14 | 121.72      | 126.32   |
| 22  | 6     | 608  | CLA  | C1-O2A-CGA  | 2.14  | 121.83      | 116.65   |
| 22  | A     | 1103 | CLA  | C3D-C2D-C1D | -2.14 | 102.91      | 105.83   |
| 22  | 6     | 602  | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 21  | A     | 1011 | CL0  | C4C-C3C-C2C | -2.14 | 104.92      | 113.37   |
| 22  | B     | 1226 | CLA  | CMA-C3A-C4A | 2.14  | 117.53      | 111.77   |
| 22  | A     | 1134 | CLA  | CMD-C2D-C3D | -2.14 | 122.78      | 127.69   |
| 22  | Z     | 605  | CLA  | CAA-C2A-C3A | -2.14 | 107.22      | 113.00   |
| 22  | 3     | 607  | CLA  | CHD-C1D-ND  | -2.14 | 121.79      | 124.80   |
| 22  | B     | 1212 | CLA  | C3D-C2D-C1D | -2.14 | 102.91      | 105.83   |
| 22  | A     | 1012 | CLA  | C1D-ND-C4D  | -2.14 | 104.81      | 106.31   |
| 22  | 9     | 609  | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 22  | B     | 1208 | CLA  | C3D-C2D-C1D | -2.14 | 102.91      | 105.83   |
| 22  | 5     | 601  | CLA  | C2C-C1C-NC  | 2.14  | 112.23      | 109.98   |
| 22  | A     | 1123 | CLA  | C2A-C1A-CHA | 2.14  | 127.58      | 123.87   |
| 22  | 1     | 601  | CLA  | O2A-CGA-CBA | 2.14  | 118.36      | 111.83   |
| 26  | 4     | 801  | LHG  | O7-C7-O9    | -2.14 | 118.71      | 123.70   |
| 22  | B     | 1227 | CLA  | CMD-C2D-C3D | -2.14 | 122.79      | 127.69   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1227 | CLA  | C1D-ND-C4D  | -2.14 | 104.81      | 106.31   |
| 22  | 5     | 605  | CLA  | CAA-CBA-CGA | -2.14 | 107.14      | 113.21   |
| 22  | B     | 1022 | CLA  | C4B-CHC-C1C | 2.14  | 131.27      | 126.25   |
| 22  | 2     | 607  | CLA  | CHD-C1D-ND  | -2.14 | 121.80      | 124.80   |
| 22  | B     | 1222 | CLA  | CMB-C2B-C3B | 2.14  | 131.58      | 126.55   |
| 40  | 4     | 610  | CHL  | C3D-C4D-ND  | -2.14 | 109.51      | 112.94   |
| 22  | A     | 1141 | CLA  | CMD-C2D-C3D | -2.14 | 122.79      | 127.69   |
| 22  | 5     | 622  | CLA  | C2A-C1A-CHA | 2.14  | 127.58      | 123.87   |
| 22  | 1     | 611  | CLA  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 22  | B     | 1202 | CLA  | C1D-ND-C4D  | -2.14 | 104.81      | 106.31   |
| 22  | A     | 1134 | CLA  | O2A-CGA-CBA | 2.14  | 118.35      | 111.83   |
| 22  | 1     | 601  | CLA  | C3D-C2D-C1D | -2.14 | 102.92      | 105.83   |
| 22  | B     | 1204 | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 22  | 4     | 608  | CLA  | CHA-C1A-NA  | -2.14 | 121.56      | 126.39   |
| 25  | 4     | 503  | BCR  | C33-C5-C6   | -2.14 | 122.15      | 124.48   |
| 22  | A     | 1114 | CLA  | C1-O2A-CGA  | 2.14  | 121.82      | 116.65   |
| 22  | B     | 1214 | CLA  | C1D-ND-C4D  | -2.13 | 104.81      | 106.31   |
| 22  | B     | 1240 | CLA  | C1D-ND-C4D  | -2.13 | 104.81      | 106.31   |
| 22  | A     | 1134 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | A     | 1108 | CLA  | C3B-C4B-NB  | -2.13 | 108.62      | 110.53   |
| 22  | 8     | 615  | CLA  | C2D-C1D-ND  | 2.13  | 112.24      | 110.13   |
| 22  | A     | 1120 | CLA  | C1-O2A-CGA  | 2.13  | 121.82      | 116.65   |
| 22  | B     | 1213 | CLA  | C3D-C2D-C1D | -2.13 | 102.92      | 105.83   |
| 22  | J     | 1901 | CLA  | C1D-ND-C4D  | -2.13 | 104.81      | 106.31   |
| 22  | Z     | 611  | CLA  | C1D-ND-C4D  | -2.13 | 104.81      | 106.31   |
| 25  | 5     | 503  | BCR  | C35-C13-C12 | 2.13  | 121.35      | 118.09   |
| 22  | A     | 1104 | CLA  | CMD-C2D-C3D | -2.13 | 122.80      | 127.69   |
| 22  | 8     | 612  | CLA  | C2D-C1D-ND  | 2.13  | 112.24      | 110.13   |
| 22  | 2     | 615  | CLA  | CAA-C2A-C3A | -2.13 | 107.24      | 113.00   |
| 22  | K     | 1402 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | Z     | 605  | CLA  | C1-O2A-CGA  | 2.13  | 121.81      | 116.65   |
| 22  | 6     | 604  | CLA  | O1A-CGA-CBA | -2.13 | 115.44      | 123.78   |
| 22  | B     | 1220 | CLA  | CAA-CBA-CGA | -2.13 | 107.16      | 113.21   |
| 22  | B     | 1228 | CLA  | C3B-C4B-NB  | -2.13 | 108.63      | 110.53   |
| 22  | 5     | 605  | CLA  | C3D-C2D-C1D | -2.13 | 102.92      | 105.83   |
| 22  | B     | 1210 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | B     | 1231 | CLA  | C1-O2A-CGA  | 2.13  | 121.81      | 116.65   |
| 22  | B     | 1220 | CLA  | C6-C5-C3    | -2.13 | 108.28      | 113.47   |
| 22  | B     | 1203 | CLA  | C3D-C2D-C1D | -2.13 | 102.92      | 105.83   |
| 22  | 2     | 601  | CLA  | CMD-C2D-C3D | -2.13 | 122.80      | 127.69   |
| 22  | B     | 1238 | CLA  | O2A-CGA-CBA | 2.13  | 118.33      | 111.83   |
| 22  | 5     | 615  | CLA  | O2A-CGA-CBA | 2.13  | 118.33      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 8     | 603  | CLA  | O2D-CGD-O1D | -2.13 | 119.70      | 123.85   |
| 22  | 4     | 606  | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | 7     | 603  | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 40  | 4     | 610  | CHL  | CMD-C2D-C3D | 2.13  | 128.94      | 124.68   |
| 22  | 1     | 611  | CLA  | C3B-C4B-NB  | -2.13 | 108.63      | 110.53   |
| 22  | 2     | 612  | CLA  | C3B-C4B-NB  | -2.13 | 108.63      | 110.53   |
| 22  | B     | 1228 | CLA  | C1D-ND-C4D  | -2.13 | 104.82      | 106.31   |
| 22  | 7     | 615  | CLA  | CMD-C2D-C3D | -2.13 | 122.81      | 127.69   |
| 22  | A     | 1104 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 40  | 5     | 610  | CHL  | CMD-C2D-C3D | 2.13  | 128.94      | 124.68   |
| 22  | 1     | 603  | CLA  | C3D-C2D-C1D | -2.13 | 102.93      | 105.83   |
| 22  | B     | 1221 | CLA  | CMA-C3A-C2A | 2.13  | 122.21      | 113.98   |
| 22  | A     | 1104 | CLA  | O1D-CGD-CBD | -2.13 | 120.32      | 124.52   |
| 22  | B     | 1240 | CLA  | O1D-CGD-CBD | -2.13 | 120.32      | 124.52   |
| 22  | A     | 1118 | CLA  | C3D-C2D-C1D | -2.13 | 102.93      | 105.83   |
| 22  | A     | 1103 | CLA  | CMD-C2D-C3D | -2.13 | 122.81      | 127.69   |
| 22  | 7     | 604  | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | B     | 1241 | CLA  | CMD-C2D-C3D | -2.13 | 122.81      | 127.69   |
| 22  | B     | 1220 | CLA  | C3D-C2D-C1D | -2.13 | 102.93      | 105.83   |
| 22  | 7     | 613  | CLA  | C3D-C2D-C1D | -2.13 | 102.93      | 105.83   |
| 22  | 2     | 615  | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 22  | 8     | 603  | CLA  | O1A-CGA-CBA | -2.13 | 115.46      | 123.78   |
| 25  | B     | 4005 | BCR  | C38-C26-C27 | 2.13  | 118.13      | 113.60   |
| 22  | B     | 1022 | CLA  | CMA-C3A-C4A | 2.13  | 117.49      | 111.77   |
| 22  | B     | 1207 | CLA  | CHA-C1A-NA  | -2.13 | 121.58      | 126.39   |
| 40  | 3     | 611  | CHL  | CMD-C2D-C3D | 2.13  | 128.93      | 124.68   |
| 22  | 2     | 608  | CLA  | C3B-C4B-NB  | -2.13 | 108.63      | 110.53   |
| 22  | B     | 1023 | CLA  | C3B-C2B-C1B | -2.13 | 104.66      | 107.17   |
| 22  | 3     | 604  | CLA  | O1A-CGA-CBA | -2.13 | 115.47      | 123.78   |
| 39  | 5     | 502  | LUT  | C35-C15-C14 | -2.13 | 119.17      | 123.52   |
| 25  | 3     | 505  | BCR  | C31-C1-C6   | -2.13 | 106.91      | 110.24   |
| 22  | 3     | 602  | CLA  | CMD-C2D-C3D | -2.13 | 122.81      | 127.69   |
| 22  | 1     | 601  | CLA  | C2A-C1A-CHA | 2.13  | 127.56      | 123.87   |
| 22  | B     | 1215 | CLA  | C3B-C4B-NB  | -2.13 | 108.63      | 110.53   |
| 22  | 3     | 602  | CLA  | C2D-C1D-ND  | 2.12  | 112.23      | 110.13   |
| 22  | 7     | 608  | CLA  | C2D-C1D-ND  | 2.12  | 112.23      | 110.13   |
| 22  | 9     | 605  | CLA  | O2A-CGA-CBA | 2.12  | 118.31      | 111.83   |
| 22  | 7     | 601  | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | 9     | 606  | CLA  | C1-O2A-CGA  | 2.12  | 121.79      | 116.65   |
| 22  | B     | 1203 | CLA  | CMD-C2D-C3D | -2.12 | 122.82      | 127.69   |
| 22  | A     | 1108 | CLA  | O2A-CGA-CBA | 2.12  | 118.31      | 111.83   |
| 22  | B     | 1234 | CLA  | C1D-ND-C4D  | -2.12 | 104.82      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 615  | CLA  | CMD-C2D-C3D | -2.12 | 122.82      | 127.69   |
| 22  | A     | 1133 | CLA  | C1-O2A-CGA  | 2.12  | 121.79      | 116.65   |
| 22  | A     | 1125 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | A     | 1116 | CLA  | CAC-C3C-C4C | 2.12  | 127.55      | 124.79   |
| 22  | 2     | 612  | CLA  | C3D-C2D-C1D | -2.12 | 102.93      | 105.83   |
| 22  | B     | 1201 | CLA  | CMB-C2B-C3B | 2.12  | 131.54      | 126.55   |
| 22  | A     | 1108 | CLA  | C1D-ND-C4D  | -2.12 | 104.82      | 106.31   |
| 22  | 4     | 602  | CLA  | CMD-C2D-C3D | -2.12 | 122.82      | 127.69   |
| 22  | 5     | 615  | CLA  | CMD-C2D-C3D | -2.12 | 122.82      | 127.69   |
| 22  | B     | 1212 | CLA  | C1-O2A-CGA  | 2.12  | 121.79      | 116.65   |
| 40  | Z     | 610  | CHL  | C4D-ND-C1D  | 2.12  | 106.83      | 105.22   |
| 40  | 5     | 610  | CHL  | C3D-C4D-ND  | -2.12 | 109.53      | 112.94   |
| 22  | A     | 1013 | CLA  | C4B-CHC-C1C | 2.12  | 131.24      | 126.25   |
| 22  | 8     | 607  | CLA  | O2A-CGA-CBA | 2.12  | 118.30      | 111.83   |
| 22  | 3     | 618  | CLA  | CHD-C1D-ND  | -2.12 | 121.82      | 124.80   |
| 22  | Z     | 615  | CLA  | C1D-ND-C4D  | -2.12 | 104.82      | 106.31   |
| 22  | 6     | 612  | CLA  | C3D-C2D-C1D | -2.12 | 102.94      | 105.83   |
| 22  | 5     | 607  | CLA  | CMD-C2D-C3D | -2.12 | 122.83      | 127.69   |
| 22  | 8     | 602  | CLA  | O2A-CGA-CBA | 2.12  | 118.30      | 111.83   |
| 22  | 9     | 604  | CLA  | C1C-C2C-C3C | -2.12 | 104.75      | 106.98   |
| 22  | 4     | 601  | CLA  | C2A-C1A-CHA | 2.12  | 127.55      | 123.87   |
| 22  | B     | 1230 | CLA  | C3D-C2D-C1D | -2.12 | 102.94      | 105.83   |
| 22  | 7     | 603  | CLA  | O2D-CGD-O1D | -2.12 | 119.72      | 123.85   |
| 22  | B     | 1209 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | 1     | 601  | CLA  | CMD-C2D-C3D | -2.12 | 122.83      | 127.69   |
| 22  | B     | 1203 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | 8     | 608  | CLA  | O2D-CGD-O1D | -2.12 | 119.72      | 123.85   |
| 40  | 6     | 610  | CHL  | C4D-ND-C1D  | 2.12  | 106.83      | 105.22   |
| 22  | A     | 1123 | CLA  | CMD-C2D-C3D | -2.12 | 122.83      | 127.69   |
| 25  | A     | 4004 | BCR  | C34-C9-C10  | -2.12 | 119.38      | 122.82   |
| 22  | 5     | 618  | CLA  | C3B-C4B-NB  | -2.12 | 108.64      | 110.53   |
| 22  | K     | 1403 | CLA  | CAA-C2A-C3A | -2.12 | 107.28      | 113.00   |
| 22  | A     | 1113 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | B     | 1220 | CLA  | CAC-C3C-C4C | 2.12  | 127.55      | 124.79   |
| 39  | 6     | 502  | LUT  | C19-C9-C8   | 2.12  | 121.32      | 118.09   |
| 22  | 5     | 602  | CLA  | CHA-C1A-NA  | -2.12 | 121.60      | 126.39   |
| 22  | B     | 1214 | CLA  | CHA-C1A-NA  | -2.12 | 121.60      | 126.39   |
| 22  | 8     | 611  | CLA  | C3D-C2D-C1D | -2.12 | 102.94      | 105.83   |
| 22  | B     | 1240 | CLA  | C2D-C1D-ND  | 2.12  | 112.22      | 110.13   |
| 22  | Z     | 615  | CLA  | C2D-C1D-ND  | 2.12  | 112.22      | 110.13   |
| 22  | 9     | 602  | CLA  | CMA-C3A-C4A | 2.12  | 117.46      | 111.77   |
| 22  | B     | 1222 | CLA  | O2D-CGD-O1D | -2.12 | 119.73      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1125 | CLA  | C1D-ND-C4D  | -2.12 | 104.83      | 106.31   |
| 22  | B     | 1203 | CLA  | C1D-ND-C4D  | -2.12 | 104.83      | 106.31   |
| 22  | B     | 1223 | CLA  | C1D-ND-C4D  | -2.12 | 104.83      | 106.31   |
| 22  | 1     | 602  | CLA  | C1D-ND-C4D  | -2.12 | 104.83      | 106.31   |
| 22  | A     | 1131 | CLA  | CMD-C2D-C3D | -2.12 | 122.84      | 127.69   |
| 22  | B     | 1206 | CLA  | C4B-CHC-C1C | 2.12  | 131.22      | 126.25   |
| 40  | 1     | 609  | CHL  | CMD-C2D-C3D | 2.12  | 128.91      | 124.68   |
| 22  | 8     | 611  | CLA  | C4B-CHC-C1C | 2.12  | 131.22      | 126.25   |
| 22  | 5     | 609  | CLA  | C1D-ND-C4D  | -2.12 | 104.83      | 106.31   |
| 40  | 5     | 611  | CHL  | C4C-CHD-C1D | 2.12  | 123.64      | 116.07   |
| 37  | J     | 4002 | C7Z  | C1-C6-C7    | 2.11  | 121.39      | 115.65   |
| 22  | 8     | 608  | CLA  | CAA-C2A-C3A | -2.11 | 107.29      | 113.00   |
| 22  | B     | 1231 | CLA  | CHA-C1A-NA  | -2.11 | 121.60      | 126.39   |
| 22  | B     | 1210 | CLA  | CAA-C2A-C3A | -2.11 | 107.29      | 113.00   |
| 22  | 5     | 609  | CLA  | CHD-C1D-ND  | -2.11 | 121.83      | 124.80   |
| 40  | 6     | 617  | CHL  | CMD-C2D-C3D | 2.11  | 128.91      | 124.68   |
| 22  | 3     | 606  | CLA  | C2D-C1D-ND  | 2.11  | 112.22      | 110.13   |
| 22  | 9     | 609  | CLA  | CMD-C2D-C3D | -2.11 | 122.84      | 127.69   |
| 22  | A     | 1121 | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 40  | 5     | 611  | CHL  | CMD-C2D-C3D | 2.11  | 128.90      | 124.68   |
| 22  | F     | 1301 | CLA  | C2A-C1A-CHA | 2.11  | 127.53      | 123.87   |
| 22  | B     | 1228 | CLA  | C2D-C1D-ND  | 2.11  | 112.22      | 110.13   |
| 25  | 3     | 503  | BCR  | C36-C18-C17 | -2.11 | 119.39      | 122.82   |
| 22  | A     | 1137 | CLA  | C3D-C2D-C1D | -2.11 | 102.95      | 105.83   |
| 22  | 7     | 604  | CLA  | C1D-ND-C4D  | -2.11 | 104.83      | 106.31   |
| 22  | 9     | 602  | CLA  | C1D-ND-C4D  | -2.11 | 104.83      | 106.31   |
| 22  | B     | 1226 | CLA  | CBA-CAA-C2A | 2.11  | 120.07      | 113.79   |
| 40  | 4     | 610  | CHL  | CMA-C3A-C2A | 2.11  | 122.28      | 114.13   |
| 25  | I     | 4001 | BCR  | C36-C18-C17 | -2.11 | 119.40      | 122.82   |
| 22  | B     | 1215 | CLA  | C2D-C1D-ND  | 2.11  | 112.21      | 110.13   |
| 22  | 1     | 604  | CLA  | O1D-CGD-CBD | -2.11 | 120.36      | 124.52   |
| 22  | 5     | 609  | CLA  | CMD-C2D-C3D | -2.11 | 122.85      | 127.69   |
| 25  | 7     | 503  | BCR  | C29-C28-C27 | 2.11  | 115.91      | 111.28   |
| 25  | K     | 4002 | BCR  | C3-C4-C5    | -2.11 | 110.30      | 114.06   |
| 22  | A     | 1116 | CLA  | C2D-C1D-ND  | 2.11  | 112.21      | 110.13   |
| 22  | 7     | 607  | CLA  | CHA-C1A-NA  | -2.11 | 121.62      | 126.39   |
| 40  | Z     | 609  | CHL  | C1C-C2C-CMC | 2.11  | 130.60      | 126.80   |
| 40  | 4     | 617  | CHL  | CMA-C3A-C4A | 2.11  | 119.15      | 114.61   |
| 22  | A     | 1111 | CLA  | C3D-C2D-C1D | -2.11 | 102.95      | 105.83   |
| 22  | A     | 1138 | CLA  | CMD-C2D-C3D | -2.11 | 122.86      | 127.69   |
| 40  | 2     | 609  | CHL  | CMD-C2D-C3D | 2.11  | 128.89      | 124.68   |
| 22  | 4     | 603  | CLA  | C1-O2A-CGA  | 2.11  | 121.75      | 116.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | G     | 1601 | CLA  | CMD-C2D-C3D | -2.11 | 122.86      | 127.69   |
| 22  | A     | 1134 | CLA  | C3D-C2D-C1D | -2.11 | 102.96      | 105.83   |
| 22  | Z     | 607  | CLA  | CMD-C2D-C3D | -2.11 | 122.86      | 127.69   |
| 22  | 5     | 605  | CLA  | C2D-C1D-ND  | 2.11  | 112.21      | 110.13   |
| 22  | 7     | 608  | CLA  | CAA-C2A-C3A | -2.11 | 107.31      | 113.00   |
| 22  | B     | 1212 | CLA  | C2A-C1A-CHA | 2.11  | 127.52      | 123.87   |
| 22  | J     | 1901 | CLA  | C3D-C2D-C1D | -2.11 | 102.96      | 105.83   |
| 22  | 7     | 603  | CLA  | C2D-C1D-ND  | 2.10  | 112.21      | 110.13   |
| 25  | 7     | 503  | BCR  | C35-C13-C12 | 2.10  | 121.30      | 118.09   |
| 22  | K     | 1402 | CLA  | CMD-C2D-C3D | -2.10 | 122.86      | 127.69   |
| 22  | B     | 1217 | CLA  | O2A-CGA-CBA | 2.10  | 118.25      | 111.83   |
| 22  | 2     | 604  | CLA  | O2A-CGA-CBA | 2.10  | 118.25      | 111.83   |
| 22  | 5     | 604  | CLA  | O2D-CGD-O1D | -2.10 | 119.75      | 123.85   |
| 37  | 1     | 503  | C7Z  | C7-C8-C9    | -2.10 | 123.12      | 126.23   |
| 39  | Z     | 501  | LUT  | C15-C14-C13 | -2.10 | 124.33      | 127.28   |
| 22  | 7     | 601  | CLA  | C2D-C1D-ND  | 2.10  | 112.21      | 110.13   |
| 22  | 6     | 607  | CLA  | CHD-C1D-ND  | -2.10 | 121.84      | 124.80   |
| 22  | 5     | 601  | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 22  | A     | 1127 | CLA  | O2A-CGA-CBA | 2.10  | 118.24      | 111.83   |
| 39  | 3     | 501  | LUT  | C26-C27-C28 | -2.10 | 121.31      | 124.58   |
| 22  | B     | 1212 | CLA  | CMA-C3A-C4A | 2.10  | 117.42      | 111.77   |
| 22  | 6     | 605  | CLA  | CMA-C3A-C4A | 2.10  | 117.42      | 111.77   |
| 25  | B     | 4005 | BCR  | C36-C18-C17 | -2.10 | 119.41      | 122.82   |
| 22  | A     | 1124 | CLA  | C1D-ND-C4D  | -2.10 | 104.84      | 106.31   |
| 39  | 7     | 501  | LUT  | C30-C31-C32 | -2.10 | 117.11      | 123.20   |
| 22  | B     | 1214 | CLA  | CAA-CBA-CGA | -2.10 | 107.24      | 113.21   |
| 22  | 3     | 601  | CLA  | C2A-C1A-CHA | 2.10  | 127.51      | 123.87   |
| 22  | B     | 1022 | CLA  | C6-C5-C3    | -2.10 | 108.35      | 113.47   |
| 39  | 9     | 502  | LUT  | C3-C4-C5    | -2.10 | 106.95      | 112.18   |
| 22  | B     | 1023 | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | G     | 1601 | CLA  | C1D-ND-C4D  | -2.10 | 104.84      | 106.31   |
| 40  | Z     | 610  | CHL  | CMD-C2D-C3D | 2.10  | 128.88      | 124.68   |
| 22  | 5     | 613  | CLA  | CHD-C1D-ND  | -2.10 | 121.85      | 124.80   |
| 22  | 7     | 613  | CLA  | CMD-C2D-C3D | -2.10 | 122.88      | 127.69   |
| 40  | 4     | 611  | CHL  | CMD-C2D-C3D | 2.10  | 128.88      | 124.68   |
| 22  | 1     | 604  | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | Z     | 615  | CLA  | CAA-C2A-C3A | -2.10 | 107.33      | 113.00   |
| 22  | B     | 1234 | CLA  | C6-C5-C3    | -2.10 | 108.36      | 113.47   |
| 22  | B     | 1229 | CLA  | C3D-C2D-C1D | -2.10 | 102.97      | 105.83   |
| 22  | 9     | 604  | CLA  | C3D-C2D-C1D | -2.10 | 102.97      | 105.83   |
| 22  | 6     | 602  | CLA  | C1D-ND-C4D  | -2.10 | 104.84      | 106.31   |
| 22  | A     | 1111 | CLA  | C1-O2A-CGA  | 2.10  | 121.72      | 116.65   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 7     | 611  | CLA  | C3B-C4B-NB  | -2.09 | 108.66      | 110.53   |
| 22  | 7     | 604  | CLA  | C3D-C2D-C1D | -2.09 | 102.97      | 105.83   |
| 25  | A     | 4004 | BCR  | C36-C18-C17 | -2.09 | 119.42      | 122.82   |
| 22  | F     | 1301 | CLA  | C1D-ND-C4D  | -2.09 | 104.84      | 106.31   |
| 40  | 6     | 613  | CHL  | CMD-C2D-C3D | 2.09  | 128.87      | 124.68   |
| 22  | 8     | 615  | CLA  | CMD-C2D-C3D | -2.09 | 122.89      | 127.69   |
| 22  | 4     | 606  | CLA  | CHA-C1A-NA  | -2.09 | 121.65      | 126.39   |
| 22  | A     | 1109 | CLA  | C2D-C1D-ND  | 2.09  | 112.20      | 110.13   |
| 25  | G     | 4001 | BCR  | C37-C22-C21 | -2.09 | 119.43      | 122.82   |
| 22  | Z     | 602  | CLA  | C1D-ND-C4D  | -2.09 | 104.84      | 106.31   |
| 22  | 4     | 604  | CLA  | C1D-ND-C4D  | -2.09 | 104.84      | 106.31   |
| 22  | A     | 1126 | CLA  | C3B-C2B-C1B | -2.09 | 104.70      | 107.17   |
| 22  | 1     | 613  | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | A     | 1122 | CLA  | O2D-CGD-O1D | -2.09 | 119.78      | 123.85   |
| 37  | 5     | 505  | C7Z  | C11-C12-C13 | -2.09 | 120.63      | 126.36   |
| 40  | 2     | 610  | CHL  | CMD-C2D-C3D | 2.09  | 128.86      | 124.68   |
| 22  | 3     | 616  | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 22  | B     | 1239 | CLA  | C2D-C1D-ND  | 2.09  | 112.19      | 110.13   |
| 22  | B     | 1218 | CLA  | O1D-CGD-CBD | -2.09 | 120.39      | 124.52   |
| 22  | 2     | 615  | CLA  | O1D-CGD-CBD | -2.09 | 120.40      | 124.52   |
| 25  | B     | 4001 | BCR  | C23-C22-C21 | -2.09 | 115.72      | 119.01   |
| 22  | 6     | 609  | CLA  | C2D-C1D-ND  | 2.09  | 112.19      | 110.13   |
| 25  | 6     | 504  | BCR  | C1-C6-C5    | -2.09 | 119.78      | 122.64   |
| 22  | A     | 1102 | CLA  | C2D-C1D-ND  | 2.09  | 112.19      | 110.13   |
| 22  | B     | 1202 | CLA  | CMA-C3A-C4A | 2.09  | 117.39      | 111.77   |
| 40  | 4     | 617  | CHL  | CMD-C2D-C3D | 2.09  | 128.86      | 124.68   |
| 22  | 7     | 602  | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | 2     | 604  | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | 1     | 602  | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 22  | 4     | 604  | CLA  | C2D-C1D-ND  | 2.09  | 112.19      | 110.13   |
| 22  | 6     | 606  | CLA  | C3B-C4B-NB  | -2.09 | 108.67      | 110.53   |
| 22  | B     | 1205 | CLA  | C1D-ND-C4D  | -2.09 | 104.85      | 106.31   |
| 22  | 7     | 615  | CLA  | C1D-ND-C4D  | -2.09 | 104.85      | 106.31   |
| 22  | A     | 1108 | CLA  | C2D-C1D-ND  | 2.09  | 112.19      | 110.13   |
| 40  | 1     | 610  | CHL  | C3D-C4D-ND  | -2.09 | 109.59      | 112.94   |
| 26  | Z     | 801  | LHG  | C5-O7-C7    | -2.09 | 112.80      | 117.80   |
| 22  | F     | 1301 | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 25  | A     | 4002 | BCR  | C19-C18-C17 | 2.09  | 122.29      | 119.01   |
| 25  | 4     | 503  | BCR  | C30-C25-C24 | 2.09  | 121.31      | 115.65   |
| 40  | 1     | 610  | CHL  | CMD-C2D-C3D | 2.09  | 128.85      | 124.68   |
| 39  | 7     | 501  | LUT  | C31-C30-C29 | -2.08 | 124.35      | 127.28   |
| 22  | 4     | 606  | CLA  | O2A-CGA-CBA | 2.08  | 118.19      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 1201 | CLA  | CHA-C1A-NA  | -2.08 | 121.67      | 126.39   |
| 22  | 2     | 601  | CLA  | CHA-C1A-NA  | -2.08 | 121.67      | 126.39   |
| 22  | A     | 1111 | CLA  | C3B-C4B-NB  | -2.08 | 108.67      | 110.53   |
| 22  | 1     | 604  | CLA  | C3B-C4B-NB  | -2.08 | 108.67      | 110.53   |
| 22  | A     | 1128 | CLA  | CHD-C1D-ND  | -2.08 | 121.87      | 124.80   |
| 22  | A     | 1101 | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 25  | J     | 4001 | BCR  | C34-C9-C10  | -2.08 | 119.44      | 122.82   |
| 22  | 3     | 603  | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 22  | 8     | 615  | CLA  | CAA-C2A-C3A | -2.08 | 107.37      | 113.00   |
| 22  | 5     | 604  | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 22  | B     | 1221 | CLA  | C2A-C1A-CHA | 2.08  | 127.48      | 123.87   |
| 22  | B     | 1237 | CLA  | C2D-C1D-ND  | 2.08  | 112.19      | 110.13   |
| 22  | A     | 1139 | CLA  | CBA-CAA-C2A | 2.08  | 119.99      | 113.79   |
| 22  | 9     | 606  | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 22  | 6     | 612  | CLA  | CHA-C1A-NA  | -2.08 | 121.68      | 126.39   |
| 22  | 6     | 603  | CLA  | O1A-CGA-CBA | -2.08 | 115.64      | 123.78   |
| 22  | 9     | 605  | CLA  | C2D-C1D-ND  | 2.08  | 112.19      | 110.13   |
| 22  | B     | 1230 | CLA  | C2C-C1C-NC  | 2.08  | 112.17      | 109.98   |
| 22  | B     | 1236 | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 22  | 6     | 603  | CLA  | C2D-C1D-ND  | 2.08  | 112.19      | 110.13   |
| 40  | 4     | 611  | CHL  | C3D-C4D-ND  | -2.08 | 109.60      | 112.94   |
| 22  | A     | 1119 | CLA  | CHA-C1A-NA  | -2.08 | 121.68      | 126.39   |
| 22  | 4     | 612  | CLA  | C1D-ND-C4D  | -2.08 | 104.85      | 106.31   |
| 22  | 6     | 604  | CLA  | C1D-ND-C4D  | -2.08 | 104.85      | 106.31   |
| 40  | 5     | 617  | CHL  | CMD-C2D-C3D | 2.08  | 128.84      | 124.68   |
| 39  | 6     | 501  | LUT  | C15-C14-C13 | -2.08 | 124.36      | 127.28   |
| 22  | 3     | 601  | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | 4     | 609  | CLA  | CHD-C1D-ND  | -2.08 | 121.88      | 124.80   |
| 22  | 9     | 612  | CLA  | CHD-C1D-ND  | -2.08 | 121.88      | 124.80   |
| 22  | 7     | 604  | CLA  | CBA-CAA-C2A | 2.08  | 119.97      | 113.79   |
| 22  | A     | 1107 | CLA  | CHD-C1D-ND  | -2.08 | 121.88      | 124.80   |
| 22  | 8     | 615  | CLA  | C3D-C2D-C1D | -2.08 | 103.00      | 105.83   |
| 22  | K     | 1401 | CLA  | C1D-ND-C4D  | -2.08 | 104.86      | 106.31   |
| 26  | A     | 5001 | LHG  | C9-C8-C7    | -2.08 | 106.09      | 113.69   |
| 22  | B     | 1211 | CLA  | CAA-CBA-CGA | -2.08 | 107.31      | 113.21   |
| 22  | 7     | 608  | CLA  | CMD-C2D-C3D | -2.08 | 122.93      | 127.69   |
| 22  | L     | 1502 | CLA  | C3D-C2D-C1D | -2.08 | 103.00      | 105.83   |
| 22  | 3     | 618  | CLA  | C3D-C2D-C1D | -2.08 | 103.00      | 105.83   |
| 25  | 7     | 504  | BCR  | C34-C9-C10  | -2.08 | 119.45      | 122.82   |
| 22  | B     | 1217 | CLA  | CMD-C2D-C3D | -2.08 | 122.93      | 127.69   |
| 22  | A     | 1137 | CLA  | C2D-C1D-ND  | 2.08  | 112.18      | 110.13   |
| 22  | B     | 1023 | CLA  | C2D-C1D-ND  | 2.08  | 112.18      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 1111 | CLA  | C1D-ND-C4D  | -2.08 | 104.86      | 106.31   |
| 22  | B     | 1238 | CLA  | C1D-ND-C4D  | -2.08 | 104.86      | 106.31   |
| 39  | 8     | 502  | LUT  | C39-C29-C28 | 2.08  | 121.26      | 118.09   |
| 22  | A     | 1103 | CLA  | C2C-C1C-NC  | 2.07  | 112.16      | 109.98   |
| 22  | A     | 1140 | CLA  | C2D-C1D-ND  | 2.07  | 112.18      | 110.13   |
| 22  | Z     | 604  | CLA  | C2D-C1D-ND  | 2.07  | 112.18      | 110.13   |
| 22  | 3     | 601  | CLA  | C3D-C2D-C1D | -2.07 | 103.00      | 105.83   |
| 22  | 3     | 613  | CLA  | C3D-C2D-C1D | -2.07 | 103.00      | 105.83   |
| 22  | B     | 1240 | CLA  | C2A-C1A-CHA | 2.07  | 127.46      | 123.87   |
| 22  | 3     | 607  | CLA  | C2A-C1A-CHA | 2.07  | 127.46      | 123.87   |
| 25  | 3     | 503  | BCR  | C33-C5-C4   | 2.07  | 118.02      | 113.60   |
| 22  | 5     | 605  | CLA  | OBD-CAD-C3D | -2.07 | 123.57      | 128.42   |
| 22  | A     | 1134 | CLA  | C2D-C1D-ND  | 2.07  | 112.18      | 110.13   |
| 22  | 4     | 607  | CLA  | C2D-C1D-ND  | 2.07  | 112.18      | 110.13   |
| 22  | 5     | 613  | CLA  | C2D-C1D-ND  | 2.07  | 112.18      | 110.13   |
| 25  | K     | 4001 | BCR  | C15-C14-C13 | -2.07 | 124.37      | 127.28   |
| 25  | 7     | 504  | BCR  | C36-C18-C17 | -2.07 | 119.46      | 122.82   |
| 22  | B     | 1235 | CLA  | CMA-C3A-C4A | 2.07  | 117.34      | 111.77   |
| 22  | 6     | 618  | CLA  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 22  | 9     | 607  | CLA  | C6-C5-C3    | -2.07 | 108.42      | 113.47   |
| 40  | 6     | 610  | CHL  | CMD-C2D-C3D | 2.07  | 128.82      | 124.68   |
| 22  | 2     | 606  | CLA  | CHD-C1D-ND  | -2.07 | 121.89      | 124.80   |
| 22  | 9     | 605  | CLA  | CHD-C1D-ND  | -2.07 | 121.89      | 124.80   |
| 22  | A     | 1109 | CLA  | C1-C2-C3    | -2.07 | 122.80      | 126.20   |
| 22  | B     | 1201 | CLA  | C1D-ND-C4D  | -2.07 | 104.86      | 106.31   |
| 22  | B     | 1201 | CLA  | CMD-C2D-C3D | -2.07 | 122.94      | 127.69   |
| 40  | 2     | 613  | CHL  | CMD-C2D-C3D | 2.07  | 128.82      | 124.68   |
| 22  | A     | 1101 | CLA  | C2D-C1D-ND  | 2.07  | 112.17      | 110.13   |
| 22  | 3     | 607  | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 40  | 6     | 611  | CHL  | C3D-C4D-ND  | -2.07 | 109.62      | 112.94   |
| 22  | B     | 1201 | CLA  | C3B-C2B-C1B | -2.07 | 104.73      | 107.17   |
| 25  | 3     | 506  | BCR  | C30-C25-C24 | 2.07  | 121.27      | 115.65   |
| 22  | A     | 1118 | CLA  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 22  | B     | 1234 | CLA  | OBD-CAD-C3D | -2.07 | 123.58      | 128.42   |
| 25  | 3     | 505  | BCR  | C19-C18-C17 | 2.07  | 122.26      | 119.01   |
| 22  | B     | 1215 | CLA  | C3D-C2D-C1D | -2.07 | 103.01      | 105.83   |
| 22  | 7     | 609  | CLA  | CAA-C2A-C3A | -2.07 | 107.41      | 113.00   |
| 22  | 8     | 608  | CLA  | C6-C5-C3    | -2.07 | 108.43      | 113.47   |
| 22  | 1     | 608  | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 22  | B     | 1219 | CLA  | C2A-C1A-CHA | 2.07  | 127.46      | 123.87   |
| 22  | B     | 1207 | CLA  | C1D-ND-C4D  | -2.07 | 104.86      | 106.31   |
| 22  | B     | 1212 | CLA  | C1D-ND-C4D  | -2.07 | 104.86      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 7     | 616  | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 25  | 4     | 503  | BCR  | C3-C4-C5    | -2.07 | 110.37      | 114.06   |
| 39  | 9     | 501  | LUT  | C22-C23-C24 | -2.07 | 108.11      | 111.18   |
| 36  | F     | 4001 | RRX  | C35-C13-C14 | -2.07 | 119.47      | 122.82   |
| 22  | A     | 1123 | CLA  | CAC-C3C-C4C | 2.07  | 127.48      | 124.79   |
| 22  | K     | 1402 | CLA  | O2A-CGA-CBA | 2.07  | 118.14      | 111.83   |
| 22  | B     | 1023 | CLA  | C4B-CHC-C1C | 2.07  | 131.11      | 126.25   |
| 39  | 4     | 502  | LUT  | C39-C29-C28 | 2.07  | 121.25      | 118.09   |
| 22  | 7     | 606  | CLA  | C1-O2A-CGA  | 2.07  | 121.65      | 116.65   |
| 22  | A     | 1116 | CLA  | C6-C5-C3    | -2.07 | 108.43      | 113.47   |
| 22  | B     | 1239 | CLA  | CMD-C2D-C3D | -2.07 | 122.95      | 127.69   |
| 40  | 9     | 613  | CHL  | CMD-C2D-C3D | 2.07  | 128.81      | 124.68   |
| 22  | B     | 1210 | CLA  | C3B-C4B-NB  | -2.07 | 108.69      | 110.53   |
| 25  | 5     | 503  | BCR  | C29-C28-C27 | 2.07  | 115.82      | 111.28   |
| 22  | A     | 1126 | CLA  | CAA-C2A-C3A | -2.07 | 107.42      | 113.00   |
| 22  | A     | 1111 | CLA  | CAA-C2A-C3A | -2.06 | 107.42      | 113.00   |
| 40  | 8     | 610  | CHL  | CMA-C3A-C4A | 2.06  | 119.06      | 114.61   |
| 22  | B     | 1239 | CLA  | C3D-C2D-C1D | -2.06 | 103.01      | 105.83   |
| 39  | 1     | 502  | LUT  | C20-C13-C12 | 2.06  | 121.24      | 118.09   |
| 22  | 7     | 607  | CLA  | O2A-CGA-CBA | 2.06  | 118.13      | 111.83   |
| 22  | 8     | 605  | CLA  | O1D-CGD-CBD | -2.06 | 120.45      | 124.52   |
| 22  | B     | 1022 | CLA  | CMD-C2D-C3D | -2.06 | 122.96      | 127.69   |
| 22  | B     | 1217 | CLA  | CHA-C1A-NA  | -2.06 | 121.72      | 126.39   |
| 25  | A     | 4002 | BCR  | C37-C22-C23 | 2.06  | 121.24      | 118.09   |
| 22  | A     | 1135 | CLA  | CMD-C2D-C3D | -2.06 | 122.96      | 127.69   |
| 22  | 5     | 609  | CLA  | C2D-C1D-ND  | 2.06  | 112.17      | 110.13   |
| 22  | A     | 1120 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 22  | 5     | 608  | CLA  | CMD-C2D-C3D | -2.06 | 122.97      | 127.69   |
| 22  | B     | 1210 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 40  | 3     | 611  | CHL  | C3D-C4D-ND  | -2.06 | 109.63      | 112.94   |
| 22  | A     | 1132 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 22  | 2     | 607  | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | 2     | 608  | CLA  | CMD-C2D-C3D | -2.06 | 122.97      | 127.69   |
| 22  | 5     | 606  | CLA  | C3B-C4B-NB  | -2.06 | 108.69      | 110.53   |
| 22  | B     | 1234 | CLA  | CHD-C1D-ND  | -2.06 | 121.91      | 124.80   |
| 40  | 6     | 611  | CHL  | CMD-C2D-C3D | 2.06  | 128.80      | 124.68   |
| 25  | B     | 4006 | BCR  | C27-C26-C25 | -2.06 | 119.92      | 122.70   |
| 22  | A     | 1117 | CLA  | CMD-C2D-C3D | -2.06 | 122.97      | 127.69   |
| 22  | B     | 1217 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 25  | K     | 4001 | BCR  | C19-C18-C17 | 2.06  | 122.25      | 119.01   |
| 22  | A     | 1138 | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | B     | 1211 | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | Z     | 604  | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 22  | A     | 1126 | CLA  | CMD-C2D-C3D | -2.06 | 122.97      | 127.69   |
| 22  | 2     | 603  | CLA  | C3B-C4B-NB  | -2.06 | 108.69      | 110.53   |
| 22  | G     | 1601 | CLA  | C2A-C1A-CHA | 2.06  | 127.44      | 123.87   |
| 22  | 4     | 604  | CLA  | C3D-C2D-C1D | -2.06 | 103.03      | 105.83   |
| 22  | 9     | 609  | CLA  | C3D-C2D-C1D | -2.06 | 103.03      | 105.83   |
| 22  | B     | 1210 | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | 6     | 619  | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | 1     | 601  | CLA  | O2D-CGD-O1D | -2.06 | 119.85      | 123.85   |
| 21  | A     | 1011 | CL0  | C4D-ND-C1D  | -2.06 | 103.66      | 105.22   |
| 22  | B     | 1214 | CLA  | CHD-C1D-ND  | -2.06 | 121.91      | 124.80   |
| 22  | 8     | 611  | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | 5     | 604  | CLA  | CMD-C2D-C3D | -2.06 | 122.98      | 127.69   |
| 25  | 8     | 503  | BCR  | C35-C13-C12 | 2.05  | 121.23      | 118.09   |
| 22  | B     | 1240 | CLA  | C3D-C2D-C1D | -2.05 | 103.03      | 105.83   |
| 22  | 8     | 604  | CLA  | C2D-C1D-ND  | 2.05  | 112.16      | 110.13   |
| 22  | G     | 1601 | CLA  | CHD-C1D-ND  | -2.05 | 121.91      | 124.80   |
| 22  | 8     | 605  | CLA  | CHD-C1D-ND  | -2.05 | 121.91      | 124.80   |
| 31  | A     | 5003 | LMG  | O7-C10-O9   | -2.05 | 118.90      | 123.70   |
| 22  | A     | 1106 | CLA  | C2D-C1D-ND  | 2.05  | 112.16      | 110.13   |
| 22  | 4     | 609  | CLA  | CHA-C1A-NA  | -2.05 | 121.74      | 126.39   |
| 22  | B     | 1237 | CLA  | C1-O2A-CGA  | 2.05  | 121.62      | 116.65   |
| 22  | A     | 1108 | CLA  | C2A-C1A-CHA | 2.05  | 127.43      | 123.87   |
| 22  | B     | 1222 | CLA  | C3D-C2D-C1D | -2.05 | 103.03      | 105.83   |
| 22  | A     | 1125 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | 1     | 612  | CLA  | C6-C5-C3    | -2.05 | 108.47      | 113.47   |
| 22  | A     | 1123 | CLA  | CHD-C1D-ND  | -2.05 | 121.92      | 124.80   |
| 22  | B     | 1207 | CLA  | C1-O2A-CGA  | 2.05  | 121.62      | 116.65   |
| 22  | 6     | 606  | CLA  | C1-O2A-CGA  | 2.05  | 121.62      | 116.65   |
| 22  | 7     | 607  | CLA  | CMD-C2D-C3D | -2.05 | 122.98      | 127.69   |
| 22  | B     | 1223 | CLA  | CAA-CBA-CGA | -2.05 | 107.38      | 113.21   |
| 39  | 2     | 503  | LUT  | C37-C21-C36 | 2.05  | 110.85      | 107.87   |
| 22  | 1     | 607  | CLA  | CMD-C2D-C3D | -2.05 | 122.99      | 127.69   |
| 22  | B     | 1214 | CLA  | C1C-C2C-C3C | -2.05 | 104.83      | 106.98   |
| 22  | 5     | 613  | CLA  | CAA-C2A-C3A | -2.05 | 107.46      | 113.00   |
| 22  | A     | 1126 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 22  | A     | 1113 | CLA  | C2D-C1D-ND  | 2.05  | 112.15      | 110.13   |
| 22  | 5     | 613  | CLA  | C1D-ND-C4D  | -2.05 | 104.88      | 106.31   |
| 22  | 3     | 604  | CLA  | C1C-C2C-C3C | -2.05 | 104.83      | 106.98   |
| 22  | A     | 1102 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 22  | K     | 1402 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 25  | A     | 4003 | BCR  | C23-C24-C25 | -2.05 | 121.53      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25  | G     | 4001 | BCR  | C12-C13-C14 | -2.05 | 115.79      | 119.01   |
| 22  | 4     | 612  | CLA  | C2D-C1D-ND  | 2.05  | 112.15      | 110.13   |
| 22  | B     | 1216 | CLA  | C1D-ND-C4D  | -2.05 | 104.88      | 106.31   |
| 22  | 5     | 608  | CLA  | C1D-ND-C4D  | -2.05 | 104.88      | 106.31   |
| 22  | 2     | 604  | CLA  | C3B-C4B-NB  | -2.05 | 108.70      | 110.53   |
| 28  | F     | 5001 | LMT  | O1'-C1'-C2' | 2.05  | 111.38      | 108.27   |
| 22  | 4     | 601  | CLA  | C2D-C1D-ND  | 2.05  | 112.15      | 110.13   |
| 22  | K     | 1404 | CLA  | CMA-C3A-C2A | 2.05  | 121.89      | 113.98   |
| 22  | 7     | 613  | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | 4     | 601  | CLA  | CHA-C1A-NA  | -2.05 | 121.76      | 126.39   |
| 22  | 1     | 612  | CLA  | C3D-C2D-C1D | -2.04 | 103.04      | 105.83   |
| 22  | A     | 1131 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | B     | 1213 | CLA  | C3B-C4B-NB  | -2.04 | 108.71      | 110.53   |
| 22  | B     | 1238 | CLA  | C2D-C1D-ND  | 2.04  | 112.15      | 110.13   |
| 22  | A     | 1113 | CLA  | CMD-C2D-C3D | -2.04 | 123.01      | 127.69   |
| 22  | 7     | 616  | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | B     | 1213 | CLA  | O1A-CGA-CBA | -2.04 | 115.80      | 123.78   |
| 39  | Z     | 502  | LUT  | C3-C4-C5    | -2.04 | 107.10      | 112.18   |
| 40  | 7     | 610  | CHL  | CMD-C2D-C3D | 2.04  | 128.76      | 124.68   |
| 22  | B     | 1201 | CLA  | C2D-C1D-ND  | 2.04  | 112.14      | 110.13   |
| 22  | B     | 1240 | CLA  | CAA-CBA-CGA | -2.04 | 107.42      | 113.21   |
| 22  | A     | 1141 | CLA  | CAC-C3C-C4C | 2.04  | 127.44      | 124.79   |
| 22  | B     | 1210 | CLA  | CAC-C3C-C4C | 2.04  | 127.44      | 124.79   |
| 22  | G     | 1602 | CLA  | C2D-C1D-ND  | 2.04  | 112.14      | 110.13   |
| 22  | 7     | 611  | CLA  | C1-O2A-CGA  | 2.04  | 121.59      | 116.65   |
| 22  | 8     | 606  | CLA  | C3B-C4B-NB  | -2.04 | 108.71      | 110.53   |
| 40  | 8     | 613  | CHL  | CMD-C2D-C3D | 2.04  | 128.76      | 124.68   |
| 22  | A     | 1115 | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | 9     | 607  | CLA  | O2D-CGD-O1D | -2.04 | 119.88      | 123.85   |
| 26  | B     | 5006 | LHG  | C5-O7-C7    | -2.04 | 112.92      | 117.80   |
| 25  | 4     | 503  | BCR  | C36-C18-C17 | -2.04 | 119.51      | 122.82   |
| 22  | 6     | 615  | CLA  | C1D-ND-C4D  | -2.04 | 104.88      | 106.31   |
| 37  | 1     | 503  | C7Z  | C38-C25-C24 | 2.04  | 118.17      | 114.42   |
| 22  | 7     | 611  | CLA  | CHA-C1A-NA  | -2.04 | 121.78      | 126.39   |
| 25  | K     | 4002 | BCR  | C23-C24-C25 | -2.04 | 121.56      | 127.00   |
| 39  | 2     | 501  | LUT  | C35-C15-C14 | -2.04 | 119.35      | 123.52   |
| 38  | K     | 5001 | SPH  | O3-C3-C2    | 2.04  | 110.74      | 107.31   |
| 22  | A     | 1129 | CLA  | C1D-ND-C4D  | -2.04 | 104.88      | 106.31   |
| 22  | A     | 1012 | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | 6     | 619  | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | 1     | 601  | CLA  | CHA-C1A-NA  | -2.04 | 121.78      | 126.39   |
| 22  | A     | 1113 | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 606  | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | 1     | 606  | CLA  | CHA-C1A-NA  | -2.04 | 121.78      | 126.39   |
| 22  | 8     | 605  | CLA  | C1D-ND-C4D  | -2.04 | 104.88      | 106.31   |
| 25  | L     | 4001 | BCR  | C34-C9-C8   | 2.04  | 121.20      | 118.09   |
| 22  | B     | 1236 | CLA  | CMD-C2D-C3D | -2.04 | 123.02      | 127.69   |
| 22  | 5     | 609  | CLA  | C3D-C2D-C1D | -2.03 | 103.05      | 105.83   |
| 22  | 5     | 601  | CLA  | O2A-CGA-CBA | 2.03  | 118.04      | 111.83   |
| 22  | B     | 1212 | CLA  | C1C-C2C-C3C | -2.03 | 104.84      | 106.98   |
| 22  | 7     | 601  | CLA  | O2D-CGD-O1D | -2.03 | 119.89      | 123.85   |
| 25  | 3     | 505  | BCR  | C34-C9-C10  | -2.03 | 119.52      | 122.82   |
| 25  | B     | 4003 | BCR  | C29-C30-C25 | 2.03  | 113.39      | 110.44   |
| 22  | 2     | 608  | CLA  | C1D-ND-C4D  | -2.03 | 104.89      | 106.31   |
| 22  | F     | 1301 | CLA  | O2A-CGA-O1A | -2.03 | 118.54      | 123.63   |
| 22  | 8     | 606  | CLA  | CHA-C1A-NA  | -2.03 | 121.79      | 126.39   |
| 22  | 1     | 613  | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | B     | 1234 | CLA  | C2D-C1D-ND  | 2.03  | 112.14      | 110.13   |
| 22  | F     | 1302 | CLA  | CMD-C2D-C3D | -2.03 | 123.03      | 127.69   |
| 22  | 2     | 615  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | 8     | 615  | CLA  | C1D-ND-C4D  | -2.03 | 104.89      | 106.31   |
| 22  | A     | 1125 | CLA  | O2A-CGA-CBA | 2.03  | 118.03      | 111.83   |
| 22  | 5     | 603  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | B     | 1215 | CLA  | CHA-C1A-NA  | -2.03 | 121.79      | 126.39   |
| 25  | B     | 4007 | BCR  | C36-C18-C17 | -2.03 | 119.53      | 122.82   |
| 40  | Z     | 613  | CHL  | CMD-C2D-C3D | 2.03  | 128.74      | 124.68   |
| 22  | 7     | 604  | CLA  | CMD-C2D-C3D | -2.03 | 123.03      | 127.69   |
| 22  | B     | 1204 | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | A     | 1114 | CLA  | CMB-C2B-C3B | 2.03  | 131.33      | 126.55   |
| 22  | 7     | 602  | CLA  | CMA-C3A-C4A | 2.03  | 117.23      | 111.77   |
| 40  | 7     | 610  | CHL  | C3D-C4D-ND  | -2.03 | 109.68      | 112.94   |
| 22  | A     | 1139 | CLA  | C2D-C1D-ND  | 2.03  | 112.14      | 110.13   |
| 22  | A     | 1126 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 39  | 1     | 502  | LUT  | C31-C30-C29 | -2.03 | 124.43      | 127.28   |
| 22  | A     | 1110 | CLA  | CHA-C1A-NA  | -2.03 | 121.80      | 126.39   |
| 22  | 1     | 611  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 39  | 7     | 502  | LUT  | C39-C29-C28 | 2.03  | 121.19      | 118.09   |
| 22  | A     | 1116 | CLA  | CMD-C2D-C3D | -2.03 | 123.04      | 127.69   |
| 22  | 6     | 615  | CLA  | C2A-C1A-CHA | 2.03  | 127.39      | 123.87   |
| 22  | Z     | 605  | CLA  | C6-C5-C3    | -2.03 | 108.53      | 113.47   |
| 22  | A     | 1131 | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | Z     | 603  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | B     | 1202 | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 22  | Z     | 611  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 7     | 606  | CLA  | C1D-ND-C4D  | -2.03 | 104.89      | 106.31   |
| 25  | A     | 4002 | BCR  | C33-C5-C4   | 2.03  | 117.92      | 113.60   |
| 22  | Z     | 615  | CLA  | C3D-C2D-C1D | -2.03 | 103.07      | 105.83   |
| 25  | A     | 4001 | BCR  | C2-C1-C6    | 2.03  | 113.38      | 110.44   |
| 22  | 1     | 602  | CLA  | CHD-C1D-ND  | -2.02 | 121.95      | 124.80   |
| 22  | 4     | 601  | CLA  | CMA-C3A-C4A | 2.02  | 117.22      | 111.77   |
| 22  | 7     | 611  | CLA  | CMD-C2D-C3D | -2.02 | 123.05      | 127.69   |
| 22  | B     | 1235 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 22  | B     | 1226 | CLA  | C2A-C1A-CHA | 2.02  | 127.38      | 123.87   |
| 25  | L     | 4001 | BCR  | C19-C18-C17 | 2.02  | 122.19      | 119.01   |
| 39  | 8     | 502  | LUT  | C18-C5-C6   | -2.02 | 122.28      | 124.48   |
| 23  | A     | 2001 | PQN  | C11-C12-C13 | -2.02 | 123.34      | 126.83   |
| 39  | Z     | 502  | LUT  | C22-C23-C24 | -2.02 | 108.18      | 111.18   |
| 25  | J     | 4001 | BCR  | C38-C26-C27 | 2.02  | 117.91      | 113.60   |
| 22  | B     | 1216 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 22  | B     | 1228 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 22  | 1     | 601  | CLA  | CMA-C3A-C4A | 2.02  | 117.21      | 111.77   |
| 22  | A     | 1132 | CLA  | C1-O2A-CGA  | 2.02  | 121.55      | 116.65   |
| 22  | Z     | 605  | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 22  | 7     | 605  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 4     | 615  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 5     | 609  | CLA  | CAA-C2A-C3A | -2.02 | 107.53      | 113.00   |
| 22  | 8     | 604  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | B     | 1218 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 22  | 7     | 612  | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 25  | B     | 4001 | BCR  | C34-C9-C8   | 2.02  | 121.18      | 118.09   |
| 22  | 2     | 606  | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 22  | 9     | 605  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 9     | 601  | CLA  | C1D-ND-C4D  | -2.02 | 104.89      | 106.31   |
| 22  | 6     | 604  | CLA  | C2D-C1D-ND  | 2.02  | 112.13      | 110.13   |
| 22  | 2     | 605  | CLA  | CHD-C1D-ND  | -2.02 | 121.96      | 124.80   |
| 22  | 4     | 602  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 2     | 605  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 3     | 618  | CLA  | C2A-C1A-CHA | 2.02  | 127.37      | 123.87   |
| 22  | B     | 1229 | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 25  | 5     | 503  | BCR  | C30-C25-C24 | 2.02  | 121.13      | 115.65   |
| 39  | 5     | 501  | LUT  | C30-C31-C32 | -2.02 | 117.35      | 123.20   |
| 25  | 6     | 504  | BCR  | C27-C26-C25 | -2.02 | 119.97      | 122.70   |
| 22  | A     | 1135 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | B     | 1214 | CLA  | C6-C5-C3    | -2.02 | 108.55      | 113.47   |
| 22  | Z     | 606  | CLA  | CHA-C1A-NA  | -2.02 | 121.82      | 126.39   |
| 22  | 2     | 607  | CLA  | C1D-ND-C4D  | -2.02 | 104.90      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 609  | CLA  | CMD-C2D-C3D | -2.02 | 123.06      | 127.69   |
| 22  | B     | 1206 | CLA  | C2A-C1A-CHA | 2.02  | 127.37      | 123.87   |
| 22  | Z     | 604  | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 22  | 7     | 602  | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 40  | 6     | 613  | CHL  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 25  | 3     | 503  | BCR  | C34-C9-C10  | -2.02 | 119.55      | 122.82   |
| 22  | A     | 1138 | CLA  | C1D-ND-C4D  | -2.02 | 104.90      | 106.31   |
| 22  | 3     | 604  | CLA  | CHA-C4D-ND  | 2.02  | 136.71      | 132.55   |
| 39  | 2     | 501  | LUT  | C16-C1-C6   | -2.02 | 107.08      | 110.24   |
| 22  | 5     | 606  | CLA  | CAC-C3C-C4C | 2.02  | 127.41      | 124.79   |
| 40  | 7     | 610  | CHL  | C4C-CHD-C1D | 2.02  | 123.28      | 116.07   |
| 39  | 5     | 502  | LUT  | C3-C4-C5    | -2.01 | 107.16      | 112.18   |
| 26  | 4     | 802  | LHG  | C5-O7-C7    | -2.01 | 112.97      | 117.80   |
| 22  | B     | 1226 | CLA  | CMB-C2B-C3B | 2.01  | 131.29      | 126.55   |
| 40  | 1     | 609  | CHL  | C1C-C2C-CMC | 2.01  | 130.43      | 126.80   |
| 22  | B     | 1224 | CLA  | C2A-C1A-CHA | 2.01  | 127.36      | 123.87   |
| 22  | B     | 1213 | CLA  | CHA-C1A-NA  | -2.01 | 121.83      | 126.39   |
| 22  | B     | 1234 | CLA  | CMD-C2D-C3D | -2.01 | 123.07      | 127.69   |
| 25  | B     | 4004 | BCR  | C37-C22-C21 | -2.01 | 119.56      | 122.82   |
| 22  | 6     | 602  | CLA  | CHD-C1D-ND  | -2.01 | 121.97      | 124.80   |
| 22  | B     | 1232 | CLA  | C2D-C1D-ND  | 2.01  | 112.12      | 110.13   |
| 39  | 6     | 502  | LUT  | C20-C13-C12 | 2.01  | 121.16      | 118.09   |
| 40  | 8     | 610  | CHL  | CMD-C2D-C3D | 2.01  | 128.70      | 124.68   |
| 22  | B     | 1022 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 22  | Z     | 607  | CLA  | C2A-C1A-CHA | 2.01  | 127.36      | 123.87   |
| 22  | 7     | 615  | CLA  | C2A-C1A-CHA | 2.01  | 127.36      | 123.87   |
| 22  | 8     | 607  | CLA  | CMA-C3A-C4A | 2.01  | 117.18      | 111.77   |
| 37  | J     | 4002 | C7Z  | C24-C25-C26 | -2.01 | 116.62      | 120.76   |
| 22  | 8     | 612  | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 4     | 608  | CLA  | C2D-C1D-ND  | 2.01  | 112.12      | 110.13   |
| 22  | 6     | 607  | CLA  | C2D-C1D-ND  | 2.01  | 112.12      | 110.13   |
| 22  | B     | 1221 | CLA  | CMA-C3A-C4A | 2.01  | 117.18      | 111.77   |
| 22  | 8     | 601  | CLA  | C2D-C1D-ND  | 2.01  | 112.11      | 110.13   |
| 22  | 7     | 607  | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 9     | 605  | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 22  | A     | 1122 | CLA  | C2D-C1D-ND  | 2.01  | 112.11      | 110.13   |
| 22  | A     | 1105 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | G     | 1601 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 4     | 612  | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 6     | 606  | CLA  | O2A-CGA-CBA | 2.01  | 117.96      | 111.83   |
| 22  | 3     | 603  | CLA  | O1A-CGA-CBA | -2.01 | 115.93      | 123.78   |
| 22  | 5     | 602  | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 8     | 606  | CLA  | CMA-C3A-C4A | 2.01  | 117.17      | 111.77   |
| 22  | B     | 1224 | CLA  | C2D-C1D-ND  | 2.01  | 112.11      | 110.13   |
| 22  | 1     | 605  | CLA  | C2D-C1D-ND  | 2.01  | 112.11      | 110.13   |
| 22  | A     | 1133 | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 25  | L     | 4002 | BCR  | C23-C24-C25 | -2.01 | 121.64      | 127.00   |
| 22  | B     | 1222 | CLA  | C3B-C4B-NB  | -2.01 | 108.74      | 110.53   |
| 22  | Z     | 602  | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 28  | 9     | 803  | LMT  | C2'-C3'-C4' | 2.01  | 114.23      | 109.68   |
| 22  | Z     | 602  | CLA  | CHD-C1D-ND  | -2.01 | 121.98      | 124.80   |
| 22  | 4     | 608  | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 6     | 615  | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | B     | 1217 | CLA  | C1D-ND-C4D  | -2.01 | 104.91      | 106.31   |
| 22  | 4     | 612  | CLA  | C2A-C1A-CHA | 2.01  | 127.35      | 123.87   |
| 22  | B     | 1214 | CLA  | CMD-C2D-C3D | -2.00 | 123.09      | 127.69   |
| 22  | 2     | 607  | CLA  | C3D-C2D-C1D | -2.00 | 103.09      | 105.83   |
| 22  | L     | 1503 | CLA  | C2D-C1D-ND  | 2.00  | 112.11      | 110.13   |
| 39  | 4     | 502  | LUT  | C19-C9-C8   | 2.00  | 121.15      | 118.09   |
| 40  | 9     | 610  | CHL  | CMD-C2D-C3D | 2.00  | 128.69      | 124.68   |
| 22  | 8     | 606  | CLA  | C3D-C2D-C1D | -2.00 | 103.10      | 105.83   |
| 22  | 6     | 602  | CLA  | CMD-C2D-C3D | -2.00 | 123.09      | 127.69   |
| 39  | 4     | 502  | LUT  | C22-C23-C24 | -2.00 | 108.21      | 111.18   |
| 22  | B     | 1222 | CLA  | CHA-C1A-NA  | -2.00 | 121.86      | 126.39   |
| 39  | 3     | 502  | LUT  | C19-C9-C8   | 2.00  | 121.15      | 118.09   |
| 25  | K     | 4001 | BCR  | C31-C1-C6   | -2.00 | 107.10      | 110.24   |
| 22  | B     | 1212 | CLA  | C3B-C4B-NB  | -2.00 | 108.74      | 110.53   |
| 22  | 1     | 612  | CLA  | C2D-C1D-ND  | 2.00  | 112.11      | 110.13   |
| 25  | 7     | 504  | BCR  | C37-C22-C21 | -2.00 | 119.57      | 122.82   |
| 22  | A     | 1108 | CLA  | C3D-C2D-C1D | -2.00 | 103.10      | 105.83   |
| 22  | A     | 1111 | CLA  | C2D-C1D-ND  | 2.00  | 112.11      | 110.13   |
| 22  | 6     | 607  | CLA  | CMD-C2D-C3D | -2.00 | 123.10      | 127.69   |
| 22  | A     | 1127 | CLA  | C1D-ND-C4D  | -2.00 | 104.91      | 106.31   |
| 22  | 2     | 604  | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |
| 22  | 6     | 602  | CLA  | CAA-C2A-C3A | -2.00 | 107.59      | 113.00   |
| 22  | 9     | 606  | CLA  | O2A-CGA-CBA | 2.00  | 117.93      | 111.83   |
| 22  | B     | 1241 | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |

All (315) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 21  | A     | 1011 | CL0  | ND   |
| 21  | A     | 1011 | CL0  | NC   |
| 21  | A     | 1011 | CL0  | NA   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | A     | 1012 | CLA  | ND   |
| 22  | A     | 1102 | CLA  | ND   |
| 22  | A     | 1103 | CLA  | ND   |
| 22  | A     | 1104 | CLA  | ND   |
| 22  | A     | 1105 | CLA  | ND   |
| 22  | A     | 1106 | CLA  | ND   |
| 22  | A     | 1107 | CLA  | ND   |
| 22  | A     | 1108 | CLA  | ND   |
| 22  | A     | 1109 | CLA  | ND   |
| 22  | A     | 1110 | CLA  | ND   |
| 22  | A     | 1111 | CLA  | ND   |
| 22  | A     | 1112 | CLA  | ND   |
| 22  | A     | 1113 | CLA  | ND   |
| 22  | A     | 1114 | CLA  | ND   |
| 22  | A     | 1115 | CLA  | ND   |
| 22  | A     | 1116 | CLA  | ND   |
| 22  | A     | 1117 | CLA  | ND   |
| 22  | A     | 1118 | CLA  | ND   |
| 22  | A     | 1119 | CLA  | ND   |
| 22  | A     | 1120 | CLA  | ND   |
| 22  | A     | 1121 | CLA  | ND   |
| 22  | A     | 1122 | CLA  | ND   |
| 22  | A     | 1123 | CLA  | ND   |
| 22  | A     | 1124 | CLA  | ND   |
| 22  | A     | 1125 | CLA  | ND   |
| 22  | A     | 1126 | CLA  | ND   |
| 22  | A     | 1127 | CLA  | ND   |
| 22  | A     | 1128 | CLA  | ND   |
| 22  | A     | 1129 | CLA  | ND   |
| 22  | A     | 1130 | CLA  | ND   |
| 22  | A     | 1131 | CLA  | ND   |
| 22  | A     | 1132 | CLA  | ND   |
| 22  | A     | 1133 | CLA  | ND   |
| 22  | A     | 1134 | CLA  | ND   |
| 22  | A     | 1135 | CLA  | ND   |
| 22  | A     | 1136 | CLA  | ND   |
| 22  | A     | 1137 | CLA  | ND   |
| 22  | A     | 1138 | CLA  | ND   |
| 22  | A     | 1139 | CLA  | ND   |
| 22  | A     | 1141 | CLA  | ND   |
| 22  | A     | 1013 | CLA  | ND   |
| 22  | A     | 1140 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | A     | 1101 | CLA  | ND   |
| 22  | B     | 1022 | CLA  | ND   |
| 22  | B     | 1237 | CLA  | ND   |
| 22  | B     | 1021 | CLA  | ND   |
| 22  | B     | 1023 | CLA  | ND   |
| 22  | B     | 1201 | CLA  | ND   |
| 22  | B     | 1202 | CLA  | ND   |
| 22  | B     | 1203 | CLA  | ND   |
| 22  | B     | 1204 | CLA  | ND   |
| 22  | B     | 1205 | CLA  | ND   |
| 22  | B     | 1206 | CLA  | ND   |
| 22  | B     | 1207 | CLA  | ND   |
| 22  | B     | 1208 | CLA  | ND   |
| 22  | B     | 1209 | CLA  | ND   |
| 22  | B     | 1210 | CLA  | ND   |
| 22  | B     | 1211 | CLA  | ND   |
| 22  | B     | 1212 | CLA  | ND   |
| 22  | B     | 1213 | CLA  | ND   |
| 22  | B     | 1214 | CLA  | ND   |
| 22  | B     | 1215 | CLA  | ND   |
| 22  | B     | 1216 | CLA  | ND   |
| 22  | B     | 1217 | CLA  | ND   |
| 22  | B     | 1218 | CLA  | ND   |
| 22  | B     | 1219 | CLA  | ND   |
| 22  | B     | 1220 | CLA  | ND   |
| 22  | B     | 1221 | CLA  | ND   |
| 22  | B     | 1222 | CLA  | ND   |
| 22  | B     | 1223 | CLA  | ND   |
| 22  | B     | 1224 | CLA  | ND   |
| 22  | B     | 1225 | CLA  | ND   |
| 22  | B     | 1226 | CLA  | ND   |
| 22  | B     | 1227 | CLA  | ND   |
| 22  | B     | 1228 | CLA  | ND   |
| 22  | B     | 1229 | CLA  | ND   |
| 22  | B     | 1230 | CLA  | ND   |
| 22  | B     | 1231 | CLA  | ND   |
| 22  | B     | 1232 | CLA  | ND   |
| 22  | B     | 1234 | CLA  | ND   |
| 22  | B     | 1235 | CLA  | ND   |
| 22  | B     | 1236 | CLA  | ND   |
| 22  | B     | 1238 | CLA  | ND   |
| 22  | B     | 1239 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | B     | 1240 | CLA  | ND   |
| 22  | B     | 1241 | CLA  | ND   |
| 22  | F     | 1301 | CLA  | ND   |
| 22  | F     | 1302 | CLA  | ND   |
| 22  | G     | 1601 | CLA  | ND   |
| 22  | G     | 1602 | CLA  | ND   |
| 22  | J     | 1901 | CLA  | ND   |
| 22  | K     | 1401 | CLA  | ND   |
| 22  | K     | 1402 | CLA  | ND   |
| 22  | K     | 1403 | CLA  | ND   |
| 22  | K     | 1404 | CLA  | ND   |
| 22  | L     | 1502 | CLA  | ND   |
| 22  | L     | 1503 | CLA  | ND   |
| 22  | 1     | 601  | CLA  | ND   |
| 22  | 1     | 602  | CLA  | ND   |
| 22  | 1     | 603  | CLA  | ND   |
| 22  | 1     | 604  | CLA  | ND   |
| 22  | 1     | 605  | CLA  | ND   |
| 22  | 1     | 606  | CLA  | ND   |
| 22  | 1     | 607  | CLA  | ND   |
| 22  | 1     | 608  | CLA  | ND   |
| 22  | 1     | 611  | CLA  | ND   |
| 22  | 1     | 612  | CLA  | ND   |
| 22  | 1     | 613  | CLA  | ND   |
| 22  | 1     | 615  | CLA  | ND   |
| 22  | Z     | 601  | CLA  | ND   |
| 22  | Z     | 602  | CLA  | ND   |
| 22  | Z     | 603  | CLA  | ND   |
| 22  | Z     | 604  | CLA  | ND   |
| 22  | Z     | 605  | CLA  | ND   |
| 22  | Z     | 606  | CLA  | ND   |
| 22  | Z     | 607  | CLA  | ND   |
| 22  | Z     | 608  | CLA  | ND   |
| 22  | Z     | 611  | CLA  | ND   |
| 22  | Z     | 612  | CLA  | ND   |
| 22  | Z     | 615  | CLA  | ND   |
| 22  | 3     | 601  | CLA  | ND   |
| 22  | 3     | 602  | CLA  | ND   |
| 22  | 3     | 603  | CLA  | ND   |
| 22  | 3     | 604  | CLA  | ND   |
| 22  | 3     | 605  | CLA  | ND   |
| 22  | 3     | 606  | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | 3     | 607 | CLA  | ND   |
| 22  | 3     | 608 | CLA  | ND   |
| 22  | 3     | 610 | CLA  | ND   |
| 22  | 3     | 612 | CLA  | ND   |
| 22  | 3     | 613 | CLA  | ND   |
| 22  | 3     | 618 | CLA  | ND   |
| 22  | 3     | 616 | CLA  | ND   |
| 22  | 7     | 609 | CLA  | ND   |
| 22  | 7     | 601 | CLA  | ND   |
| 22  | 7     | 602 | CLA  | ND   |
| 22  | 7     | 603 | CLA  | ND   |
| 22  | 7     | 604 | CLA  | ND   |
| 22  | 7     | 605 | CLA  | ND   |
| 22  | 7     | 606 | CLA  | ND   |
| 22  | 7     | 607 | CLA  | ND   |
| 22  | 7     | 608 | CLA  | ND   |
| 22  | 7     | 611 | CLA  | ND   |
| 22  | 7     | 612 | CLA  | ND   |
| 22  | 7     | 613 | CLA  | ND   |
| 22  | 7     | 615 | CLA  | ND   |
| 22  | 7     | 616 | CLA  | ND   |
| 22  | 8     | 605 | CLA  | ND   |
| 22  | 8     | 609 | CLA  | ND   |
| 22  | 8     | 601 | CLA  | ND   |
| 22  | 8     | 602 | CLA  | ND   |
| 22  | 8     | 603 | CLA  | ND   |
| 22  | 8     | 604 | CLA  | ND   |
| 22  | 8     | 606 | CLA  | ND   |
| 22  | 8     | 607 | CLA  | ND   |
| 22  | 8     | 608 | CLA  | ND   |
| 22  | 8     | 611 | CLA  | ND   |
| 22  | 8     | 612 | CLA  | ND   |
| 22  | 8     | 615 | CLA  | ND   |
| 22  | 4     | 601 | CLA  | ND   |
| 22  | 4     | 602 | CLA  | ND   |
| 22  | 4     | 603 | CLA  | ND   |
| 22  | 4     | 604 | CLA  | ND   |
| 22  | 4     | 605 | CLA  | ND   |
| 22  | 4     | 606 | CLA  | ND   |
| 22  | 4     | 607 | CLA  | ND   |
| 22  | 4     | 608 | CLA  | ND   |
| 22  | 4     | 612 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | 4     | 615 | CLA  | ND   |
| 22  | 4     | 609 | CLA  | ND   |
| 22  | 5     | 601 | CLA  | ND   |
| 22  | 5     | 602 | CLA  | ND   |
| 22  | 5     | 603 | CLA  | ND   |
| 22  | 5     | 604 | CLA  | ND   |
| 22  | 5     | 605 | CLA  | ND   |
| 22  | 5     | 606 | CLA  | ND   |
| 22  | 5     | 607 | CLA  | ND   |
| 22  | 5     | 608 | CLA  | ND   |
| 22  | 5     | 609 | CLA  | ND   |
| 22  | 5     | 612 | CLA  | ND   |
| 22  | 5     | 613 | CLA  | ND   |
| 22  | 5     | 615 | CLA  | ND   |
| 22  | 5     | 618 | CLA  | ND   |
| 22  | 5     | 622 | CLA  | ND   |
| 22  | 6     | 608 | CLA  | ND   |
| 22  | 6     | 609 | CLA  | ND   |
| 22  | 6     | 601 | CLA  | ND   |
| 22  | 6     | 602 | CLA  | ND   |
| 22  | 6     | 603 | CLA  | ND   |
| 22  | 6     | 604 | CLA  | ND   |
| 22  | 6     | 605 | CLA  | ND   |
| 22  | 6     | 606 | CLA  | ND   |
| 22  | 6     | 607 | CLA  | ND   |
| 22  | 6     | 612 | CLA  | ND   |
| 22  | 6     | 615 | CLA  | ND   |
| 22  | 6     | 618 | CLA  | ND   |
| 22  | 6     | 619 | CLA  | ND   |
| 22  | 2     | 601 | CLA  | ND   |
| 22  | 2     | 602 | CLA  | ND   |
| 22  | 2     | 603 | CLA  | ND   |
| 22  | 2     | 604 | CLA  | ND   |
| 22  | 2     | 605 | CLA  | ND   |
| 22  | 2     | 606 | CLA  | ND   |
| 22  | 2     | 607 | CLA  | ND   |
| 22  | 2     | 608 | CLA  | ND   |
| 22  | 2     | 612 | CLA  | ND   |
| 22  | 2     | 615 | CLA  | ND   |
| 22  | 9     | 601 | CLA  | ND   |
| 22  | 9     | 602 | CLA  | ND   |
| 22  | 9     | 603 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 22  | 9     | 604  | CLA  | ND   |
| 22  | 9     | 606  | CLA  | ND   |
| 22  | 9     | 607  | CLA  | ND   |
| 22  | 9     | 608  | CLA  | ND   |
| 22  | 9     | 609  | CLA  | ND   |
| 22  | 9     | 612  | CLA  | ND   |
| 36  | F     | 4001 | RRX  | C28  |
| 37  | J     | 4002 | C7Z  | C3   |
| 37  | 1     | 503  | C7Z  | C3   |
| 37  | 5     | 505  | C7Z  | C3   |
| 39  | 2     | 501  | LUT  | C26  |
| 39  | 2     | 503  | LUT  | C26  |
| 40  | 1     | 610  | CHL  | ND   |
| 40  | 1     | 610  | CHL  | NC   |
| 40  | 1     | 610  | CHL  | NA   |
| 40  | 1     | 609  | CHL  | C8   |
| 40  | 1     | 609  | CHL  | ND   |
| 40  | 1     | 609  | CHL  | NC   |
| 40  | 1     | 609  | CHL  | NA   |
| 40  | Z     | 610  | CHL  | C8   |
| 40  | Z     | 610  | CHL  | ND   |
| 40  | Z     | 610  | CHL  | NC   |
| 40  | Z     | 610  | CHL  | NA   |
| 40  | Z     | 613  | CHL  | ND   |
| 40  | Z     | 613  | CHL  | NC   |
| 40  | Z     | 613  | CHL  | NA   |
| 40  | Z     | 609  | CHL  | C8   |
| 40  | Z     | 609  | CHL  | ND   |
| 40  | Z     | 609  | CHL  | NC   |
| 40  | Z     | 609  | CHL  | NA   |
| 40  | 3     | 611  | CHL  | C8   |
| 40  | 3     | 611  | CHL  | ND   |
| 40  | 3     | 611  | CHL  | NC   |
| 40  | 3     | 611  | CHL  | NA   |
| 40  | 7     | 610  | CHL  | ND   |
| 40  | 7     | 610  | CHL  | NC   |
| 40  | 7     | 610  | CHL  | NA   |
| 40  | 8     | 610  | CHL  | C8   |
| 40  | 8     | 610  | CHL  | ND   |
| 40  | 8     | 610  | CHL  | NC   |
| 40  | 8     | 610  | CHL  | NA   |
| 40  | 8     | 613  | CHL  | C8   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 40  | 8     | 613 | CHL  | ND   |
| 40  | 8     | 613 | CHL  | C3A  |
| 40  | 8     | 613 | CHL  | NA   |
| 40  | 8     | 613 | CHL  | NC   |
| 40  | 4     | 610 | CHL  | NC   |
| 40  | 4     | 610 | CHL  | ND   |
| 40  | 4     | 610 | CHL  | C3A  |
| 40  | 4     | 610 | CHL  | NA   |
| 40  | 4     | 611 | CHL  | ND   |
| 40  | 4     | 611 | CHL  | NC   |
| 40  | 4     | 611 | CHL  | NA   |
| 40  | 4     | 613 | CHL  | C8   |
| 40  | 4     | 613 | CHL  | ND   |
| 40  | 4     | 613 | CHL  | NC   |
| 40  | 4     | 613 | CHL  | NA   |
| 40  | 4     | 617 | CHL  | ND   |
| 40  | 4     | 617 | CHL  | NC   |
| 40  | 4     | 617 | CHL  | NA   |
| 40  | 5     | 610 | CHL  | C8   |
| 40  | 5     | 610 | CHL  | ND   |
| 40  | 5     | 610 | CHL  | NC   |
| 40  | 5     | 610 | CHL  | NA   |
| 40  | 5     | 611 | CHL  | ND   |
| 40  | 5     | 611 | CHL  | NC   |
| 40  | 5     | 611 | CHL  | NA   |
| 40  | 5     | 617 | CHL  | ND   |
| 40  | 5     | 617 | CHL  | NC   |
| 40  | 5     | 617 | CHL  | NA   |
| 40  | 6     | 610 | CHL  | C8   |
| 40  | 6     | 610 | CHL  | ND   |
| 40  | 6     | 610 | CHL  | NC   |
| 40  | 6     | 610 | CHL  | NA   |
| 40  | 6     | 611 | CHL  | ND   |
| 40  | 6     | 611 | CHL  | NC   |
| 40  | 6     | 611 | CHL  | NA   |
| 40  | 6     | 613 | CHL  | C8   |
| 40  | 6     | 613 | CHL  | ND   |
| 40  | 6     | 613 | CHL  | NC   |
| 40  | 6     | 613 | CHL  | NA   |
| 40  | 6     | 617 | CHL  | ND   |
| 40  | 6     | 617 | CHL  | NC   |
| 40  | 6     | 617 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 40  | 2     | 609 | CHL  | ND   |
| 40  | 2     | 609 | CHL  | NC   |
| 40  | 2     | 609 | CHL  | NA   |
| 40  | 2     | 610 | CHL  | NC   |
| 40  | 2     | 610 | CHL  | ND   |
| 40  | 2     | 610 | CHL  | C3A  |
| 40  | 2     | 610 | CHL  | NA   |
| 40  | 2     | 613 | CHL  | ND   |
| 40  | 2     | 613 | CHL  | NC   |
| 40  | 2     | 613 | CHL  | NA   |
| 40  | 9     | 610 | CHL  | C8   |
| 40  | 9     | 610 | CHL  | ND   |
| 40  | 9     | 610 | CHL  | NC   |
| 40  | 9     | 610 | CHL  | NA   |
| 40  | 9     | 613 | CHL  | ND   |
| 40  | 9     | 613 | CHL  | NC   |
| 40  | 9     | 613 | CHL  | NA   |
| 42  | Z     | 504 | QTB  | C11  |

All (3861) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1012 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1102 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1102 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1103 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1103 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1105 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1105 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1106 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1106 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 1106 | CLA  | CHA-CBD-CGD-O2D |
| 22  | A     | 1108 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1108 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1109 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1111 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1111 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1114 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1116 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1116 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1116 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1116 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1117 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1117 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1120 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1120 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1121 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1121 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1123 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1123 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1123 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1123 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1125 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1128 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1129 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1129 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1129 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1130 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1132 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1132 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1135 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1136 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1136 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1136 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1136 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1137 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1138 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1138 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1139 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1139 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1139 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1139 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1140 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1101 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1101 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1101 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1022 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1237 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1021 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1023 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1023 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1201 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1202 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1202 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1204 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1205 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1205 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1206 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1206 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1207 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1208 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1208 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1208 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1209 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1211 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1211 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1212 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1212 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1213 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1214 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1214 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1214 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1214 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1215 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1215 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1215 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1215 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1216 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1216 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1216 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1216 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1217 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1217 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1217 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1219 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1219 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1219 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1220 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1220 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1223 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1223 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1224 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1224 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1224 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1224 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1225 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1225 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1226 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1226 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1226 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1228 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1229 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1230 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 1230 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 1231 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1234 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1234 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1234 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1235 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1235 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1235 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1235 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1236 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1240 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1241 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 1301 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 1301 | CLA  | CAD-CBD-CGD-O1D |
| 22  | F     | 1301 | CLA  | CAD-CBD-CGD-O2D |
| 22  | F     | 1302 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 1601 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 1602 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 1602 | CLA  | C2B-C3B-CAB-CBB |
| 22  | G     | 1602 | CLA  | C4B-C3B-CAB-CBB |
| 22  | J     | 1901 | CLA  | C1A-C2A-CAA-CBA |
| 22  | J     | 1901 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 1401 | CLA  | CBA-CGA-O2A-C1  |
| 22  | K     | 1402 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 1402 | CLA  | C3A-C2A-CAA-CBA |
| 22  | K     | 1403 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 1404 | CLA  | CBD-CGD-O2D-CED |
| 22  | L     | 1502 | CLA  | C1A-C2A-CAA-CBA |
| 22  | L     | 1502 | CLA  | C3A-C2A-CAA-CBA |
| 22  | L     | 1503 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 601  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 601  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 602  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 604  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 607 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 607 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 608 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 613 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 615 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 615 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 601 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 615 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 615 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 605 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 606 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 607 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 608 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 610 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 618 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 616 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 616 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 605 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 605 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 605 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 606 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 613 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 615 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 615 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 615 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 616 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 616 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 616 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 22  | 8     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 606 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 607 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 607 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 611 | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 611 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 612 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 615 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 602 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 602 | CLA  | C3-C5-C6-C7     |
| 22  | 4     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 605 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 607 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 612 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 601 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 601 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 601 | CLA  | C4-C3-C5-C6     |
| 22  | 5     | 602 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 603 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 607 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 612 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 613 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 5     | 613  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 618  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 622  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 601  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 605  | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 612  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 615  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 615  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 618  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 619  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 602  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 603  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 603  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 2     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 604  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 2     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 612  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 615  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 601  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 603  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 609  | CLA  | C4B-C3B-CAB-CBB |
| 25  | A     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | A     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | A     | 4001 | BCR  | C10-C11-C12-C13 |
| 25  | A     | 4001 | BCR  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | A     | 4001 | BCR  | C11-C12-C13-C35 |
| 25  | A     | 4002 | BCR  | C7-C8-C9-C10    |
| 25  | A     | 4002 | BCR  | C7-C8-C9-C34    |
| 25  | A     | 4002 | BCR  | C11-C10-C9-C8   |
| 25  | A     | 4002 | BCR  | C11-C10-C9-C34  |
| 25  | A     | 4002 | BCR  | C10-C11-C12-C13 |
| 25  | A     | 4003 | BCR  | C5-C6-C7-C8     |
| 25  | A     | 4003 | BCR  | C7-C8-C9-C10    |
| 25  | A     | 4003 | BCR  | C7-C8-C9-C34    |
| 25  | A     | 4004 | BCR  | C7-C8-C9-C10    |
| 25  | A     | 4004 | BCR  | C7-C8-C9-C34    |
| 25  | A     | 4004 | BCR  | C11-C10-C9-C8   |
| 25  | A     | 4004 | BCR  | C11-C10-C9-C34  |
| 25  | A     | 4004 | BCR  | C23-C24-C25-C26 |
| 25  | A     | 4005 | BCR  | C7-C8-C9-C10    |
| 25  | A     | 4005 | BCR  | C11-C10-C9-C8   |
| 25  | A     | 4005 | BCR  | C11-C10-C9-C34  |
| 25  | A     | 4005 | BCR  | C36-C18-C19-C20 |
| 25  | A     | 4005 | BCR  | C21-C22-C23-C24 |
| 25  | A     | 4005 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | B     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | B     | 4001 | BCR  | C17-C18-C19-C20 |
| 25  | B     | 4001 | BCR  | C36-C18-C19-C20 |
| 25  | B     | 4001 | BCR  | C21-C22-C23-C24 |
| 25  | B     | 4001 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 4002 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 4002 | BCR  | C11-C10-C9-C8   |
| 25  | B     | 4002 | BCR  | C11-C10-C9-C34  |
| 25  | B     | 4002 | BCR  | C10-C11-C12-C13 |
| 25  | B     | 4002 | BCR  | C21-C22-C23-C24 |
| 25  | B     | 4002 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 4004 | BCR  | C7-C8-C9-C10    |
| 25  | B     | 4004 | BCR  | C11-C10-C9-C8   |
| 25  | B     | 4004 | BCR  | C11-C10-C9-C34  |
| 25  | B     | 4004 | BCR  | C10-C11-C12-C13 |
| 25  | B     | 4005 | BCR  | C11-C10-C9-C8   |
| 25  | B     | 4005 | BCR  | C11-C10-C9-C34  |
| 25  | B     | 4005 | BCR  | C10-C11-C12-C13 |
| 25  | B     | 4005 | BCR  | C11-C12-C13-C14 |
| 25  | B     | 4007 | BCR  | C11-C10-C9-C8   |
| 25  | B     | 4007 | BCR  | C11-C10-C9-C34  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 4007 | BCR  | C9-C10-C11-C12  |
| 25  | B     | 4007 | BCR  | C10-C11-C12-C13 |
| 25  | B     | 4006 | BCR  | C10-C11-C12-C13 |
| 25  | G     | 4001 | BCR  | C7-C8-C9-C10    |
| 25  | G     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | G     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | G     | 4001 | BCR  | C10-C11-C12-C13 |
| 25  | I     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | I     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | I     | 4001 | BCR  | C10-C11-C12-C13 |
| 25  | I     | 4001 | BCR  | C17-C18-C19-C20 |
| 25  | J     | 4001 | BCR  | C7-C8-C9-C10    |
| 25  | J     | 4001 | BCR  | C7-C8-C9-C34    |
| 25  | J     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | J     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | J     | 4001 | BCR  | C10-C11-C12-C13 |
| 25  | J     | 4001 | BCR  | C11-C12-C13-C14 |
| 25  | J     | 4001 | BCR  | C17-C18-C19-C20 |
| 25  | J     | 4001 | BCR  | C21-C22-C23-C24 |
| 25  | J     | 4001 | BCR  | C37-C22-C23-C24 |
| 25  | K     | 4001 | BCR  | C7-C8-C9-C34    |
| 25  | K     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | K     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | K     | 4001 | BCR  | C10-C11-C12-C13 |
| 25  | K     | 4001 | BCR  | C21-C22-C23-C24 |
| 25  | K     | 4001 | BCR  | C37-C22-C23-C24 |
| 25  | K     | 4001 | BCR  | C23-C24-C25-C26 |
| 25  | K     | 4001 | BCR  | C23-C24-C25-C30 |
| 25  | K     | 4002 | BCR  | C11-C10-C9-C8   |
| 25  | K     | 4002 | BCR  | C11-C10-C9-C34  |
| 25  | K     | 4002 | BCR  | C10-C11-C12-C13 |
| 25  | L     | 4001 | BCR  | C7-C8-C9-C10    |
| 25  | L     | 4001 | BCR  | C11-C10-C9-C8   |
| 25  | L     | 4001 | BCR  | C11-C10-C9-C34  |
| 25  | L     | 4001 | BCR  | C10-C11-C12-C13 |
| 25  | L     | 4001 | BCR  | C23-C24-C25-C26 |
| 25  | L     | 4001 | BCR  | C23-C24-C25-C30 |
| 25  | L     | 4002 | BCR  | C11-C10-C9-C8   |
| 25  | L     | 4002 | BCR  | C11-C10-C9-C34  |
| 25  | 3     | 503  | BCR  | C5-C6-C7-C8     |
| 25  | 3     | 503  | BCR  | C7-C8-C9-C10    |
| 25  | 3     | 503  | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 3     | 503 | BCR  | C11-C10-C9-C8   |
| 25  | 3     | 503 | BCR  | C11-C10-C9-C34  |
| 25  | 3     | 504 | BCR  | C7-C8-C9-C10    |
| 25  | 3     | 504 | BCR  | C11-C10-C9-C8   |
| 25  | 3     | 504 | BCR  | C11-C10-C9-C34  |
| 25  | 3     | 504 | BCR  | C21-C22-C23-C24 |
| 25  | 3     | 504 | BCR  | C37-C22-C23-C24 |
| 25  | 3     | 505 | BCR  | C7-C8-C9-C10    |
| 25  | 3     | 505 | BCR  | C7-C8-C9-C34    |
| 25  | 3     | 505 | BCR  | C11-C10-C9-C8   |
| 25  | 3     | 505 | BCR  | C11-C10-C9-C34  |
| 25  | 3     | 505 | BCR  | C10-C11-C12-C13 |
| 25  | 3     | 506 | BCR  | C7-C8-C9-C10    |
| 25  | 3     | 506 | BCR  | C7-C8-C9-C34    |
| 25  | 3     | 506 | BCR  | C11-C10-C9-C8   |
| 25  | 3     | 506 | BCR  | C11-C10-C9-C34  |
| 25  | 3     | 506 | BCR  | C10-C11-C12-C13 |
| 25  | 3     | 506 | BCR  | C21-C22-C23-C24 |
| 25  | 3     | 506 | BCR  | C23-C24-C25-C26 |
| 25  | 3     | 506 | BCR  | C23-C24-C25-C30 |
| 25  | 7     | 503 | BCR  | C11-C10-C9-C8   |
| 25  | 7     | 503 | BCR  | C11-C10-C9-C34  |
| 25  | 7     | 503 | BCR  | C10-C11-C12-C13 |
| 25  | 7     | 503 | BCR  | C23-C24-C25-C26 |
| 25  | 7     | 503 | BCR  | C23-C24-C25-C30 |
| 25  | 7     | 504 | BCR  | C11-C10-C9-C8   |
| 25  | 7     | 504 | BCR  | C11-C10-C9-C34  |
| 25  | 7     | 504 | BCR  | C9-C10-C11-C12  |
| 25  | 7     | 504 | BCR  | C10-C11-C12-C13 |
| 25  | 8     | 503 | BCR  | C5-C6-C7-C8     |
| 25  | 8     | 503 | BCR  | C7-C8-C9-C34    |
| 25  | 8     | 503 | BCR  | C11-C10-C9-C8   |
| 25  | 8     | 503 | BCR  | C11-C10-C9-C34  |
| 25  | 8     | 503 | BCR  | C10-C11-C12-C13 |
| 25  | 4     | 503 | BCR  | C11-C10-C9-C8   |
| 25  | 4     | 503 | BCR  | C11-C10-C9-C34  |
| 25  | 4     | 503 | BCR  | C10-C11-C12-C13 |
| 25  | 4     | 503 | BCR  | C21-C22-C23-C24 |
| 25  | 4     | 503 | BCR  | C37-C22-C23-C24 |
| 25  | 4     | 503 | BCR  | C23-C24-C25-C26 |
| 25  | 4     | 503 | BCR  | C23-C24-C25-C30 |
| 25  | 5     | 503 | BCR  | C11-C10-C9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | 5     | 503  | BCR  | C11-C10-C9-C34  |
| 25  | 5     | 503  | BCR  | C9-C10-C11-C12  |
| 25  | 5     | 503  | BCR  | C10-C11-C12-C13 |
| 25  | 5     | 503  | BCR  | C23-C24-C25-C26 |
| 25  | 5     | 504  | BCR  | C10-C11-C12-C13 |
| 25  | 6     | 504  | BCR  | C7-C8-C9-C10    |
| 25  | 6     | 504  | BCR  | C9-C10-C11-C12  |
| 25  | 6     | 504  | BCR  | C11-C12-C13-C14 |
| 25  | 6     | 504  | BCR  | C11-C12-C13-C35 |
| 25  | 6     | 503  | BCR  | C7-C8-C9-C10    |
| 25  | 6     | 503  | BCR  | C11-C10-C9-C8   |
| 25  | 6     | 503  | BCR  | C11-C10-C9-C34  |
| 25  | 6     | 503  | BCR  | C10-C11-C12-C13 |
| 26  | A     | 5001 | LHG  | C4-O6-P-O3      |
| 26  | A     | 5001 | LHG  | C4-O6-P-O4      |
| 26  | A     | 5001 | LHG  | C4-O6-P-O5      |
| 26  | A     | 5001 | LHG  | O6-C4-C5-O7     |
| 26  | A     | 5002 | LHG  | C3-O3-P-O4      |
| 26  | A     | 5002 | LHG  | C3-O3-P-O6      |
| 26  | A     | 5002 | LHG  | C4-O6-P-O3      |
| 26  | A     | 5002 | LHG  | C4-O6-P-O4      |
| 26  | B     | 5001 | LHG  | C4-O6-P-O3      |
| 26  | B     | 5001 | LHG  | C4-O6-P-O4      |
| 26  | B     | 5001 | LHG  | C4-O6-P-O5      |
| 26  | B     | 5001 | LHG  | O9-C7-O7-C5     |
| 26  | B     | 5001 | LHG  | C8-C7-O7-C5     |
| 26  | B     | 5002 | LHG  | C3-O3-P-O5      |
| 26  | B     | 5002 | LHG  | C3-O3-P-O6      |
| 26  | B     | 5002 | LHG  | O9-C7-O7-C5     |
| 26  | B     | 5006 | LHG  | C1-C2-C3-O3     |
| 26  | B     | 5006 | LHG  | C3-O3-P-O5      |
| 26  | B     | 5006 | LHG  | C4-O6-P-O3      |
| 26  | B     | 5006 | LHG  | C4-O6-P-O4      |
| 26  | B     | 5006 | LHG  | O9-C7-O7-C5     |
| 26  | 1     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 1     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 1     | 801  | LHG  | C4-O6-P-O3      |
| 26  | Z     | 801  | LHG  | C1-C2-C3-O3     |
| 26  | Z     | 801  | LHG  | C4-O6-P-O3      |
| 26  | Z     | 801  | LHG  | C4-O6-P-O5      |
| 26  | Z     | 801  | LHG  | C8-C7-O7-C5     |
| 26  | 3     | 801  | LHG  | C1-C2-C3-O3     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | 3     | 801  | LHG  | C4-O6-P-O5      |
| 26  | 3     | 801  | LHG  | O9-C7-O7-C5     |
| 26  | 7     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 7     | 801  | LHG  | C4-O6-P-O3      |
| 26  | 7     | 801  | LHG  | C4-O6-P-O4      |
| 26  | 8     | 801  | LHG  | C1-C2-C3-O3     |
| 26  | 8     | 801  | LHG  | C4-O6-P-O3      |
| 26  | 8     | 801  | LHG  | C4-O6-P-O4      |
| 26  | 4     | 801  | LHG  | O2-C2-C3-O3     |
| 26  | 4     | 801  | LHG  | C4-O6-P-O5      |
| 26  | 4     | 801  | LHG  | C8-C7-O7-C5     |
| 26  | 4     | 802  | LHG  | O1-C1-C2-C3     |
| 26  | 4     | 802  | LHG  | C1-C2-C3-O3     |
| 26  | 4     | 802  | LHG  | C3-O3-P-O4      |
| 26  | 4     | 802  | LHG  | C3-O3-P-O5      |
| 26  | 4     | 802  | LHG  | C3-O3-P-O6      |
| 26  | 4     | 802  | LHG  | C4-O6-P-O3      |
| 26  | 4     | 802  | LHG  | C4-O6-P-O4      |
| 26  | 4     | 802  | LHG  | C4-O6-P-O5      |
| 26  | 4     | 802  | LHG  | O7-C5-C6-O8     |
| 26  | 5     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 5     | 801  | LHG  | C1-C2-C3-O3     |
| 26  | 5     | 801  | LHG  | O2-C2-C3-O3     |
| 26  | 5     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 5     | 801  | LHG  | C4-O6-P-O3      |
| 26  | 5     | 801  | LHG  | C4-O6-P-O4      |
| 26  | 5     | 801  | LHG  | C4-O6-P-O5      |
| 26  | 5     | 801  | LHG  | O7-C5-C6-O8     |
| 26  | 6     | 801  | LHG  | C1-C2-C3-O3     |
| 26  | 6     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 6     | 801  | LHG  | C3-O3-P-O6      |
| 26  | 6     | 801  | LHG  | C4-O6-P-O5      |
| 26  | 6     | 801  | LHG  | O6-C4-C5-O7     |
| 26  | 6     | 801  | LHG  | C8-C7-O7-C5     |
| 26  | 2     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 9     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 9     | 801  | LHG  | C1-C2-C3-O3     |
| 26  | 9     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 9     | 801  | LHG  | C3-O3-P-O6      |
| 27  | A     | 5004 | NKP  | CAG-CAH-CAI-OAJ |
| 27  | 3     | 802  | NKP  | OAF-CAG-CAH-CAI |
| 27  | 8     | 802  | NKP  | CAG-OAF-PAC-OAA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 27  | 8     | 802  | NKP  | CAG-OAF-PAC-OAB |
| 27  | 8     | 802  | NKP  | OAF-CAG-CAH-CAI |
| 27  | 8     | 802  | NKP  | OBC-CAH-CAI-OAJ |
| 28  | B     | 5005 | LMT  | C2-C1-O1'-C1'   |
| 28  | F     | 5001 | LMT  | C2-C1-O1'-C1'   |
| 28  | 9     | 803  | LMT  | O5'-C1'-O1'-C1  |
| 31  | A     | 5003 | LMG  | C2-C1-O1-C7     |
| 31  | A     | 5003 | LMG  | O6-C1-O1-C7     |
| 31  | J     | 5001 | LMG  | C11-C10-O7-C8   |
| 32  | A     | 5005 | DGA  | CG1-CG2-CG3-OXT |
| 32  | A     | 5005 | DGA  | OG2-CG2-CG3-OXT |
| 32  | 9     | 802  | DGA  | CG1-CG2-CG3-OXT |
| 32  | 9     | 802  | DGA  | OG2-CG2-CG3-OXT |
| 33  | B     | 5003 | DGD  | O1B-C1B-O2G-C2G |
| 37  | J     | 4002 | C7Z  | C31-C32-C33-C40 |
| 37  | 5     | 505  | C7Z  | C11-C12-C13-C20 |
| 37  | 5     | 505  | C7Z  | C11-C12-C13-C14 |
| 37  | 5     | 505  | C7Z  | C27-C28-C29-C30 |
| 37  | 5     | 505  | C7Z  | C27-C28-C29-C39 |
| 38  | K     | 5001 | SPH  | C1-C2-C3-O3     |
| 38  | K     | 5001 | SPH  | C1-C2-C3-C4     |
| 38  | K     | 5001 | SPH  | N2-C2-C3-O3     |
| 38  | K     | 5001 | SPH  | N2-C2-C3-C4     |
| 38  | 7     | 803  | SPH  | C1-C2-C3-O3     |
| 38  | 7     | 803  | SPH  | C1-C2-C3-C4     |
| 38  | 7     | 803  | SPH  | N2-C2-C3-O3     |
| 38  | 7     | 803  | SPH  | N2-C2-C3-C4     |
| 38  | 7     | 803  | SPH  | C2-C3-C4-C5     |
| 38  | 7     | 803  | SPH  | O3-C3-C4-C5     |
| 39  | Z     | 503  | LUT  | C5-C6-C7-C8     |
| 39  | Z     | 503  | LUT  | C25-C26-C27-C28 |
| 39  | 7     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | 8     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | 4     | 501  | LUT  | C25-C26-C27-C28 |
| 39  | 4     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | 5     | 501  | LUT  | C21-C26-C27-C28 |
| 39  | 5     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | 6     | 501  | LUT  | C25-C26-C27-C28 |
| 39  | 6     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | 2     | 501  | LUT  | C21-C26-C27-C28 |
| 39  | 2     | 502  | LUT  | C7-C8-C9-C10    |
| 39  | 2     | 502  | LUT  | C25-C26-C27-C28 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 39  | 2     | 503  | LUT  | C7-C8-C9-C10    |
| 39  | 2     | 503  | LUT  | C7-C8-C9-C19    |
| 39  | 2     | 503  | LUT  | C21-C26-C27-C28 |
| 39  | 2     | 503  | LUT  | C25-C26-C27-C28 |
| 39  | 9     | 502  | LUT  | C25-C26-C27-C28 |
| 40  | 1     | 610  | CHL  | C4C-C3C-CAC-CBC |
| 40  | Z     | 613  | CHL  | C1A-C2A-CAA-CBA |
| 40  | 8     | 613  | CHL  | C1A-C2A-CAA-CBA |
| 40  | 4     | 613  | CHL  | C1A-C2A-CAA-CBA |
| 40  | 5     | 617  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 5     | 617  | CHL  | CHA-CBD-CGD-O2D |
| 40  | 6     | 611  | CHL  | C3A-C2A-CAA-CBA |
| 40  | 2     | 613  | CHL  | C3A-C2A-CAA-CBA |
| 41  | 1     | 802  | SQD  | C8-C7-O47-C45   |
| 41  | 2     | 803  | SQD  | C5-C6-S-O7      |
| 41  | 2     | 803  | SQD  | C5-C6-S-O9      |
| 42  | Z     | 504  | QTB  | C03-C02-C09-C10 |
| 43  | 8     | 806  | 3PH  | C1-O11-P-O13    |
| 43  | 8     | 806  | 3PH  | C1-O11-P-O14    |
| 43  | 8     | 806  | 3PH  | C1-O11-P-O12    |
| 43  | 8     | 806  | 3PH  | O22-C21-O21-C2  |
| 43  | 8     | 806  | 3PH  | C22-C21-O21-C2  |
| 43  | 5     | 802  | 3PH  | O11-C1-C2-O21   |
| 43  | 5     | 802  | 3PH  | O22-C21-O21-C2  |
| 43  | 5     | 802  | 3PH  | C22-C21-O21-C2  |
| 43  | 6     | 802  | 3PH  | O22-C21-O21-C2  |
| 43  | 6     | 802  | 3PH  | C22-C21-O21-C2  |
| 43  | 2     | 802  | 3PH  | C1-O11-P-O13    |
| 43  | 2     | 802  | 3PH  | C1-O11-P-O14    |
| 43  | 2     | 802  | 3PH  | C1-O11-P-O12    |
| 43  | 2     | 802  | 3PH  | O32-C31-O31-C3  |
| 45  | 8     | 803  | LPX  | O1-C3-C4-O5     |
| 45  | 8     | 803  | LPX  | C3-O1-P1-O3     |
| 45  | 8     | 803  | LPX  | C3-O1-P1-O2     |
| 45  | 8     | 803  | LPX  | C1-O2-P1-O1     |
| 45  | 8     | 803  | LPX  | C1-O2-P1-O3     |
| 45  | 8     | 803  | LPX  | C1-O2-P1-O4     |
| 22  | A     | 1138 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1140 | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 1402 | CLA  | O1D-CGD-O2D-CED |
| 22  | L     | 1503 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 603  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 5     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1021 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1023 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 619  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1109 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1115 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1119 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1126 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1131 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1138 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1141 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1203 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1205 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1206 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1216 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1218 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1232 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1236 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1239 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1241 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 1402 | CLA  | CBD-CGD-O2D-CED |
| 22  | L     | 1503 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 611  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 612  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 602  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 607  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 611  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 612  | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 618  | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 605  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 7     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 611  | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 615  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 602  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 615  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 609  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 615  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 602  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 612  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 618  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 607  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 602  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 605  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 609  | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1113 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1133 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1207 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1222 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 615  | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 1401 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 615  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 615  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 615  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 609  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1126 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1232 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 611  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1113 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 612  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 1502 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 603  | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1104 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1114 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1101 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1202 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1206 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1218 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1220 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1228 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1240 | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 1404 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 27  | A     | 5004 | NKP  | OAE-CAK-OAJ-CAI |
| 27  | 3     | 802  | NKP  | OAE-CAK-OAJ-CAI |
| 31  | A     | 5003 | LMG  | O10-C28-O8-C9   |
| 41  | 1     | 802  | SQD  | O10-C23-O48-C46 |
| 41  | 2     | 803  | SQD  | O10-C23-O48-C46 |
| 43  | 7     | 802  | 3PH  | O32-C31-O31-C3  |
| 43  | 8     | 806  | 3PH  | O32-C31-O31-C3  |
| 22  | G     | 1602 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 613  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1114 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1123 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1132 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1141 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1201 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1207 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1213 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1217 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1241 | CLA  | O1D-CGD-O2D-CED |
| 22  | F     | 1302 | CLA  | O1D-CGD-O2D-CED |
| 22  | J     | 1901 | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 1403 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 611  | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 613  | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 616  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 616  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 611  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 622  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1012 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1116 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1022 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1214 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1224 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1226 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1234 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 605  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 3     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 613  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 613  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1139 | CLA  | CBD-CGD-O2D-CED |
| 26  | 1     | 801  | LHG  | O9-C7-O7-C5     |
| 26  | 6     | 801  | LHG  | O9-C7-O7-C5     |
| 31  | J     | 5001 | LMG  | O9-C10-O7-C8    |
| 41  | 1     | 802  | SQD  | O49-C7-O47-C45  |
| 43  | 7     | 802  | 3PH  | O22-C21-O21-C2  |
| 22  | 1     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1115 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1118 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1124 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1126 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1131 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1136 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1237 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1215 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1224 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1226 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1240 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1241 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 605  | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 611  | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 605  | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 607  | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 608  | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 607  | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 610  | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 616  | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 605  | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 606  | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 615  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 7     | 616  | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 605  | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 607  | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 608  | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 603  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1121 | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 1404 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 613  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1104 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1130 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1133 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1139 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1101 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1202 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1207 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1218 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1222 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1227 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1228 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1240 | CLA  | CBA-CGA-O2A-C1  |
| 22  | K     | 1404 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 615  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 603  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 613  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 612  | CLA  | CBA-CGA-O2A-C1  |
| 27  | A     | 5004 | NKP  | CAL-CAK-OAJ-CAI |
| 31  | A     | 5003 | LMG  | C29-C28-O8-C9   |
| 41  | 2     | 803  | SQD  | C24-C23-O48-C46 |
| 43  | 7     | 802  | 3PH  | C32-C31-O31-C3  |
| 43  | 2     | 802  | 3PH  | C32-C31-O31-C3  |
| 22  | A     | 1105 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1107 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1113 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1129 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1133 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1136 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1137 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1237 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1212 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1223 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1228 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1229 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1230 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1231 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1235 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1238 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 1602 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 1401 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 604  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 607  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 604  | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 607  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 609  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 604  | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 615  | CLA  | CBD-CGD-O2D-CED |
| 26  | B     | 5006 | LHG  | C8-C7-O7-C5     |
| 26  | 1     | 801  | LHG  | C8-C7-O7-C5     |
| 33  | B     | 5003 | DGD  | C2B-C1B-O2G-C2G |
| 43  | 7     | 802  | 3PH  | C22-C21-O21-C2  |
| 22  | A     | 1115 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1128 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1131 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1203 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1208 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1219 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 1601 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 618  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 611  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | F     | 1301 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 618  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 618  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 9     | 609  | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1211 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 609  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1012 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1122 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1226 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1240 | CLA  | C4-C3-C5-C6     |
| 22  | 8     | 601  | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1012 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1136 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1226 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1235 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1240 | CLA  | C2-C3-C5-C6     |
| 22  | 8     | 601  | CLA  | C2-C3-C5-C6     |
| 22  | 5     | 601  | CLA  | C2-C3-C5-C6     |
| 22  | 3     | 618  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1130 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1215 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 602  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 609  | CLA  | O1D-CGD-O2D-CED |
| 28  | B     | 5005 | LMT  | O5'-C5'-C6'-O6' |
| 22  | A     | 1121 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 602  | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 603  | CLA  | C2A-CAA-CBA-CGA |
| 40  | 1     | 610  | CHL  | C2A-CAA-CBA-CGA |
| 40  | 4     | 610  | CHL  | C2A-CAA-CBA-CGA |
| 22  | A     | 1123 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1127 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1134 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1140 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1206 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1236 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 607  | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 607  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 5     | 609  | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1239 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1111 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1114 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1119 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1123 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1124 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1128 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1129 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1237 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1203 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1206 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1216 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1220 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1230 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1231 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 27  | 3     | 802  | NKP  | CAL-CAK-OAJ-CAI |
| 32  | A     | 5005 | DGA  | CA2-CA1-OG1-CG1 |
| 41  | 1     | 802  | SQD  | C24-C23-O48-C46 |
| 43  | 8     | 806  | 3PH  | C32-C31-O31-C3  |
| 25  | K     | 4001 | BCR  | C19-C20-C21-C22 |
| 25  | 3     | 505  | BCR  | C9-C10-C11-C12  |
| 25  | 8     | 503  | BCR  | C13-C14-C15-C16 |
| 25  | 6     | 504  | BCR  | C13-C14-C15-C16 |
| 25  | 6     | 503  | BCR  | C9-C10-C11-C12  |
| 36  | F     | 4001 | RRX  | C19-C20-C21-C22 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 37  | J     | 4002 | C7Z  | C9-C10-C11-C12  |
| 37  | 5     | 505  | C7Z  | C13-C14-C15-C35 |
| 39  | 2     | 501  | LUT  | C29-C30-C31-C32 |
| 22  | A     | 1119 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1126 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1129 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1130 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1139 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1237 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1203 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1227 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 603  | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 608  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 32  | A     | 5005 | DGA  | OA1-CA1-OG1-CG1 |
| 26  | Z     | 801  | LHG  | O9-C7-O7-C5     |
| 26  | 4     | 801  | LHG  | O9-C7-O7-C5     |
| 22  | 2     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 33  | B     | 5003 | DGD  | CBA-CCA-CDA-CEA |
| 22  | A     | 1119 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1216 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1218 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 605  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1120 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1204 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1209 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1228 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1229 | CLA  | C3-C5-C6-C7     |
| 22  | L     | 1502 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 604  | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 601  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1106 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1209 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 606  | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 608  | CLA  | CBD-CGD-O2D-CED |
| 33  | B     | 5003 | DGD  | C8A-C9A-CAA-CBA |
| 26  | A     | 5001 | LHG  | O2-C2-C3-O3     |
| 26  | Z     | 801  | LHG  | O2-C2-C3-O3     |
| 26  | 8     | 801  | LHG  | O2-C2-C3-O3     |
| 26  | 2     | 801  | LHG  | O2-C2-C3-O3     |
| 26  | 9     | 801  | LHG  | O2-C2-C3-O3     |
| 27  | 3     | 802  | NKP  | OAF-CAG-CAH-OBC |
| 22  | A     | 1109 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1206 | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1117 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1121 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1126 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1137 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1215 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1236 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 613  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 611  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 608  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 28  | 4     | 803  | LMT  | O5'-C5'-C6'-O6' |
| 22  | A     | 1111 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1128 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 613  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 28  | 9     | 803  | LMT  | C4B-C5B-C6B-O6B |
| 22  | B     | 1205 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 618  | CLA  | O1D-CGD-O2D-CED |
| 28  | 1     | 803  | LMT  | O5B-C5B-C6B-O6B |
| 28  | 8     | 805  | LMT  | O5'-C5'-C6'-O6' |
| 22  | A     | 1124 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 622  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1137 | CLA  | O1A-CGA-O2A-C1  |
| 28  | B     | 5005 | LMT  | C4'-C5'-C6'-O6' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 6     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 612  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1103 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1202 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1240 | CLA  | CBD-CGD-O2D-CED |
| 22  | F     | 1301 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1236 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1210 | CLA  | CBA-CGA-O2A-C1  |
| 22  | F     | 1301 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 608  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 618  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 612  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1115 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1115 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1122 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1121 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1124 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1215 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1230 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 613  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 611  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 28  | A     | 5006 | LMT  | O5'-C5'-C6'-O6' |
| 28  | 9     | 803  | LMT  | O5B-C5B-C6B-O6B |
| 22  | A     | 1133 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1207 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1133 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 603  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1117 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1210 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1216 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1231 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1236 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 28  | A     | 5006 | LMT  | O5'-C1'-O1'-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 41  | 2     | 803  | SQD  | O5-C1-O6-C44    |
| 22  | L     | 1502 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1131 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1217 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1104 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1110 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1117 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1101 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1221 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1227 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 609  | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 607  | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 609  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 615  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 604  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 608  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1136 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1139 | CLA  | O1D-CGD-O2D-CED |
| 28  | 4     | 803  | LMT  | C4B-C5B-C6B-O6B |
| 22  | 7     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 609  | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 607  | CLA  | CBD-CGD-O2D-CED |
| 32  | 9     | 802  | DGA  | CB2-CB1-OG2-CG2 |
| 28  | 8     | 805  | LMT  | O5B-C5B-C6B-O6B |
| 25  | I     | 4001 | BCR  | C15-C16-C17-C18 |
| 22  | B     | 1217 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 7     | 801  | LHG  | C1-C2-C3-O3     |
| 22  | 4     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1106 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1108 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1116 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1120 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1211 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1214 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1219 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1224 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1229 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1239 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | K     | 1403 | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 1502 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 610  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 609  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 612  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 32  | 9     | 802  | DGA  | CA2-CA1-OG1-CG1 |
| 26  | 5     | 801  | LHG  | C28-C29-C30-C31 |
| 28  | 8     | 805  | LMT  | C4B-C5B-C6B-O6B |
| 22  | A     | 1105 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1137 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1237 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1229 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 604  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 604  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1104 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1217 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1218 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 611  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1013 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1104 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1110 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1121 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1209 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1215 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 611  | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 604  | CLA  | C14-C13-C15-C16 |
| 22  | 8     | 605  | CLA  | C14-C13-C15-C16 |
| 22  | 5     | 609  | CLA  | C11-C10-C8-C9   |
| 22  | 9     | 603  | CLA  | C6-C7-C8-C9     |
| 40  | Z     | 610  | CHL  | C11-C12-C13-C14 |
| 40  | Z     | 609  | CHL  | C14-C13-C15-C16 |
| 28  | 4     | 803  | LMT  | C4'-C5'-C6'-O6' |
| 22  | B     | 1212 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1228 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 1602 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 604  | CLA  | O1D-CGD-O2D-CED |
| 28  | A     | 5006 | LMT  | C2'-C1'-O1'-C1  |
| 41  | 2     | 803  | SQD  | C2-C1-O6-C44    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | A     | 5002 | LHG  | C7-C8-C9-C10    |
| 26  | 4     | 801  | LHG  | C7-C8-C9-C10    |
| 26  | B     | 5006 | LHG  | O2-C2-C3-O3     |
| 26  | 7     | 801  | LHG  | O2-C2-C3-O3     |
| 26  | 6     | 801  | LHG  | O2-C2-C3-O3     |
| 27  | 8     | 802  | NKP  | OAF-CAG-CAH-OBC |
| 22  | B     | 1231 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1120 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1214 | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 1403 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1112 | CLA  | CBD-CGD-O2D-CED |
| 25  | A     | 4005 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 4001 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 4002 | BCR  | C36-C18-C19-C20 |
| 25  | B     | 4004 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 4005 | BCR  | C11-C12-C13-C35 |
| 25  | B     | 4006 | BCR  | C11-C12-C13-C35 |
| 25  | G     | 4001 | BCR  | C7-C8-C9-C34    |
| 25  | I     | 4001 | BCR  | C7-C8-C9-C34    |
| 25  | I     | 4001 | BCR  | C36-C18-C19-C20 |
| 25  | J     | 4001 | BCR  | C11-C12-C13-C35 |
| 25  | J     | 4001 | BCR  | C36-C18-C19-C20 |
| 25  | L     | 4001 | BCR  | C7-C8-C9-C34    |
| 25  | L     | 4001 | BCR  | C37-C22-C23-C24 |
| 25  | 3     | 504  | BCR  | C7-C8-C9-C34    |
| 25  | 3     | 506  | BCR  | C37-C22-C23-C24 |
| 25  | 7     | 504  | BCR  | C7-C8-C9-C34    |
| 25  | 7     | 504  | BCR  | C37-C22-C23-C24 |
| 25  | 5     | 503  | BCR  | C37-C22-C23-C24 |
| 25  | 6     | 504  | BCR  | C7-C8-C9-C34    |
| 25  | 6     | 503  | BCR  | C7-C8-C9-C34    |
| 36  | F     | 4001 | RRX  | C36-C18-C19-C20 |
| 37  | J     | 4002 | C7Z  | C7-C8-C9-C19    |
| 37  | J     | 4002 | C7Z  | C27-C28-C29-C39 |
| 39  | Z     | 503  | LUT  | C27-C28-C29-C39 |
| 39  | 2     | 501  | LUT  | C27-C28-C29-C39 |
| 39  | 2     | 502  | LUT  | C7-C8-C9-C19    |
| 42  | Z     | 504  | QTB  | C01-C02-C09-C10 |
| 25  | A     | 4004 | BCR  | C21-C22-C23-C24 |
| 25  | A     | 4005 | BCR  | C17-C18-C19-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 4002 | BCR  | C7-C8-C9-C10    |
| 25  | B     | 4006 | BCR  | C11-C12-C13-C14 |
| 25  | I     | 4001 | BCR  | C7-C8-C9-C10    |
| 25  | K     | 4001 | BCR  | C7-C8-C9-C10    |
| 25  | L     | 4001 | BCR  | C21-C22-C23-C24 |
| 25  | 7     | 504  | BCR  | C7-C8-C9-C10    |
| 25  | 7     | 504  | BCR  | C21-C22-C23-C24 |
| 25  | 8     | 503  | BCR  | C7-C8-C9-C10    |
| 25  | 5     | 503  | BCR  | C21-C22-C23-C24 |
| 36  | F     | 4001 | RRX  | C17-C18-C19-C20 |
| 37  | J     | 4002 | C7Z  | C7-C8-C9-C10    |
| 37  | J     | 4002 | C7Z  | C11-C12-C13-C14 |
| 37  | J     | 4002 | C7Z  | C31-C32-C33-C34 |
| 37  | J     | 4002 | C7Z  | C27-C28-C29-C30 |
| 39  | 2     | 501  | LUT  | C27-C28-C29-C30 |
| 22  | B     | 1228 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1240 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 8     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1113 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1106 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1108 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1211 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1219 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1229 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1239 | CLA  | O1A-CGA-O2A-C1  |
| 22  | L     | 1502 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 28  | 8     | 805  | LMT  | C4'-C5'-C6'-O6' |
| 26  | 4     | 801  | LHG  | O6-C4-C5-O7     |
| 22  | 5     | 618  | CLA  | CBD-CGD-O2D-CED |
| 26  | 2     | 801  | LHG  | C8-C7-O7-C5     |
| 32  | 9     | 802  | DGA  | OG1-CG1-CG2-OG2 |
| 22  | 3     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 607  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 616  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1125 | CLA  | C8-C10-C11-C12  |
| 22  | 3     | 610  | CLA  | C5-C6-C7-C8     |
| 22  | 8     | 609  | CLA  | C15-C16-C17-C18 |
| 21  | A     | 1011 | CL0  | C2-C1-O2A-CGA   |
| 22  | A     | 1012 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1112 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1114 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1122 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1126 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1128 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1130 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1205 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1216 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1226 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1227 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1230 | CLA  | C2-C1-O2A-CGA   |
| 22  | G     | 1601 | CLA  | C2-C1-O2A-CGA   |
| 22  | K     | 1403 | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 605  | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 601  | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 601  | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 602  | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 615  | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 609  | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 602  | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 608  | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 601  | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 603  | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 2     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | 2     | 612  | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 601  | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1107 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1223 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1235 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1238 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 609  | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 615  | CLA  | O1D-CGD-O2D-CED |
| 21  | A     | 1011 | CL0  | C5-C6-C7-C8     |
| 22  | B     | 1203 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1210 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 3     | 603  | CLA  | C13-C15-C16-C17 |
| 22  | 3     | 612  | CLA  | C8-C10-C11-C12  |
| 22  | 8     | 606  | CLA  | C8-C10-C11-C12  |
| 40  | Z     | 609  | CHL  | C5-C6-C7-C8     |
| 22  | Z     | 606  | CLA  | C3-C5-C6-C7     |
| 22  | K     | 1401 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 610  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 612  | CLA  | CBD-CGD-O2D-CED |
| 28  | 4     | 803  | LMT  | O5B-C5B-C6B-O6B |
| 28  | 1     | 803  | LMT  | C4B-C5B-C6B-O6B |
| 22  | A     | 1124 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 607  | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1023 | CLA  | CBA-CGA-O2A-C1  |
| 28  | 4     | 803  | LMT  | O1'-C1-C2-C3    |
| 22  | B     | 1236 | CLA  | C4-C3-C5-C6     |
| 22  | 3     | 603  | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1129 | CLA  | O1D-CGD-O2D-CED |
| 26  | A     | 5002 | LHG  | C23-C24-C25-C26 |
| 26  | 7     | 801  | LHG  | C7-C8-C9-C10    |
| 43  | 8     | 806  | 3PH  | C31-C32-C33-C34 |
| 25  | B     | 4007 | BCR  | C13-C14-C15-C16 |
| 25  | 3     | 504  | BCR  | C9-C10-C11-C12  |
| 25  | 7     | 503  | BCR  | C9-C10-C11-C12  |
| 25  | 7     | 504  | BCR  | C13-C14-C15-C16 |
| 37  | 1     | 503  | C7Z  | C29-C30-C31-C32 |
| 39  | Z     | 503  | LUT  | C29-C30-C31-C32 |
| 22  | 5     | 622  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1130 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1230 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 606  | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 603  | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1213 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1224 | CLA  | C13-C15-C16-C17 |
| 22  | 6     | 609  | CLA  | C8-C10-C11-C12  |
| 22  | 9     | 603  | CLA  | C5-C6-C7-C8     |
| 40  | Z     | 609  | CHL  | C13-C15-C16-C17 |
| 26  | 6     | 801  | LHG  | C23-C24-C25-C26 |
| 26  | 9     | 801  | LHG  | C7-C8-C9-C10    |
| 35  | B     | 5004 | T7X  | C10-C12-C13-C14 |
| 35  | B     | 5004 | T7X  | C11-C31-C32-C33 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 1     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 607  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1134 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1104 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1110 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1117 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1136 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1021 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1204 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1207 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1213 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1222 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1231 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1241 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 611  | CLA  | C15-C16-C17-C18 |
| 22  | 1     | 612  | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 607  | CLA  | C10-C11-C12-C13 |
| 22  | 7     | 603  | CLA  | C15-C16-C17-C18 |
| 22  | 2     | 603  | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1105 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1106 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1111 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1119 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1120 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1122 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1127 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1131 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1141 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1206 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1211 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1214 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1226 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1238 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1239 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Z     | 607  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 8     | 609  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 8     | 612  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 615  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 2     | 601  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 2     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 2     | 607  | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 40  | 8     | 613  | CHL  | C2A-CAA-CBA-CGA |
| 40  | 9     | 610  | CHL  | C2A-CAA-CBA-CGA |
| 22  | B     | 1209 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1106 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1107 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1116 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1118 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1119 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1131 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1205 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1209 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1220 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1229 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1236 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1239 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1241 | CLA  | C10-C11-C12-C13 |
| 22  | F     | 1301 | CLA  | C10-C11-C12-C13 |
| 22  | Z     | 604  | CLA  | C10-C11-C12-C13 |
| 22  | 3     | 601  | CLA  | C13-C15-C16-C17 |
| 22  | 3     | 601  | CLA  | C15-C16-C17-C18 |
| 22  | 8     | 601  | CLA  | C10-C11-C12-C13 |
| 22  | 6     | 609  | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 619  | CLA  | C8-C10-C11-C12  |
| 26  | 2     | 801  | LHG  | C7-C8-C9-C10    |
| 26  | 9     | 801  | LHG  | C23-C24-C25-C26 |
| 22  | B     | 1215 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 608  | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1224 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 609  | CLA  | O1A-CGA-O2A-C1  |
| 32  | 9     | 802  | DGA  | OA1-CA1-OG1-CG1 |
| 22  | 1     | 615  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1012 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1107 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1109 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1113 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1120 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1122 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1124 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1127 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1128 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1128 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1130 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1101 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1210 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1216 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1216 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1218 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1230 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1241 | CLA  | C15-C16-C17-C18 |
| 22  | 1     | 601  | CLA  | C15-C16-C17-C18 |
| 22  | 1     | 612  | CLA  | C13-C15-C16-C17 |
| 22  | 1     | 615  | CLA  | C15-C16-C17-C18 |
| 22  | Z     | 605  | CLA  | C8-C10-C11-C12  |
| 22  | Z     | 611  | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 610  | CLA  | C10-C11-C12-C13 |
| 22  | 7     | 615  | CLA  | C5-C6-C7-C8     |
| 22  | 8     | 605  | CLA  | C13-C15-C16-C17 |
| 22  | 9     | 601  | CLA  | C10-C11-C12-C13 |
| 26  | A     | 5002 | LHG  | C28-C29-C30-C31 |
| 26  | B     | 5002 | LHG  | O2-C2-C3-O3     |
| 26  | 3     | 801  | LHG  | O2-C2-C3-O3     |
| 22  | 1     | 608  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 601  | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 607  | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1116 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1131 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 4     | 801  | LHG  | C23-C24-C25-C26 |
| 26  | 5     | 801  | LHG  | C23-C24-C25-C26 |
| 27  | 8     | 802  | NKP  | CAK-CAL-CAM-CAN |
| 22  | A     | 1109 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1111 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1138 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1013 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1240 | CLA  | C10-C11-C12-C13 |
| 22  | K     | 1404 | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 605  | CLA  | C15-C16-C17-C18 |
| 22  | 4     | 601  | CLA  | C8-C10-C11-C12  |
| 26  | 2     | 801  | LHG  | O9-C7-O7-C5     |
| 32  | 9     | 802  | DGA  | OB1-CB1-OG2-CG2 |
| 22  | F     | 1301 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1111 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 606  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1101 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1203 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1236 | CLA  | C13-C15-C16-C17 |
| 22  | F     | 1301 | CLA  | C5-C6-C7-C8     |
| 22  | Z     | 612  | CLA  | C10-C11-C12-C13 |
| 22  | 7     | 607  | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 606  | CLA  | C5-C6-C7-C8     |
| 23  | A     | 2001 | PQN  | C25-C26-C27-C28 |
| 22  | 3     | 616  | CLA  | O1A-CGA-O2A-C1  |
| 28  | 1     | 803  | LMT  | O1'-C1-C2-C3    |
| 22  | A     | 1106 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1124 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1133 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1203 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1224 | CLA  | C15-C16-C17-C18 |
| 22  | 7     | 616  | CLA  | C8-C10-C11-C12  |
| 22  | 4     | 605  | CLA  | C15-C16-C17-C18 |
| 22  | 5     | 609  | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 601  | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 619  | CLA  | C10-C11-C12-C13 |
| 40  | Z     | 610  | CHL  | C13-C15-C16-C17 |
| 22  | B     | 1212 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 608  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 27  | 8     | 802  | NKP  | CAL-CAK-OAJ-CAI |
| 31  | A     | 5003 | LMG  | C11-C10-O7-C8   |
| 22  | 3     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 618  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 605  | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 603  | CLA  | C3-C5-C6-C7     |
| 40  | 1     | 609  | CHL  | C8-C10-C11-C12  |
| 25  | A     | 4005 | BCR  | C19-C20-C21-C22 |
| 25  | B     | 4005 | BCR  | C19-C20-C21-C22 |
| 25  | 3     | 503  | BCR  | C13-C14-C15-C16 |
| 25  | 3     | 506  | BCR  | C9-C10-C11-C12  |
| 25  | 5     | 504  | BCR  | C9-C10-C11-C12  |
| 42  | Z     | 504  | QTB  | C02-C03-C04-C05 |
| 22  | B     | 1231 | CLA  | C15-C16-C17-C18 |
| 22  | Z     | 612  | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 607  | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | B     | 5002 | LHG  | C24-C23-O8-C6   |
| 31  | A     | 5003 | LMG  | O9-C10-O7-C8    |
| 26  | A     | 5001 | LHG  | C1-C2-C3-O3     |
| 26  | B     | 5002 | LHG  | C1-C2-C3-O3     |
| 26  | 4     | 801  | LHG  | C1-C2-C3-O3     |
| 45  | 8     | 803  | LPX  | O1-C3-C4-C5     |
| 22  | B     | 1241 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 615  | CLA  | C2A-CAA-CBA-CGA |
| 40  | 6     | 611  | CHL  | C2A-CAA-CBA-CGA |
| 22  | A     | 1112 | CLA  | CBA-CGA-O2A-C1  |
| 22  | K     | 1402 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1012 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1111 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1112 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1121 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1125 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1132 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1136 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1207 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1210 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1215 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1217 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1221 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1228 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 606  | CLA  | C5-C6-C7-C8     |
| 22  | Z     | 601  | CLA  | C10-C11-C12-C13 |
| 22  | 7     | 607  | CLA  | C15-C16-C17-C18 |
| 22  | K     | 1402 | CLA  | C3-C5-C6-C7     |
| 44  | 7     | 805  | PLM  | C1-C2-C3-C4     |
| 22  | B     | 1220 | CLA  | C10-C11-C12-C13 |
| 22  | 1     | 612  | CLA  | C10-C11-C12-C13 |
| 22  | Z     | 612  | CLA  | C15-C16-C17-C18 |
| 22  | 3     | 606  | CLA  | C15-C16-C17-C18 |
| 22  | 8     | 605  | CLA  | C8-C10-C11-C12  |
| 22  | 8     | 605  | CLA  | C10-C11-C12-C13 |
| 22  | 4     | 603  | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1102 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1110 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1112 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1219 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1225 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1231 | CLA  | C13-C15-C16-C17 |
| 22  | Z     | 612  | CLA  | C8-C10-C11-C12  |
| 22  | 3     | 606  | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 605  | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 616  | CLA  | C5-C6-C7-C8     |
| 22  | 4     | 601  | CLA  | C10-C11-C12-C13 |
| 22  | 6     | 619  | CLA  | C5-C6-C7-C8     |
| 22  | 2     | 601  | CLA  | C5-C6-C7-C8     |
| 22  | 9     | 604  | CLA  | C10-C11-C12-C13 |
| 22  | 1     | 611  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 608  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1128 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1216 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1229 | CLA  | C15-C16-C17-C18 |
| 22  | 7     | 601  | CLA  | C8-C10-C11-C12  |
| 22  | 8     | 601  | CLA  | C8-C10-C11-C12  |
| 22  | 5     | 602  | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 615  | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 612  | CLA  | CBD-CGD-O2D-CED |
| 40  | 9     | 610  | CHL  | C11-C12-C13-C14 |
| 22  | A     | 1103 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1124 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1226 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 615  | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1102 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1213 | CLA  | C16-C17-C18-C19 |
| 22  | 1     | 612  | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1107 | CLA  | C5-C6-C7-C8     |
| 22  | 4     | 609  | CLA  | C5-C6-C7-C8     |
| 25  | A     | 4003 | BCR  | C11-C10-C9-C34  |
| 25  | B     | 4003 | BCR  | C11-C10-C9-C34  |
| 22  | B     | 1231 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 4001 | BCR  | C36-C18-C19-C20 |
| 25  | A     | 4004 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 4005 | BCR  | C36-C18-C19-C20 |
| 25  | B     | 4007 | BCR  | C7-C8-C9-C34    |
| 25  | B     | 4006 | BCR  | C36-C18-C19-C20 |
| 25  | G     | 4001 | BCR  | C37-C22-C23-C24 |
| 25  | K     | 4002 | BCR  | C7-C8-C9-C34    |
| 25  | 4     | 503  | BCR  | C7-C8-C9-C34    |
| 25  | 4     | 503  | BCR  | C11-C12-C13-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | 5     | 504  | BCR  | C37-C22-C23-C24 |
| 25  | 6     | 504  | BCR  | C37-C22-C23-C24 |
| 25  | 6     | 503  | BCR  | C36-C18-C19-C20 |
| 26  | 7     | 801  | LHG  | C2-C3-O3-P      |
| 36  | F     | 4001 | RRX  | C37-C22-C23-C24 |
| 37  | J     | 4002 | C7Z  | C11-C12-C13-C20 |
| 37  | 1     | 503  | C7Z  | C7-C8-C9-C19    |
| 37  | 5     | 505  | C7Z  | C31-C32-C33-C40 |
| 39  | Z     | 503  | LUT  | C31-C32-C33-C40 |
| 39  | 2     | 502  | LUT  | C31-C32-C33-C40 |
| 39  | 2     | 503  | LUT  | C11-C12-C13-C20 |
| 22  | B     | 1212 | CLA  | C8-C10-C11-C12  |
| 22  | Z     | 606  | CLA  | C8-C10-C11-C12  |
| 25  | B     | 4001 | BCR  | C7-C8-C9-C10    |
| 25  | B     | 4005 | BCR  | C17-C18-C19-C20 |
| 25  | G     | 4001 | BCR  | C21-C22-C23-C24 |
| 25  | 5     | 504  | BCR  | C21-C22-C23-C24 |
| 25  | 6     | 504  | BCR  | C21-C22-C23-C24 |
| 36  | F     | 4001 | RRX  | C21-C22-C23-C24 |
| 22  | B     | 1023 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 608  | CLA  | O1A-CGA-O2A-C1  |
| 27  | 8     | 802  | NKP  | OAE-CAK-OAJ-CAI |
| 22  | A     | 1104 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1216 | CLA  | C2A-CAA-CBA-CGA |
| 22  | K     | 1404 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 610  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 612  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 8     | 602  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 4     | 608  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 612  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 9     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 9     | 608  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1108 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1238 | CLA  | C5-C6-C7-C8     |
| 22  | L     | 1502 | CLA  | C10-C11-C12-C13 |
| 22  | Z     | 604  | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 603  | CLA  | C8-C10-C11-C12  |
| 22  | 5     | 601  | CLA  | C10-C11-C12-C13 |
| 27  | A     | 5004 | NKP  | OBC-CAH-CAI-OAJ |
| 26  | A     | 5001 | LHG  | O1-C1-C2-C3     |
| 26  | B     | 5002 | LHG  | O1-C1-C2-C3     |
| 26  | Z     | 801  | LHG  | O1-C1-C2-C3     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | 3     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 8     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 4     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 6     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 2     | 801  | LHG  | O1-C1-C2-C3     |
| 26  | 2     | 801  | LHG  | C23-C24-C25-C26 |
| 32  | A     | 5005 | DGA  | CB9-CAB-CBB-CCB |
| 22  | A     | 1107 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1110 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1126 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 1133 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1236 | CLA  | C16-C17-C18-C20 |
| 22  | 1     | 612  | CLA  | C16-C17-C18-C19 |
| 22  | 3     | 607  | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 607  | CLA  | C16-C17-C18-C19 |
| 22  | 7     | 616  | CLA  | C11-C12-C13-C14 |
| 22  | 6     | 609  | CLA  | C16-C17-C18-C19 |
| 40  | 6     | 613  | CHL  | C6-C7-C8-C10    |
| 22  | A     | 1110 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1212 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1216 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 606  | CLA  | C3-C5-C6-C7     |
| 22  | 9     | 603  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1013 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1206 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 4003 | BCR  | C11-C10-C9-C8   |
| 25  | B     | 4003 | BCR  | C11-C10-C9-C8   |
| 28  | B     | 6101 | LMT  | O5'-C1'-O1'-C1  |
| 28  | 4     | 803  | LMT  | O5'-C1'-O1'-C1  |
| 41  | 1     | 802  | SQD  | O5-C1-O6-C44    |
| 26  | 5     | 801  | LHG  | C8-C7-O7-C5     |
| 22  | 2     | 601  | CLA  | C8-C10-C11-C12  |
| 28  | F     | 5001 | LMT  | O5'-C5'-C6'-O6' |
| 42  | Z     | 504  | QTB  | C04-C05-C06-C08 |
| 42  | Z     | 504  | QTB  | C04-C05-C06-O07 |
| 22  | B     | 1202 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1221 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1240 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1122 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 605  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 6     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 26  | B     | 5006 | LHG  | C7-C8-C9-C10    |
| 26  | 7     | 801  | LHG  | C23-C24-C25-C26 |
| 22  | A     | 1103 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1120 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1121 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1125 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1134 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1022 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1210 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1213 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1215 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1220 | CLA  | C2-C1-O2A-CGA   |
| 22  | L     | 1502 | CLA  | C2-C1-O2A-CGA   |
| 22  | L     | 1503 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 611  | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 607  | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 608  | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 611  | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 612  | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 603  | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 605  | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 613  | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 601  | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 609  | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 604  | CLA  | C2-C1-O2A-CGA   |
| 22  | 2     | 605  | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1102 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1115 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1133 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1134 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1223 | CLA  | C16-C17-C18-C19 |
| 22  | 4     | 604  | CLA  | C11-C12-C13-C15 |
| 22  | 5     | 613  | CLA  | C6-C7-C8-C10    |
| 40  | 8     | 610  | CHL  | C6-C7-C8-C9     |
| 40  | 8     | 610  | CHL  | C6-C7-C8-C10    |
| 40  | 6     | 613  | CHL  | C6-C7-C8-C9     |
| 22  | B     | 1227 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 6     | 615  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1124 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1126 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1216 | CLA  | C15-C16-C17-C18 |
| 22  | Z     | 604  | CLA  | C15-C16-C17-C18 |
| 26  | A     | 5001 | LHG  | C11-C10-C9-C8   |
| 32  | 9     | 802  | DGA  | CB9-CAB-CBB-CCB |
| 22  | 8     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1117 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 5002 | LHG  | C25-C26-C27-C28 |
| 26  | B     | 5002 | LHG  | O1-C1-C2-O2     |
| 26  | 1     | 801  | LHG  | O1-C1-C2-O2     |
| 26  | Z     | 801  | LHG  | O1-C1-C2-O2     |
| 26  | 8     | 801  | LHG  | O1-C1-C2-O2     |
| 26  | 4     | 801  | LHG  | O1-C1-C2-O2     |
| 26  | 5     | 801  | LHG  | O1-C1-C2-O2     |
| 26  | 2     | 801  | LHG  | O1-C1-C2-O2     |
| 28  | 8     | 805  | LMT  | C2-C1-O1'-C1'   |
| 22  | A     | 1113 | CLA  | C3-C5-C6-C7     |
| 32  | A     | 5005 | DGA  | CCA-CDA-CEA-CFA |
| 22  | A     | 1104 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1101 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 609  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 609  | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1209 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1109 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1112 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1118 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1122 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1131 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1134 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1135 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1022 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1205 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1214 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1227 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1238 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1240 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 1402 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 615  | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | Z     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 611  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 612  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 615  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 612  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 609  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 615  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 618  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 615  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 43  | 2     | 802  | 3PH  | C21-C22-C23-C24 |
| 26  | 8     | 801  | LHG  | C12-C13-C14-C15 |
| 26  | 5     | 801  | LHG  | C11-C12-C13-C14 |
| 27  | A     | 5004 | NKP  | CAX-CAY-CAZ-CBA |
| 43  | 7     | 802  | 3PH  | C22-C23-C24-C25 |
| 22  | A     | 1107 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 1110 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1236 | CLA  | C16-C17-C18-C19 |
| 22  | 3     | 607  | CLA  | C11-C12-C13-C14 |
| 22  | 7     | 616  | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 609  | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1125 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1023 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 8     | 607  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 2     | 604  | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1223 | CLA  | C10-C11-C12-C13 |
| 22  | 1     | 603  | CLA  | C8-C10-C11-C12  |
| 22  | 1     | 603  | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 5     | 602  | CLA  | C5-C6-C7-C8     |
| 26  | A     | 5002 | LHG  | C8-C7-O7-C5     |
| 22  | B     | 1203 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 603  | CLA  | C11-C10-C8-C7   |
| 26  | Z     | 801  | LHG  | C28-C29-C30-C31 |
| 26  | 4     | 802  | LHG  | O2-C2-C3-O3     |
| 26  | 8     | 801  | LHG  | C23-C24-C25-C26 |
| 22  | A     | 1109 | CLA  | CBA-CGA-O2A-C1  |
| 28  | B     | 6101 | LMT  | C1-C2-C3-C4     |
| 26  | 8     | 801  | LHG  | C28-C29-C30-C31 |
| 32  | A     | 5005 | DGA  | CA7-CA8-CA9-CAA |
| 41  | 2     | 803  | SQD  | C9-C10-C11-C12  |
| 22  | A     | 1112 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 611  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 608  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1104 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1108 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1109 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1125 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1131 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1135 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1101 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1207 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1212 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1236 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1241 | CLA  | C3A-C2A-CAA-CBA |
| 22  | K     | 1404 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 613  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 608  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 618  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 603  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 604  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 602  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 603  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 604  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 605  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 609  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 608  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 601  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 618  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 2     | 602  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 9     | 603  | CLA  | C3A-C2A-CAA-CBA |
| 40  | Z     | 613  | CHL  | C3A-C2A-CAA-CBA |
| 40  | 8     | 613  | CHL  | C3A-C2A-CAA-CBA |
| 40  | 4     | 613  | CHL  | C3A-C2A-CAA-CBA |
| 22  | 7     | 601  | CLA  | O1D-CGD-O2D-CED |
| 26  | A     | 5001 | LHG  | C9-C10-C11-C12  |
| 41  | 1     | 802  | SQD  | C17-C18-C19-C20 |
| 22  | B     | 1214 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1228 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1230 | CLA  | C8-C10-C11-C12  |
| 22  | F     | 1301 | CLA  | C8-C10-C11-C12  |
| 22  | 5     | 618  | CLA  | C8-C10-C11-C12  |
| 26  | 4     | 802  | LHG  | C23-C24-C25-C26 |
| 22  | A     | 1013 | CLA  | O1D-CGD-O2D-CED |
| 43  | 7     | 802  | 3PH  | C21-C22-C23-C24 |
| 25  | 8     | 503  | BCR  | C9-C10-C11-C12  |
| 39  | 9     | 502  | LUT  | C29-C30-C31-C32 |
| 22  | A     | 1117 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 1117 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1126 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1207 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1207 | CLA  | C16-C17-C18-C20 |
| 22  | 7     | 607  | CLA  | C16-C17-C18-C20 |
| 22  | 4     | 601  | CLA  | C11-C12-C13-C15 |
| 22  | 5     | 613  | CLA  | C6-C7-C8-C9     |
| 22  | K     | 1402 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 615  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 609  | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 607  | CLA  | CBD-CGD-O2D-CED |
| 26  | 4     | 801  | LHG  | C28-C29-C30-C31 |
| 26  | 2     | 801  | LHG  | C1-C2-C3-O3     |
| 22  | A     | 1115 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1013 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 26  | 6     | 801  | LHG  | C12-C13-C14-C15 |
| 26  | 6     | 801  | LHG  | C16-C17-C18-C19 |
| 26  | 6     | 801  | LHG  | C30-C31-C32-C33 |
| 22  | B     | 1212 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 612  | CLA  | C3-C5-C6-C7     |
| 26  | 1     | 801  | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 7     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1214 | CLA  | C10-C11-C12-C13 |
| 26  | Z     | 801  | LHG  | C13-C14-C15-C16 |
| 26  | 4     | 802  | LHG  | C11-C10-C9-C8   |
| 26  | 4     | 802  | LHG  | C11-C12-C13-C14 |
| 26  | 6     | 801  | LHG  | C11-C10-C9-C8   |
| 28  | 1     | 803  | LMT  | C11-C10-C9-C8   |
| 32  | 9     | 802  | DGA  | CDB-CEB-CFB-CGB |
| 38  | 7     | 804  | SPH  | C9-C10-C11-C12  |
| 22  | Z     | 608  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 8     | 801  | LHG  | C25-C26-C27-C28 |
| 38  | K     | 5001 | SPH  | C12-C13-C14-C15 |
| 26  | 6     | 801  | LHG  | C11-C12-C13-C14 |
| 28  | 4     | 803  | LMT  | C1-C2-C3-C4     |
| 22  | 4     | 609  | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 607  | CLA  | O1D-CGD-O2D-CED |
| 26  | 7     | 801  | LHG  | C28-C29-C30-C31 |
| 26  | 6     | 801  | LHG  | C34-C35-C36-C37 |
| 38  | 7     | 804  | SPH  | C10-C11-C12-C13 |
| 22  | A     | 1115 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1134 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1216 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1223 | CLA  | C16-C17-C18-C20 |
| 22  | 4     | 604  | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1118 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1122 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1132 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1135 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1240 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 605  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 607  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 5     | 609  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 609  | CLA  | C2B-C3B-CAB-CBB |
| 25  | A     | 4003 | BCR  | C1-C6-C7-C8     |
| 25  | A     | 4004 | BCR  | C1-C6-C7-C8     |
| 25  | A     | 4004 | BCR  | C5-C6-C7-C8     |
| 25  | A     | 4004 | BCR  | C23-C24-C25-C30 |
| 25  | B     | 4005 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 4005 | BCR  | C23-C24-C25-C30 |
| 25  | B     | 4006 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 4006 | BCR  | C23-C24-C25-C30 |
| 25  | I     | 4001 | BCR  | C1-C6-C7-C8     |
| 25  | I     | 4001 | BCR  | C5-C6-C7-C8     |
| 25  | J     | 4001 | BCR  | C23-C24-C25-C26 |
| 25  | J     | 4001 | BCR  | C23-C24-C25-C30 |
| 25  | K     | 4002 | BCR  | C23-C24-C25-C26 |
| 25  | K     | 4002 | BCR  | C23-C24-C25-C30 |
| 25  | L     | 4002 | BCR  | C1-C6-C7-C8     |
| 25  | L     | 4002 | BCR  | C5-C6-C7-C8     |
| 25  | 3     | 503  | BCR  | C1-C6-C7-C8     |
| 25  | 8     | 503  | BCR  | C1-C6-C7-C8     |
| 25  | 4     | 503  | BCR  | C1-C6-C7-C8     |
| 25  | 4     | 503  | BCR  | C5-C6-C7-C8     |
| 25  | 5     | 503  | BCR  | C23-C24-C25-C30 |
| 25  | 5     | 504  | BCR  | C23-C24-C25-C30 |
| 25  | 6     | 504  | BCR  | C23-C24-C25-C26 |
| 25  | 6     | 504  | BCR  | C23-C24-C25-C30 |
| 36  | F     | 4001 | RRX  | C23-C24-C25-C30 |
| 36  | F     | 4001 | RRX  | C23-C24-C25-C26 |
| 37  | 1     | 503  | C7Z  | C25-C26-C27-C28 |
| 39  | Z     | 503  | LUT  | C1-C6-C7-C8     |
| 22  | G     | 1601 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 1124 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1213 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 603  | CLA  | C5-C6-C7-C8     |
| 22  | 8     | 606  | CLA  | C10-C11-C12-C13 |
| 22  | 8     | 607  | CLA  | C5-C6-C7-C8     |
| 26  | 1     | 801  | LHG  | C11-C10-C9-C8   |
| 22  | 5     | 618  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1118 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1128 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1237 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 616  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 26  | A     | 5001 | LHG  | C23-C24-C25-C26 |
| 43  | 7     | 802  | 3PH  | C31-C32-C33-C34 |
| 22  | B     | 1234 | CLA  | C5-C6-C7-C8     |
| 22  | 9     | 603  | CLA  | C8-C10-C11-C12  |
| 28  | A     | 5006 | LMT  | C3-C4-C5-C6     |
| 22  | A     | 1122 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1226 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 27  | 8     | 802  | NKP  | CAM-CAN-CAO-CAP |
| 32  | 9     | 802  | DGA  | CAB-CBB-CCB-CDB |
| 26  | 5     | 801  | LHG  | O9-C7-O7-C5     |
| 41  | 1     | 802  | SQD  | C10-C11-C12-C13 |
| 25  | A     | 4004 | BCR  | C10-C11-C12-C13 |
| 25  | L     | 4002 | BCR  | C10-C11-C12-C13 |
| 22  | K     | 1402 | CLA  | C5-C6-C7-C8     |
| 22  | 9     | 603  | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1128 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1216 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1236 | CLA  | C2-C3-C5-C6     |
| 26  | 5     | 801  | LHG  | C11-C10-C9-C8   |
| 26  | 6     | 801  | LHG  | C13-C14-C15-C16 |
| 22  | 1     | 603  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 609  | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 5002 | LHG  | C24-C23-O8-C6   |
| 27  | 8     | 802  | NKP  | CAG-CAH-CAI-OAJ |
| 26  | 8     | 801  | LHG  | C11-C10-C9-C8   |
| 28  | 4     | 803  | LMT  | C3-C4-C5-C6     |
| 38  | 7     | 804  | SPH  | C6-C7-C8-C9     |
| 26  | 7     | 801  | LHG  | C11-C12-C13-C14 |
| 28  | A     | 5006 | LMT  | C5-C6-C7-C8     |
| 22  | B     | 1220 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 1115 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1023 | CLA  | C13-C15-C16-C17 |
| 22  | 7     | 604  | CLA  | C13-C15-C16-C17 |
| 22  | 8     | 602  | CLA  | C13-C15-C16-C17 |
| 22  | 7     | 602  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 1     | 612  | CLA  | C8-C10-C11-C12  |
| 22  | 9     | 606  | CLA  | CBA-CGA-O2A-C1  |
| 25  | A     | 4001 | BCR  | C9-C10-C11-C12  |
| 25  | B     | 4003 | BCR  | C19-C20-C21-C22 |
| 39  | 7     | 502  | LUT  | C29-C30-C31-C32 |
| 26  | 7     | 801  | LHG  | C8-C7-O7-C5     |
| 26  | 4     | 802  | LHG  | C8-C7-O7-C5     |
| 41  | 2     | 803  | SQD  | C8-C7-O47-C45   |
| 22  | A     | 1013 | CLA  | O1A-CGA-O2A-C1  |
| 43  | 5     | 802  | 3PH  | C21-C22-C23-C24 |
| 32  | 9     | 802  | DGA  | CA6-CA7-CA8-CA9 |
| 43  | 7     | 802  | 3PH  | C25-C26-C27-C28 |
| 21  | A     | 1011 | CL0  | C15-C16-C17-C18 |
| 22  | A     | 1105 | CLA  | C13-C15-C16-C17 |
| 26  | 6     | 801  | LHG  | C31-C32-C33-C34 |
| 41  | 1     | 802  | SQD  | C9-C10-C11-C12  |
| 32  | 9     | 802  | DGA  | CB5-CB6-CB7-CB8 |
| 22  | A     | 1137 | CLA  | C10-C11-C12-C13 |
| 37  | 1     | 503  | C7Z  | C27-C28-C29-C39 |
| 26  | 4     | 801  | LHG  | C11-C12-C13-C14 |
| 43  | 2     | 802  | 3PH  | C36-C37-C38-C39 |
| 22  | A     | 1110 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1219 | CLA  | C3-C5-C6-C7     |
| 22  | 2     | 601  | CLA  | C3-C5-C6-C7     |
| 22  | 9     | 605  | CLA  | C3-C5-C6-C7     |
| 28  | 8     | 805  | LMT  | C1-C2-C3-C4     |
| 37  | 1     | 503  | C7Z  | C27-C28-C29-C30 |
| 39  | 2     | 502  | LUT  | C31-C32-C33-C34 |
| 26  | A     | 5002 | LHG  | C13-C14-C15-C16 |
| 22  | 8     | 606  | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1210 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1225 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 1     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1216 | CLA  | C16-C17-C18-C19 |
| 22  | 4     | 601  | CLA  | C11-C12-C13-C14 |
| 22  | 2     | 601  | CLA  | C11-C12-C13-C14 |
| 22  | 2     | 601  | CLA  | C11-C12-C13-C15 |
| 32  | A     | 5005 | DGA  | CB4-CB5-CB6-CB7 |
| 22  | 6     | 603  | CLA  | C4-C3-C5-C6     |
| 22  | 6     | 605  | CLA  | C4-C3-C5-C6     |
| 22  | 6     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 4     | 801  | LHG  | C10-C11-C12-C13 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 1     | 607  | CLA  | C5-C6-C7-C8     |
| 28  | F     | 5001 | LMT  | C2-C3-C4-C5     |
| 22  | 1     | 603  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 609  | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 611  | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 604  | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 604  | CLA  | C8-C10-C11-C12  |
| 26  | 4     | 801  | LHG  | C29-C30-C31-C32 |
| 28  | F     | 5001 | LMT  | C1-C2-C3-C4     |
| 22  | B     | 1238 | CLA  | CBA-CGA-O2A-C1  |
| 26  | 1     | 801  | LHG  | C7-C8-C9-C10    |
| 26  | Z     | 801  | LHG  | C7-C8-C9-C10    |
| 44  | 7     | 805  | PLM  | C2-C3-C4-C5     |
| 26  | A     | 5002 | LHG  | O9-C7-O7-C5     |
| 26  | 1     | 801  | LHG  | O6-C4-C5-O7     |
| 22  | A     | 1126 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 601  | CLA  | C10-C11-C12-C13 |
| 22  | 6     | 605  | CLA  | C5-C6-C7-C8     |
| 26  | 4     | 801  | LHG  | C13-C14-C15-C16 |
| 22  | A     | 1115 | CLA  | O1A-CGA-O2A-C1  |
| 43  | 6     | 802  | 3PH  | C22-C23-C24-C25 |
| 41  | 1     | 802  | SQD  | C7-C8-C9-C10    |
| 26  | B     | 5002 | LHG  | O10-C23-O8-C6   |
| 22  | A     | 1104 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1222 | CLA  | C10-C11-C12-C13 |
| 22  | 5     | 605  | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 606  | CLA  | C13-C15-C16-C17 |
| 26  | 4     | 801  | LHG  | C30-C31-C32-C33 |
| 21  | A     | 1011 | CL0  | CBA-CGA-O2A-C1  |
| 22  | A     | 1109 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 4     | 801  | LHG  | C9-C10-C11-C12  |
| 32  | A     | 5005 | DGA  | CB7-CB8-CB9-CAB |
| 38  | K     | 5001 | SPH  | C11-C12-C13-C14 |
| 43  | 7     | 802  | 3PH  | C24-C25-C26-C27 |
| 22  | B     | 1205 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1239 | CLA  | C13-C15-C16-C17 |
| 41  | 1     | 802  | SQD  | C11-C12-C13-C14 |
| 22  | B     | 1206 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1218 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 602  | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 615  | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 6     | 607  | CLA  | C2-C1-O2A-CGA   |
| 22  | 2     | 601  | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1213 | CLA  | C16-C17-C18-C20 |
| 32  | A     | 5005 | DGA  | CA6-CA7-CA8-CA9 |
| 22  | A     | 1125 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1231 | CLA  | C2-C3-C5-C6     |
| 41  | 2     | 803  | SQD  | O49-C7-O47-C45  |
| 26  | A     | 5001 | LHG  | C11-C12-C13-C14 |
| 22  | B     | 1022 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 607  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 612  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 618  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 615  | CLA  | C2A-CAA-CBA-CGA |
| 40  | Z     | 613  | CHL  | C2A-CAA-CBA-CGA |
| 40  | 5     | 611  | CHL  | C2A-CAA-CBA-CGA |
| 22  | 3     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 32  | 9     | 802  | DGA  | CB2-CB3-CB4-CB5 |
| 22  | A     | 1112 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 612  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 601  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1133 | CLA  | C10-C11-C12-C13 |
| 22  | 3     | 603  | CLA  | C15-C16-C17-C18 |
| 22  | 4     | 609  | CLA  | C8-C10-C11-C12  |
| 42  | Z     | 504  | QTB  | C09-C10-C11-C12 |
| 26  | A     | 5001 | LHG  | C7-C8-C9-C10    |
| 26  | 4     | 802  | LHG  | O1-C1-C2-O2     |
| 26  | 6     | 801  | LHG  | O1-C1-C2-O2     |
| 26  | 9     | 801  | LHG  | O1-C1-C2-O2     |
| 22  | G     | 1601 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 609  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 26  | A     | 5002 | LHG  | O10-C23-O8-C6   |
| 22  | B     | 1231 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 612  | CLA  | C3-C5-C6-C7     |
| 27  | 8     | 802  | NKP  | CAL-CAM-CAN-CAO |
| 22  | A     | 1104 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1106 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1118 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1122 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1126 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1131 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1132 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1207 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1209 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1227 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1229 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1239 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1240 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 1404 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 611  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 613  | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 601  | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 604  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 610  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 612  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 609  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 612  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 615  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 602  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 605  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 618  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 609  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 612  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 601  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 602  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1111 | CLA  | C8-C10-C11-C12  |
| 22  | 1     | 601  | CLA  | C10-C11-C12-C13 |
| 26  | A     | 5001 | LHG  | C13-C14-C15-C16 |
| 28  | F     | 5001 | LMT  | C3-C4-C5-C6     |
| 35  | B     | 5004 | T7X  | C12-C13-C14-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 38  | K     | 5001 | SPH  | C7-C8-C9-C10    |
| 26  | 4     | 801  | LHG  | O6-C4-C5-C6     |
| 26  | 6     | 801  | LHG  | O6-C4-C5-C6     |
| 43  | 5     | 802  | 3PH  | O11-C1-C2-C3    |
| 22  | A     | 1102 | CLA  | CBD-CGD-O2D-CED |
| 26  | 7     | 801  | LHG  | O9-C7-O7-C5     |
| 26  | A     | 5002 | LHG  | C31-C32-C33-C34 |
| 22  | B     | 1203 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 603  | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1012 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1105 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1110 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1114 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1128 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1130 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1132 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1101 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1023 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1203 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1204 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1207 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1209 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1210 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1223 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1228 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1231 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1234 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1234 | CLA  | C11-C10-C8-C7   |
| 22  | 3     | 603  | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 607  | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 610  | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 607  | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 602  | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 609  | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 619  | CLA  | C11-C10-C8-C7   |
| 22  | 9     | 604  | CLA  | C11-C10-C8-C7   |
| 23  | B     | 2002 | PQN  | C17-C18-C20-C21 |
| 40  | 8     | 613  | CHL  | C11-C12-C13-C15 |
| 22  | 6     | 605  | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 601  | CLA  | C5-C6-C7-C8     |
| 22  | 4     | 601  | CLA  | C5-C6-C7-C8     |
| 22  | J     | 1901 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | 1     | 801  | LHG  | C27-C28-C29-C30 |
| 26  | Z     | 801  | LHG  | C23-C24-C25-C26 |
| 26  | 4     | 802  | LHG  | C7-C8-C9-C10    |
| 22  | 6     | 603  | CLA  | C2-C3-C5-C6     |
| 22  | 6     | 605  | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1137 | CLA  | C5-C6-C7-C8     |
| 22  | L     | 1502 | CLA  | C13-C15-C16-C17 |
| 22  | 1     | 607  | CLA  | C8-C10-C11-C12  |
| 26  | B     | 5001 | LHG  | C7-C8-C9-C10    |
| 22  | A     | 1133 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1012 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1107 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1013 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 606  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 609  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1105 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1107 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 1110 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1114 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1117 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 1117 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1119 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1121 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1122 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1126 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1128 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1130 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 1132 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1133 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1138 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1101 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1101 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1204 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1207 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1209 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1212 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1213 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1223 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1235 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1236 | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 603  | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 610  | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 3     | 616  | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 607  | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 602  | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 603  | CLA  | C14-C13-C15-C16 |
| 22  | 2     | 601  | CLA  | C6-C7-C8-C9     |
| 22  | 9     | 604  | CLA  | C11-C10-C8-C9   |
| 40  | 5     | 610  | CHL  | C11-C10-C8-C9   |
| 22  | Z     | 601  | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1222 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 608  | CLA  | O1D-CGD-O2D-CED |
| 28  | B     | 6101 | LMT  | C2'-C1'-O1'-C1  |
| 22  | B     | 1223 | CLA  | C8-C10-C11-C12  |
| 22  | 4     | 603  | CLA  | C8-C10-C11-C12  |
| 22  | 5     | 604  | CLA  | C5-C6-C7-C8     |
| 22  | 2     | 604  | CLA  | C11-C10-C8-C9   |
| 26  | B     | 5006 | LHG  | C4-C5-C6-O8     |
| 26  | 1     | 801  | LHG  | C4-C5-C6-O8     |
| 26  | Z     | 801  | LHG  | C4-C5-C6-O8     |
| 26  | 4     | 801  | LHG  | C4-C5-C6-O8     |
| 32  | 9     | 802  | DGA  | OG1-CG1-CG2-CG3 |
| 33  | B     | 5003 | DGD  | O1G-C1G-C2G-C3G |
| 35  | B     | 5004 | T7X  | C7-C8-C9-O18    |
| 43  | 8     | 806  | 3PH  | C34-C35-C36-C37 |
| 22  | B     | 1224 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 1228 | CLA  | C15-C16-C17-C18 |
| 22  | 3     | 605  | CLA  | C8-C10-C11-C12  |
| 38  | K     | 5001 | SPH  | C9-C10-C11-C12  |
| 22  | 3     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 21  | A     | 1011 | CL0  | C16-C17-C18-C20 |
| 22  | 6     | 605  | CLA  | C6-C7-C8-C10    |
| 26  | 9     | 801  | LHG  | C11-C10-C9-C8   |
| 27  | A     | 5004 | NKP  | CAV-CAW-CAX-CAY |
| 31  | J     | 5001 | LMG  | C8-C9-O8-C28    |
| 22  | A     | 1137 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1134 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 604  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 607  | CLA  | O1D-CGD-O2D-CED |
| 40  | 4     | 611  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 4     | 611  | CHL  | CHA-CBD-CGD-O2D |
| 40  | 4     | 613  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 4     | 613  | CHL  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 3     | 606  | CLA  | C10-C11-C12-C13 |
| 22  | 8     | 602  | CLA  | C15-C16-C17-C18 |
| 26  | 6     | 801  | LHG  | C7-C8-C9-C10    |
| 43  | 5     | 802  | 3PH  | C22-C23-C24-C25 |
| 22  | A     | 1125 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1231 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1102 | CLA  | C2-C3-C5-C6     |
| 22  | 8     | 605  | CLA  | C2-C3-C5-C6     |
| 22  | 6     | 618  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1104 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1123 | CLA  | C13-C15-C16-C17 |
| 22  | 7     | 616  | CLA  | C10-C11-C12-C13 |
| 22  | 4     | 608  | CLA  | C5-C6-C7-C8     |
| 22  | 5     | 609  | CLA  | C10-C11-C12-C13 |
| 25  | B     | 4006 | BCR  | C37-C22-C23-C24 |
| 39  | Z     | 503  | LUT  | C7-C8-C9-C19    |
| 26  | 4     | 802  | LHG  | O9-C7-O7-C5     |
| 22  | 8     | 607  | CLA  | C6-C7-C8-C10    |
| 25  | B     | 4006 | BCR  | C21-C22-C23-C24 |
| 39  | Z     | 503  | LUT  | C27-C28-C29-C30 |
| 22  | 9     | 606  | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 604  | CLA  | C13-C15-C16-C17 |
| 22  | 6     | 603  | CLA  | C13-C15-C16-C17 |
| 27  | 8     | 802  | NKP  | CAG-OAF-PAC-OAD |
| 43  | 5     | 802  | 3PH  | C1-O11-P-O12    |
| 32  | A     | 5005 | DGA  | CA2-CA3-CA4-CA5 |
| 22  | 7     | 601  | CLA  | C10-C11-C12-C13 |
| 26  | 4     | 801  | LHG  | C19-C20-C21-C22 |
| 28  | A     | 5006 | LMT  | C4'-C5'-C6'-O6' |
| 31  | J     | 5001 | LMG  | C7-C8-O7-C10    |
| 43  | 7     | 802  | 3PH  | C3-C2-O21-C21   |
| 26  | 2     | 801  | LHG  | C25-C26-C27-C28 |
| 22  | A     | 1133 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1204 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1213 | CLA  | C10-C11-C12-C13 |
| 22  | 8     | 609  | CLA  | C13-C15-C16-C17 |
| 25  | A     | 4002 | BCR  | C13-C14-C15-C16 |
| 25  | B     | 4005 | BCR  | C9-C10-C11-C12  |
| 25  | I     | 4001 | BCR  | C9-C10-C11-C12  |
| 25  | I     | 4001 | BCR  | C19-C20-C21-C22 |
| 25  | J     | 4001 | BCR  | C9-C10-C11-C12  |
| 25  | 3     | 505  | BCR  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 39  | Z     | 502  | LUT  | C29-C30-C31-C32 |
| 39  | 3     | 502  | LUT  | C29-C30-C31-C32 |
| 39  | 4     | 502  | LUT  | C29-C30-C31-C32 |
| 21  | A     | 1011 | CL0  | O1A-CGA-O2A-C1  |
| 22  | A     | 1121 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1220 | CLA  | C3-C5-C6-C7     |
| 38  | 7     | 804  | SPH  | C7-C8-C9-C10    |
| 43  | 8     | 806  | 3PH  | C37-C38-C39-C3A |
| 22  | B     | 1241 | CLA  | CBA-CGA-O2A-C1  |
| 31  | J     | 5001 | LMG  | C29-C28-O8-C9   |
| 32  | 9     | 802  | DGA  | CB3-CB4-CB5-CB6 |
| 26  | 4     | 802  | LHG  | C13-C14-C15-C16 |
| 22  | B     | 1021 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 1102 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1237 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1116 | CLA  | C11-C12-C13-C14 |
| 32  | A     | 5005 | DGA  | CA5-CA6-CA7-CA8 |
| 43  | 2     | 802  | 3PH  | C22-C23-C24-C25 |
| 26  | B     | 5001 | LHG  | C24-C23-O8-C6   |
| 22  | A     | 1127 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1205 | CLA  | CAA-CBA-CGA-O2A |
| 26  | 1     | 801  | LHG  | C31-C32-C33-C34 |
| 43  | 6     | 802  | 3PH  | C29-C2A-C2B-C2C |
| 22  | A     | 1141 | CLA  | C2-C1-O2A-CGA   |
| 22  | K     | 1404 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 607  | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1238 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 6     | 801  | LHG  | C19-C20-C21-C22 |
| 26  | 6     | 801  | LHG  | C28-C29-C30-C31 |
| 22  | 8     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1219 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 7     | 606  | CLA  | C5-C6-C7-C8     |
| 28  | B     | 6101 | LMT  | C9-C10-C11-C12  |
| 26  | 9     | 801  | LHG  | C11-C12-C13-C14 |
| 22  | A     | 1128 | CLA  | C10-C11-C12-C13 |
| 22  | 5     | 612  | CLA  | O1D-CGD-O2D-CED |
| 25  | 8     | 503  | BCR  | C19-C20-C21-C22 |
| 22  | 6     | 608  | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1132 | CLA  | C4-C3-C5-C6     |
| 22  | 1     | 603  | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 8     | 605  | CLA  | C4-C3-C5-C6     |
| 22  | 5     | 602  | CLA  | C4-C3-C5-C6     |
| 22  | Z     | 601  | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1211 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1221 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1110 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1012 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1108 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1109 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1130 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1021 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1023 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1203 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1205 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1210 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1216 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1223 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1228 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1234 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1234 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1235 | CLA  | C14-C13-C15-C16 |
| 22  | L     | 1502 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 603  | CLA  | C11-C10-C8-C9   |
| 22  | 3     | 606  | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 607  | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 609  | CLA  | C14-C13-C15-C16 |
| 22  | 7     | 603  | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 603  | CLA  | C14-C13-C15-C16 |
| 22  | 5     | 601  | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 602  | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 609  | CLA  | C11-C12-C13-C14 |
| 22  | 5     | 618  | CLA  | C14-C13-C15-C16 |
| 22  | 6     | 606  | CLA  | C14-C13-C15-C16 |
| 22  | 6     | 619  | CLA  | C11-C10-C8-C9   |
| 22  | 9     | 601  | CLA  | C11-C10-C8-C9   |
| 40  | Z     | 609  | CHL  | C11-C10-C8-C9   |
| 40  | 8     | 613  | CHL  | C11-C12-C13-C14 |
| 40  | 9     | 610  | CHL  | C11-C10-C8-C9   |
| 22  | 5     | 607  | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1104 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1116 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1121 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1124 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1126 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1133 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1141 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1237 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1023 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1203 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1220 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1224 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1230 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1241 | CLA  | C4B-C3B-CAB-CBB |
| 22  | F     | 1302 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 1403 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 1404 | CLA  | C4B-C3B-CAB-CBB |
| 22  | L     | 1502 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 605  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 611  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 612  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 605  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 613  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 618  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 611  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 622  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 612  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 603  | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 2     | 605  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 26  | 1     | 801  | LHG  | C11-C12-C13-C14 |
| 38  | 7     | 803  | SPH  | C7-C8-C9-C10    |
| 22  | B     | 1215 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 611  | CLA  | C13-C15-C16-C17 |
| 26  | A     | 5002 | LHG  | C11-C12-C13-C14 |
| 30  | A     | 5007 | DAO  | C3-C4-C5-C6     |
| 26  | 5     | 801  | LHG  | C13-C14-C15-C16 |
| 22  | 4     | 612  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 610  | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 615  | CLA  | C8-C10-C11-C12  |
| 22  | 9     | 604  | CLA  | C13-C15-C16-C17 |
| 28  | B     | 6101 | LMT  | C2-C3-C4-C5     |
| 22  | A     | 1013 | CLA  | C3-C5-C6-C7     |
| 26  | 4     | 801  | LHG  | C35-C36-C37-C38 |
| 26  | B     | 5001 | LHG  | O6-C4-C5-C6     |
| 26  | 1     | 801  | LHG  | O6-C4-C5-C6     |
| 26  | 4     | 802  | LHG  | O6-C4-C5-C6     |
| 26  | 5     | 801  | LHG  | O6-C4-C5-C6     |
| 43  | 7     | 802  | 3PH  | O11-C1-C2-C3    |
| 43  | 6     | 802  | 3PH  | O11-C1-C2-C3    |
| 38  | 7     | 803  | SPH  | C9-C10-C11-C12  |
| 22  | A     | 1012 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1104 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1104 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1107 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1108 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1109 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1117 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1117 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1117 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1119 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1121 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1122 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1126 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1130 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1133 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1136 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1137 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1138 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1138 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1101 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1101 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1021 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1023 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1205 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1212 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1213 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1216 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1223 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1235 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1235 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1236 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1240 | CLA  | C11-C12-C13-C15 |
| 22  | L     | 1502 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 606  | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 611  | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 611  | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 612  | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 606  | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 616  | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 609  | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 609  | CLA  | C12-C13-C15-C16 |
| 22  | 7     | 603  | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 603  | CLA  | C12-C13-C15-C16 |
| 22  | 8     | 605  | CLA  | C11-C12-C13-C15 |
| 22  | 8     | 605  | CLA  | C12-C13-C15-C16 |
| 22  | 8     | 602  | CLA  | C11-C10-C8-C7   |
| 22  | 8     | 602  | CLA  | C12-C13-C15-C16 |
| 22  | 5     | 601  | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 618  | CLA  | C12-C13-C15-C16 |
| 22  | 6     | 603  | CLA  | C12-C13-C15-C16 |
| 22  | 6     | 606  | CLA  | C12-C13-C15-C16 |
| 22  | 2     | 601  | CLA  | C6-C7-C8-C10    |
| 22  | 9     | 601  | CLA  | C11-C10-C8-C7   |
| 40  | Z     | 610  | CHL  | C11-C12-C13-C15 |
| 40  | Z     | 609  | CHL  | C11-C10-C8-C7   |
| 40  | 5     | 610  | CHL  | C11-C10-C8-C7   |
| 40  | 9     | 610  | CHL  | C11-C10-C8-C7   |
| 22  | B     | 1220 | CLA  | C15-C16-C17-C18 |
| 22  | 8     | 603  | CLA  | C15-C16-C17-C18 |
| 43  | 8     | 806  | 3PH  | C3A-C3B-C3C-C3D |
| 22  | A     | 1116 | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | 2     | 801  | LHG  | C28-C29-C30-C31 |
| 22  | B     | 1214 | CLA  | C11-C12-C13-C14 |
| 38  | 7     | 804  | SPH  | C15-C16-C17-C18 |
| 21  | A     | 1011 | CL0  | C4-C3-C5-C6     |
| 22  | A     | 1117 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1126 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1130 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1133 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1134 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1141 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1204 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1209 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1209 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1221 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1230 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 606  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 607  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 606  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 616  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 606  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 615  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 609  | CLA  | C3A-C2A-CAA-CBA |
| 40  | 7     | 610  | CHL  | C3A-C2A-CAA-CBA |
| 40  | 5     | 611  | CHL  | C3A-C2A-CAA-CBA |
| 22  | A     | 1121 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1229 | CLA  | C5-C6-C7-C8     |
| 22  | 5     | 618  | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1235 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1209 | CLA  | C2-C3-C5-C6     |
| 22  | 1     | 603  | CLA  | C2-C3-C5-C6     |
| 22  | Z     | 607  | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1241 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 605  | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 607  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1132 | CLA  | CBA-CGA-O2A-C1  |
| 25  | A     | 4002 | BCR  | C9-C10-C11-C12  |
| 25  | B     | 4007 | BCR  | C19-C20-C21-C22 |
| 25  | I     | 4001 | BCR  | C13-C14-C15-C16 |
| 25  | K     | 4002 | BCR  | C19-C20-C21-C22 |
| 25  | L     | 4001 | BCR  | C13-C14-C15-C16 |
| 25  | L     | 4002 | BCR  | C13-C14-C15-C16 |
| 25  | 4     | 503  | BCR  | C9-C10-C11-C12  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | 5     | 503  | BCR  | C15-C16-C17-C18 |
| 25  | 6     | 503  | BCR  | C19-C20-C21-C22 |
| 37  | J     | 4002 | C7Z  | C29-C30-C31-C32 |
| 39  | 1     | 502  | LUT  | C29-C30-C31-C32 |
| 39  | 7     | 501  | LUT  | C29-C30-C31-C32 |
| 39  | 6     | 501  | LUT  | C29-C30-C31-C32 |
| 39  | 9     | 501  | LUT  | C29-C30-C31-C32 |
| 25  | A     | 4004 | BCR  | C36-C18-C19-C20 |
| 26  | B     | 5006 | LHG  | C11-C12-C13-C14 |
| 26  | 2     | 801  | LHG  | C11-C12-C13-C14 |
| 43  | 8     | 806  | 3PH  | C3C-C3D-C3E-C3F |
| 42  | Z     | 504  | QTB  | C09-C10-C11-C17 |
| 31  | J     | 5001 | LMG  | O10-C28-O8-C9   |
| 26  | 8     | 801  | LHG  | C30-C31-C32-C33 |
| 39  | Z     | 503  | LUT  | C31-C32-C33-C34 |
| 40  | Z     | 610  | CHL  | C2A-CAA-CBA-CGA |
| 40  | 4     | 611  | CHL  | C2A-CAA-CBA-CGA |
| 26  | 4     | 802  | LHG  | C4-C5-C6-O8     |
| 31  | J     | 5001 | LMG  | O1-C7-C8-C9     |
| 41  | 2     | 803  | SQD  | O6-C44-C45-C46  |
| 22  | 6     | 608  | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1138 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1209 | CLA  | C10-C11-C12-C13 |
| 22  | 8     | 603  | CLA  | C8-C10-C11-C12  |
| 40  | 2     | 613  | CHL  | C1A-C2A-CAA-CBA |
| 22  | B     | 1211 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1224 | CLA  | C4-C3-C5-C6     |
| 26  | 4     | 801  | LHG  | C18-C19-C20-C21 |
| 22  | A     | 1132 | CLA  | C2-C3-C5-C6     |
| 32  | 9     | 802  | DGA  | CB4-CB5-CB6-CB7 |
| 22  | 6     | 606  | CLA  | C16-C17-C18-C20 |
| 26  | A     | 5002 | LHG  | O6-C4-C5-O7     |
| 26  | Z     | 801  | LHG  | O6-C4-C5-O7     |
| 26  | 9     | 801  | LHG  | O6-C4-C5-O7     |
| 26  | 6     | 801  | LHG  | C35-C36-C37-C38 |
| 22  | 8     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 622  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 605  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 25  | A     | 4003 | BCR  | C23-C24-C25-C30 |
| 25  | B     | 4001 | BCR  | C1-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | B     | 4001 | BCR  | C23-C24-C25-C30 |
| 25  | B     | 4004 | BCR  | C23-C24-C25-C30 |
| 25  | G     | 4001 | BCR  | C1-C6-C7-C8     |
| 25  | G     | 4001 | BCR  | C23-C24-C25-C30 |
| 25  | L     | 4002 | BCR  | C23-C24-C25-C30 |
| 25  | 3     | 503  | BCR  | C23-C24-C25-C30 |
| 25  | 7     | 504  | BCR  | C23-C24-C25-C30 |
| 37  | 5     | 505  | C7Z  | C21-C26-C27-C28 |
| 22  | A     | 1013 | CLA  | C8-C10-C11-C12  |
| 33  | B     | 5003 | DGD  | CAA-CBA-CCA-CDA |
| 22  | A     | 1108 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1122 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 1126 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1220 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1229 | CLA  | C10-C11-C12-C13 |
| 21  | A     | 1011 | CL0  | C16-C17-C18-C19 |
| 40  | 2     | 613  | CHL  | C2A-CAA-CBA-CGA |
| 26  | A     | 5002 | LHG  | O7-C5-C6-O8     |
| 26  | Z     | 801  | LHG  | O7-C5-C6-O8     |
| 33  | B     | 5003 | DGD  | O1G-C1G-C2G-O2G |
| 33  | B     | 5003 | DGD  | O2G-C2G-C3G-O3G |
| 43  | 8     | 806  | 3PH  | O21-C2-C3-O31   |
| 43  | 6     | 802  | 3PH  | O21-C2-C3-O31   |
| 26  | 8     | 801  | LHG  | C13-C14-C15-C16 |
| 31  | J     | 5001 | LMG  | C30-C31-C32-C33 |
| 43  | 8     | 806  | 3PH  | C39-C3A-C3B-C3C |
| 35  | B     | 5004 | T7X  | C15-C16-C17-C18 |
| 35  | B     | 5004 | T7X  | C21-C22-C23-C24 |
| 35  | B     | 5004 | T7X  | C22-C23-C24-C25 |
| 26  | 2     | 801  | LHG  | C26-C27-C28-C29 |
| 22  | 6     | 604  | CLA  | C13-C15-C16-C17 |
| 26  | 7     | 801  | LHG  | C25-C26-C27-C28 |
| 21  | A     | 1011 | CL0  | C2-C3-C5-C6     |
| 22  | A     | 1117 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1141 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1224 | CLA  | C2-C3-C5-C6     |
| 22  | 5     | 602  | CLA  | C2-C3-C5-C6     |
| 26  | A     | 5002 | LHG  | C29-C30-C31-C32 |
| 41  | 2     | 803  | SQD  | C7-C8-C9-C10    |
| 26  | Z     | 801  | LHG  | C16-C17-C18-C19 |
| 22  | A     | 1012 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 1104 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1130 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1136 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1137 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1237 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1023 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1210 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1231 | CLA  | C14-C13-C15-C16 |
| 22  | 8     | 602  | CLA  | C14-C13-C15-C16 |
| 22  | 6     | 603  | CLA  | C15-C16-C17-C18 |
| 26  | 1     | 801  | LHG  | C16-C17-C18-C19 |
| 22  | B     | 1240 | CLA  | C16-C17-C18-C19 |
| 28  | B     | 6101 | LMT  | O1'-C1-C2-C3    |
| 22  | B     | 1227 | CLA  | C2A-CAA-CBA-CGA |
| 41  | 1     | 802  | SQD  | C16-C17-C18-C19 |
| 26  | A     | 5002 | LHG  | O1-C1-C2-O2     |
| 26  | 7     | 801  | LHG  | O1-C1-C2-O2     |
| 37  | 1     | 503  | C7Z  | C13-C14-C15-C35 |
| 39  | 8     | 502  | LUT  | C29-C30-C31-C32 |
| 28  | B     | 5005 | LMT  | C4-C5-C6-C7     |
| 26  | Z     | 801  | LHG  | C11-C10-C9-C8   |
| 25  | 5     | 504  | BCR  | C11-C10-C9-C34  |
| 22  | A     | 1139 | CLA  | C10-C11-C12-C13 |
| 22  | 6     | 609  | CLA  | C15-C16-C17-C18 |
| 26  | A     | 5001 | LHG  | O6-C4-C5-C6     |
| 26  | A     | 5002 | LHG  | O6-C4-C5-C6     |
| 26  | 3     | 801  | LHG  | O6-C4-C5-C6     |
| 22  | A     | 1105 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1127 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1239 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 603  | CLA  | C10-C11-C12-C13 |
| 22  | 6     | 603  | CLA  | C5-C6-C7-C8     |
| 25  | A     | 4003 | BCR  | C37-C22-C23-C24 |
| 25  | L     | 4002 | BCR  | C37-C22-C23-C24 |
| 25  | 7     | 503  | BCR  | C37-C22-C23-C24 |
| 22  | A     | 1122 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1126 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1136 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1013 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1237 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1216 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1216 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1218 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1223 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1236 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1241 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 612  | CLA  | C11-C10-C8-C7   |
| 22  | Z     | 608  | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 603  | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 607  | CLA  | C11-C12-C13-C15 |
| 22  | 8     | 609  | CLA  | C12-C13-C15-C16 |
| 22  | 5     | 612  | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 604  | CLA  | C11-C12-C13-C15 |
| 22  | 9     | 603  | CLA  | C6-C7-C8-C10    |
| 22  | 9     | 603  | CLA  | C11-C10-C8-C7   |
| 23  | B     | 2002 | PQN  | C16-C17-C18-C20 |
| 40  | 8     | 613  | CHL  | C11-C10-C8-C7   |
| 40  | 5     | 610  | CHL  | C12-C13-C15-C16 |
| 33  | B     | 5003 | DGD  | C1A-C2A-C3A-C4A |
| 26  | 1     | 801  | LHG  | C9-C10-C11-C12  |
| 26  | A     | 5002 | LHG  | C35-C36-C37-C38 |
| 28  | B     | 5005 | LMT  | C3-C4-C5-C6     |
| 22  | A     | 1114 | CLA  | C5-C6-C7-C8     |
| 35  | B     | 5004 | T7X  | C27-C28-C29-C30 |
| 25  | A     | 4003 | BCR  | C21-C22-C23-C24 |
| 25  | B     | 4002 | BCR  | C17-C18-C19-C20 |
| 25  | B     | 4007 | BCR  | C7-C8-C9-C10    |
| 25  | B     | 4006 | BCR  | C17-C18-C19-C20 |
| 25  | K     | 4001 | BCR  | C17-C18-C19-C20 |
| 25  | K     | 4002 | BCR  | C7-C8-C9-C10    |
| 25  | L     | 4002 | BCR  | C21-C22-C23-C24 |
| 25  | 7     | 503  | BCR  | C21-C22-C23-C24 |
| 25  | 4     | 503  | BCR  | C7-C8-C9-C10    |
| 25  | 4     | 503  | BCR  | C11-C12-C13-C14 |
| 37  | 1     | 503  | C7Z  | C7-C8-C9-C10    |
| 37  | 5     | 505  | C7Z  | C31-C32-C33-C34 |
| 39  | Z     | 503  | LUT  | C7-C8-C9-C10    |
| 39  | 2     | 503  | LUT  | C11-C12-C13-C14 |
| 22  | 3     | 605  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 604  | CLA  | CBA-CGA-O2A-C1  |
| 31  | J     | 5001 | LMG  | C8-C7-O1-C1     |
| 41  | 2     | 803  | SQD  | C5-C6-S-O8      |
| 22  | F     | 1302 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Z     | 604  | CLA  | C2A-CAA-CBA-CGA |
| 21  | A     | 1011 | CL0  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1228 | CLA  | C4-C3-C5-C6     |
| 22  | 8     | 602  | CLA  | C4-C3-C5-C6     |
| 22  | K     | 1402 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1132 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1229 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1230 | CLA  | C10-C11-C12-C13 |
| 40  | 6     | 610  | CHL  | C3-C5-C6-C7     |
| 22  | B     | 1219 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1223 | CLA  | C13-C15-C16-C17 |
| 22  | 3     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 4     | 802  | LHG  | C12-C13-C14-C15 |
| 22  | 4     | 604  | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 615  | CLA  | C5-C6-C7-C8     |
| 25  | G     | 4001 | BCR  | C9-C10-C11-C12  |
| 39  | Z     | 501  | LUT  | C29-C30-C31-C32 |
| 39  | 6     | 502  | LUT  | C29-C30-C31-C32 |
| 26  | 4     | 802  | LHG  | C9-C10-C11-C12  |
| 22  | 8     | 607  | CLA  | C6-C7-C8-C9     |
| 25  | 5     | 504  | BCR  | C11-C10-C9-C8   |
| 22  | 7     | 607  | CLA  | C8-C10-C11-C12  |
| 26  | B     | 5006 | LHG  | O6-C4-C5-O7     |
| 26  | 4     | 802  | LHG  | O6-C4-C5-O7     |
| 26  | 5     | 801  | LHG  | O6-C4-C5-O7     |
| 43  | 7     | 802  | 3PH  | O11-C1-C2-O21   |
| 26  | A     | 5002 | LHG  | C4-C5-C6-O8     |
| 26  | 3     | 801  | LHG  | C4-C5-C6-O8     |
| 26  | 8     | 801  | LHG  | C4-C5-C6-O8     |
| 26  | 5     | 801  | LHG  | C4-C5-C6-O8     |
| 41  | 2     | 803  | SQD  | C44-C45-C46-O48 |
| 43  | 6     | 802  | 3PH  | C1-C2-C3-O31    |
| 26  | 4     | 801  | LHG  | C31-C32-C33-C34 |
| 22  | B     | 1202 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1229 | CLA  | C4-C3-C5-C6     |
| 22  | Z     | 602  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 601  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 605  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1128 | CLA  | C3-C5-C6-C7     |
| 26  | B     | 5001 | LHG  | O7-C5-C6-O8     |
| 26  | 3     | 801  | LHG  | O7-C5-C6-O8     |
| 26  | 6     | 801  | LHG  | O7-C5-C6-O8     |
| 41  | 2     | 803  | SQD  | O6-C44-C45-O47  |
| 22  | A     | 1105 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1106 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1013 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1209 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1216 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1223 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1241 | CLA  | C11-C10-C8-C9   |
| 22  | 3     | 603  | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 609  | CLA  | C14-C13-C15-C16 |
| 22  | 5     | 612  | CLA  | C11-C12-C13-C14 |
| 23  | B     | 2002 | PQN  | C16-C17-C18-C19 |
| 40  | 8     | 613  | CHL  | C11-C10-C8-C9   |
| 26  | A     | 5001 | LHG  | C10-C11-C12-C13 |
| 32  | 9     | 802  | DGA  | CBB-CAB-CB9-CB8 |
| 22  | B     | 1211 | CLA  | C10-C11-C12-C13 |
| 22  | L     | 1502 | CLA  | C15-C16-C17-C18 |
| 22  | 8     | 601  | CLA  | C5-C6-C7-C8     |
| 22  | 5     | 609  | CLA  | C13-C15-C16-C17 |
| 39  | 2     | 501  | LUT  | C26-C27-C28-C29 |
| 38  | 7     | 803  | SPH  | C11-C12-C13-C14 |
| 28  | 9     | 803  | LMT  | C3-C4-C5-C6     |
| 22  | A     | 1105 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1204 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1223 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 608  | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 603  | CLA  | C2-C1-O2A-CGA   |
| 27  | 3     | 802  | NKP  | OBC-CAH-CAI-OAJ |
| 28  | 9     | 803  | LMT  | C2'-C1'-O1'-C1  |
| 41  | 1     | 802  | SQD  | C2-C1-O6-C44    |
| 22  | A     | 1118 | CLA  | C11-C12-C13-C14 |
| 22  | 4     | 605  | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1121 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1206 | CLA  | C8-C10-C11-C12  |
| 43  | 6     | 802  | 3PH  | C24-C25-C26-C27 |
| 22  | B     | 1220 | CLA  | C8-C10-C11-C12  |
| 38  | K     | 5001 | SPH  | C6-C7-C8-C9     |
| 22  | 1     | 608  | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 601  | CLA  | C16-C17-C18-C19 |
| 22  | 4     | 603  | CLA  | C16-C17-C18-C19 |
| 22  | 6     | 619  | CLA  | C16-C17-C18-C20 |
| 43  | 7     | 802  | 3PH  | C39-C3A-C3B-C3C |
| 26  | A     | 5002 | LHG  | C16-C17-C18-C19 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 40  | 5     | 610  | CHL  | C4C-C3C-CAC-CBC |
| 22  | B     | 1222 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 1221 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 606  | CLA  | C16-C17-C18-C19 |
| 26  | 3     | 801  | LHG  | O1-C1-C2-O2     |
| 22  | 3     | 605  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1114 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1222 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 619  | CLA  | C3-C5-C6-C7     |
| 25  | A     | 4001 | BCR  | C37-C22-C23-C24 |
| 25  | 3     | 504  | BCR  | C36-C18-C19-C20 |
| 25  | 7     | 503  | BCR  | C11-C12-C13-C35 |
| 22  | A     | 1107 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1139 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1101 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1217 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1230 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1231 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1232 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1232 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1239 | CLA  | C4B-C3B-CAB-CBB |
| 22  | G     | 1601 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 1401 | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 611  | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 615  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 616  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 609  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 615  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 606  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 607  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 615  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 615  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 608  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 2     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 26  | Z     | 801  | LHG  | C30-C31-C32-C33 |
| 22  | A     | 1108 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1110 | CLA  | C4-C3-C5-C6     |
| 40  | 7     | 610  | CHL  | C4-C3-C5-C6     |
| 26  | 5     | 801  | LHG  | O8-C23-C24-C25  |
| 25  | 7     | 503  | BCR  | C11-C12-C13-C14 |
| 25  | 6     | 503  | BCR  | C17-C18-C19-C20 |
| 32  | A     | 5005 | DGA  | CB5-CB6-CB7-CB8 |
| 33  | B     | 5003 | DGD  | C7A-C8A-C9A-CAA |
| 38  | 7     | 804  | SPH  | C12-C13-C14-C15 |
| 22  | A     | 1109 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1102 | CLA  | O1D-CGD-O2D-CED |
| 26  | B     | 5006 | LHG  | O6-C4-C5-C6     |
| 26  | 7     | 801  | LHG  | O6-C4-C5-C6     |
| 26  | 9     | 801  | LHG  | O6-C4-C5-C6     |
| 28  | 9     | 803  | LMT  | C11-C10-C9-C8   |
| 32  | 9     | 802  | DGA  | CA7-CA8-CA9-CAA |
| 22  | 5     | 612  | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1105 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1106 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1125 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 1203 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1206 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1206 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1208 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1215 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1217 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1219 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1220 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1221 | CLA  | C12-C13-C15-C16 |
| 22  | 1     | 604  | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 611  | CLA  | C12-C13-C15-C16 |
| 22  | Z     | 604  | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 612  | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 612  | CLA  | C11-C10-C8-C7   |
| 22  | 4     | 609  | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 602  | CLA  | C11-C12-C13-C15 |
| 43  | 7     | 802  | 3PH  | C27-C28-C29-C2A |
| 22  | B     | 1210 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1226 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1240 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1208 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 609  | CLA  | C13-C15-C16-C17 |
| 22  | 5     | 604  | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 9     | 605  | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1228 | CLA  | C2-C3-C5-C6     |
| 26  | B     | 5001 | LHG  | O6-C4-C5-O7     |
| 26  | 3     | 801  | LHG  | O6-C4-C5-O7     |
| 26  | 7     | 801  | LHG  | O6-C4-C5-O7     |
| 43  | 6     | 802  | 3PH  | O11-C1-C2-O21   |
| 22  | 6     | 608  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1117 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1122 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1218 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1236 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 606  | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 612  | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 607  | CLA  | C11-C12-C13-C14 |
| 22  | 4     | 609  | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 604  | CLA  | C11-C12-C13-C14 |
| 22  | 9     | 603  | CLA  | C11-C10-C8-C9   |
| 40  | 5     | 610  | CHL  | C14-C13-C15-C16 |
| 22  | 2     | 604  | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 609  | CLA  | C13-C15-C16-C17 |
| 25  | B     | 4002 | BCR  | C9-C10-C11-C12  |
| 25  | B     | 4002 | BCR  | C13-C14-C15-C16 |
| 25  | B     | 4006 | BCR  | C9-C10-C11-C12  |
| 25  | J     | 4001 | BCR  | C19-C20-C21-C22 |
| 25  | 3     | 503  | BCR  | C19-C20-C21-C22 |
| 25  | 4     | 503  | BCR  | C19-C20-C21-C22 |
| 39  | 8     | 501  | LUT  | C29-C30-C31-C32 |
| 22  | A     | 1140 | CLA  | C8-C10-C11-C12  |
| 26  | 4     | 801  | LHG  | C33-C34-C35-C36 |
| 35  | B     | 5004 | T7X  | C31-C32-C33-C34 |
| 22  | 6     | 608  | CLA  | C3-C5-C6-C7     |
| 26  | B     | 5006 | LHG  | O7-C5-C6-O8     |
| 26  | 1     | 801  | LHG  | O7-C5-C6-O8     |
| 26  | 8     | 801  | LHG  | O7-C5-C6-O8     |
| 26  | 4     | 801  | LHG  | O7-C5-C6-O8     |
| 31  | A     | 5003 | LMG  | O1-C7-C8-O7     |
| 35  | B     | 5004 | T7X  | O16-C8-C9-O18   |
| 41  | 2     | 803  | SQD  | O47-C45-C46-O48 |
| 43  | 7     | 802  | 3PH  | O21-C2-C3-O31   |
| 26  | 6     | 801  | LHG  | C27-C28-C29-C30 |
| 22  | B     | 1021 | CLA  | C16-C17-C18-C20 |
| 26  | B     | 5001 | LHG  | C4-C5-C6-O8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | 7     | 802  | 3PH  | C1-C2-C3-O31    |
| 43  | 8     | 806  | 3PH  | C1-C2-C3-O31    |
| 22  | A     | 1122 | CLA  | C15-C16-C17-C18 |
| 22  | 8     | 612  | CLA  | O1D-CGD-O2D-CED |
| 33  | B     | 5003 | DGD  | C1B-C2B-C3B-C4B |
| 22  | Z     | 605  | CLA  | CAD-CBD-CGD-O2D |
| 22  | Z     | 606  | CLA  | CAD-CBD-CGD-O2D |
| 22  | 7     | 609  | CLA  | CAD-CBD-CGD-O2D |
| 22  | 6     | 615  | CLA  | CAD-CBD-CGD-O2D |
| 22  | 2     | 605  | CLA  | CAD-CBD-CGD-O2D |
| 22  | 2     | 606  | CLA  | CAD-CBD-CGD-O2D |
| 40  | 1     | 610  | CHL  | CAD-CBD-CGD-O2D |
| 22  | B     | 1234 | CLA  | O1A-CGA-O2A-C1  |
| 41  | 1     | 802  | SQD  | C13-C14-C15-C16 |
| 22  | A     | 1122 | CLA  | C16-C17-C18-C20 |
| 22  | 1     | 612  | CLA  | C2A-CAA-CBA-CGA |
| 28  | A     | 5006 | LMT  | C2-C3-C4-C5     |
| 22  | A     | 1118 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 607  | CLA  | C10-C11-C12-C13 |
| 28  | 9     | 803  | LMT  | C2B-C1B-O1B-C4' |
| 26  | 1     | 801  | LHG  | C26-C27-C28-C29 |
| 22  | A     | 1135 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1208 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 1234 | CLA  | CAD-CBD-CGD-O1D |
| 22  | 1     | 604  | CLA  | CHA-CBD-CGD-O1D |
| 22  | 1     | 604  | CLA  | CHA-CBD-CGD-O2D |
| 22  | Z     | 605  | CLA  | CAD-CBD-CGD-O1D |
| 22  | Z     | 606  | CLA  | CAD-CBD-CGD-O1D |
| 22  | 7     | 609  | CLA  | CAD-CBD-CGD-O1D |
| 22  | 8     | 609  | CLA  | CAD-CBD-CGD-O1D |
| 22  | 6     | 615  | CLA  | CAD-CBD-CGD-O1D |
| 22  | 2     | 605  | CLA  | CAD-CBD-CGD-O1D |
| 22  | 2     | 606  | CLA  | CAD-CBD-CGD-O1D |
| 25  | A     | 4002 | BCR  | C19-C20-C21-C22 |
| 25  | A     | 4004 | BCR  | C19-C20-C21-C22 |
| 25  | K     | 4001 | BCR  | C15-C16-C17-C18 |
| 25  | 3     | 505  | BCR  | C15-C16-C17-C18 |
| 25  | 6     | 503  | BCR  | C15-C16-C17-C18 |
| 26  | A     | 5002 | LHG  | C4-O6-P-O5      |
| 26  | B     | 5002 | LHG  | C4-O6-P-O4      |
| 26  | 1     | 801  | LHG  | C4-O6-P-O5      |
| 26  | Z     | 801  | LHG  | C3-O3-P-O5      |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | 8     | 801  | LHG  | C3-O3-P-O5      |
| 26  | 4     | 801  | LHG  | C3-O3-P-O5      |
| 37  | 5     | 505  | C7Z  | C9-C10-C11-C12  |
| 37  | 5     | 505  | C7Z  | C33-C34-C35-C15 |
| 39  | 1     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | Z     | 502  | LUT  | C25-C26-C27-C28 |
| 39  | 3     | 501  | LUT  | C29-C30-C31-C32 |
| 39  | 5     | 502  | LUT  | C29-C30-C31-C32 |
| 40  | 1     | 610  | CHL  | CAD-CBD-CGD-O1D |
| 40  | 3     | 611  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 3     | 611  | CHL  | CHA-CBD-CGD-O2D |
| 40  | 8     | 610  | CHL  | CHA-CBD-CGD-O2D |
| 22  | B     | 1210 | CLA  | C16-C17-C18-C20 |
| 43  | 6     | 802  | 3PH  | C28-C29-C2A-C2B |
| 22  | B     | 1204 | CLA  | C13-C15-C16-C17 |
| 22  | 7     | 609  | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1104 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1109 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1112 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1116 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1121 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1131 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1134 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1101 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1022 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1205 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1214 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1227 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1238 | CLA  | C2B-C3B-CAB-CBB |
| 22  | F     | 1302 | CLA  | C2B-C3B-CAB-CBB |
| 22  | G     | 1601 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 1402 | CLA  | C2B-C3B-CAB-CBB |
| 22  | L     | 1502 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 601  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 611  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 612  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 612  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 3     | 618  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 609  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 613  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 618  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 601  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 25  | K     | 4001 | BCR  | C1-C6-C7-C8     |
| 25  | 3     | 505  | BCR  | C23-C24-C25-C30 |
| 25  | 6     | 503  | BCR  | C23-C24-C25-C30 |
| 37  | J     | 4002 | C7Z  | C21-C26-C27-C28 |
| 28  | F     | 5001 | LMT  | C11-C10-C9-C8   |
| 22  | B     | 1237 | CLA  | C2-C3-C5-C6     |
| 22  | B     | 1202 | CLA  | C2-C3-C5-C6     |
| 22  | 8     | 602  | CLA  | C2-C3-C5-C6     |
| 22  | 3     | 612  | CLA  | C5-C6-C7-C8     |
| 25  | K     | 4001 | BCR  | C36-C18-C19-C20 |
| 25  | 5     | 503  | BCR  | C36-C18-C19-C20 |
| 26  | B     | 5002 | LHG  | C2-C3-O3-P      |
| 26  | 1     | 801  | LHG  | C2-C3-O3-P      |
| 26  | Z     | 801  | LHG  | C2-C3-O3-P      |
| 26  | 8     | 801  | LHG  | C2-C3-O3-P      |
| 26  | 6     | 801  | LHG  | C2-C3-O3-P      |
| 45  | 8     | 803  | LPX  | C4-C3-O1-P1     |
| 22  | A     | 1137 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1125 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 608  | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1135 | CLA  | O1A-CGA-O2A-C1  |
| 32  | 9     | 802  | DGA  | CB6-CB7-CB8-CB9 |
| 22  | B     | 1202 | CLA  | C15-C16-C17-C18 |
| 22  | L     | 1502 | CLA  | C8-C10-C11-C12  |
| 25  | B     | 4005 | BCR  | C18-C19-C20-C21 |
| 25  | 3     | 506  | BCR  | C18-C19-C20-C21 |
| 25  | 5     | 504  | BCR  | C18-C19-C20-C21 |
| 25  | 6     | 504  | BCR  | C18-C19-C20-C21 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1123 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1132 | CLA  | C10-C11-C12-C13 |
| 22  | 5     | 607  | CLA  | C10-C11-C12-C13 |
| 22  | 5     | 618  | CLA  | C15-C16-C17-C18 |
| 21  | A     | 1011 | CL0  | O1D-CGD-O2D-CED |
| 22  | 8     | 612  | CLA  | CBD-CGD-O2D-CED |
| 25  | B     | 4004 | BCR  | C19-C20-C21-C22 |
| 25  | 3     | 505  | BCR  | C19-C20-C21-C22 |
| 22  | A     | 1121 | CLA  | C16-C17-C18-C20 |
| 22  | 5     | 613  | CLA  | C5-C6-C7-C8     |
| 26  | 6     | 801  | LHG  | C10-C11-C12-C13 |
| 45  | 8     | 803  | LPX  | C11-C12-C13-C14 |
| 22  | B     | 1234 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1221 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 1103 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1124 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 1126 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1138 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1216 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1240 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 612  | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 604  | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 608  | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 609  | CLA  | C11-C12-C13-C14 |
| 22  | 7     | 604  | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 605  | CLA  | C11-C12-C13-C14 |
| 22  | 4     | 604  | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 602  | CLA  | C11-C12-C13-C14 |
| 40  | Z     | 609  | CHL  | C11-C12-C13-C14 |
| 40  | 3     | 611  | CHL  | C6-C7-C8-C9     |
| 22  | A     | 1120 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1103 | CLA  | C11-C12-C13-C15 |
| 22  | 4     | 604  | CLA  | C11-C10-C8-C7   |
| 27  | A     | 5004 | NKP  | CAK-CAL-CAM-CAN |
| 26  | Z     | 801  | LHG  | C11-C12-C13-C14 |
| 26  | 8     | 801  | LHG  | C26-C27-C28-C29 |
| 22  | 3     | 601  | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1234 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1230 | CLA  | C4-C3-C5-C6     |
| 22  | 1     | 612  | CLA  | C4-C3-C5-C6     |
| 26  | 6     | 801  | LHG  | C33-C34-C35-C36 |
| 22  | 3     | 613  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1118 | CLA  | C11-C12-C13-C15 |
| 22  | 4     | 603  | CLA  | C16-C17-C18-C20 |
| 26  | 3     | 801  | LHG  | C2-C3-O3-P      |
| 31  | J     | 5001 | LMG  | O1-C7-C8-O7     |
| 41  | 1     | 802  | SQD  | O47-C45-C46-O48 |
| 25  | A     | 4001 | BCR  | C15-C16-C17-C18 |
| 25  | 7     | 503  | BCR  | C15-C16-C17-C18 |
| 22  | 1     | 608  | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1220 | CLA  | O1D-CGD-O2D-CED |
| 38  | 7     | 803  | SPH  | C13-C14-C15-C16 |
| 43  | 8     | 806  | 3PH  | C38-C39-C3A-C3B |
| 22  | B     | 1221 | CLA  | CAA-CBA-CGA-O2A |
| 40  | 8     | 610  | CHL  | CAA-CBA-CGA-O2A |
| 22  | 6     | 609  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1110 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1127 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1136 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 611  | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 603  | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 619  | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1213 | CLA  | C4-C3-C5-C6     |
| 22  | 5     | 618  | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1136 | CLA  | CAA-CBA-CGA-O2A |
| 33  | B     | 5003 | DGD  | C1G-C2G-C3G-O3G |
| 41  | 1     | 802  | SQD  | C44-C45-C46-O48 |
| 32  | 9     | 802  | DGA  | CB1-CB2-CB3-CB4 |
| 26  | B     | 5006 | LHG  | O8-C23-C24-C25  |
| 25  | A     | 4003 | BCR  | C36-C18-C19-C20 |
| 25  | 3     | 504  | BCR  | C11-C12-C13-C35 |
| 25  | A     | 4001 | BCR  | C17-C18-C19-C20 |
| 22  | B     | 1235 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1208 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 605  | CLA  | C2A-CAA-CBA-CGA |
| 39  | 7     | 502  | LUT  | C9-C10-C11-C12  |
| 22  | B     | 1213 | CLA  | C2-C3-C5-C6     |
| 28  | B     | 6101 | LMT  | C2-C1-O1'-C1'   |
| 22  | A     | 1120 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 1228 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1111 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1125 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1203 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1206 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | B     | 1208 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1217 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1219 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 604  | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 607  | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 611  | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 611  | CLA  | C14-C13-C15-C16 |
| 22  | Z     | 612  | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 609  | CLA  | C6-C7-C8-C9     |
| 23  | B     | 2002 | PQN  | C21-C22-C23-C24 |
| 30  | A     | 5007 | DAO  | C6-C7-C8-C9     |
| 22  | A     | 1122 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 1012 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1129 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1204 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1219 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1235 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 602  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 8     | 612  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 603  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 612  | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1108 | CLA  | C5-C6-C7-C8     |
| 26  | 6     | 801  | LHG  | C24-C25-C26-C27 |
| 22  | A     | 1125 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 1235 | CLA  | C13-C15-C16-C17 |
| 22  | 1     | 607  | CLA  | C10-C11-C12-C13 |
| 32  | 9     | 802  | DGA  | CB7-CB8-CB9-CAB |
| 35  | B     | 5004 | T7X  | O16-C10-C12-C13 |
| 38  | K     | 5001 | SPH  | C10-C11-C12-C13 |
| 22  | A     | 1108 | CLA  | C2-C3-C5-C6     |
| 40  | 7     | 610  | CHL  | C2-C3-C5-C6     |
| 35  | B     | 5004 | T7X  | C13-C14-C15-C16 |
| 28  | B     | 6101 | LMT  | C7-C8-C9-C10    |
| 26  | 5     | 801  | LHG  | C12-C13-C14-C15 |
| 25  | L     | 4001 | BCR  | C9-C10-C11-C12  |
| 39  | 2     | 503  | LUT  | C9-C10-C11-C12  |
| 22  | 4     | 605  | CLA  | C16-C17-C18-C19 |
| 22  | 6     | 619  | CLA  | C16-C17-C18-C19 |
| 43  | 6     | 802  | 3PH  | C27-C28-C29-C2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1104 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1111 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1112 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1209 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 607  | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 606  | CLA  | C11-C10-C8-C7   |
| 22  | 4     | 603  | CLA  | C11-C12-C13-C15 |
| 22  | B     | 1203 | CLA  | C13-C15-C16-C17 |
| 22  | 8     | 604  | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 612  | CLA  | CBA-CGA-O2A-C1  |
| 28  | A     | 5006 | LMT  | C5'-C4'-O1B-C1B |
| 32  | A     | 5005 | DGA  | OB1-CB1-OG2-CG2 |
| 22  | 4     | 608  | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 604  | CLA  | C16-C17-C18-C19 |
| 22  | B     | 1228 | CLA  | C8-C10-C11-C12  |
| 26  | B     | 5001 | LHG  | O10-C23-O8-C6   |
| 32  | A     | 5005 | DGA  | OG1-CG1-CG2-OG2 |
| 22  | A     | 1110 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 1128 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1220 | CLA  | C4-C3-C5-C6     |
| 22  | L     | 1503 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 616  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 603  | CLA  | C3A-C2A-CAA-CBA |
| 40  | Z     | 609  | CHL  | C3A-C2A-CAA-CBA |
| 22  | 1     | 612  | CLA  | C2-C3-C5-C6     |
| 25  | A     | 4005 | BCR  | C16-C17-C18-C36 |
| 25  | B     | 4003 | BCR  | C20-C21-C22-C37 |
| 25  | 5     | 504  | BCR  | C16-C17-C18-C36 |
| 36  | F     | 4001 | RRX  | C35-C13-C14-C15 |
| 39  | 2     | 503  | LUT  | C40-C33-C34-C35 |
| 22  | A     | 1119 | CLA  | C13-C15-C16-C17 |
| 22  | 3     | 605  | CLA  | C10-C11-C12-C13 |
| 26  | A     | 5002 | LHG  | C32-C33-C34-C35 |
| 22  | 9     | 602  | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1237 | CLA  | C10-C11-C12-C13 |
| 22  | 7     | 607  | CLA  | C2-C1-O2A-CGA   |
| 25  | L     | 4002 | BCR  | C19-C20-C21-C22 |
| 25  | 7     | 503  | BCR  | C13-C14-C15-C16 |
| 25  | 7     | 504  | BCR  | C19-C20-C21-C22 |
| 22  | B     | 1211 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 1210 | CLA  | C15-C16-C17-C18 |
| 22  | 3     | 606  | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 23  | A     | 2001 | PQN  | C15-C16-C17-C18 |
| 26  | 4     | 802  | LHG  | C2-C3-O3-P      |
| 22  | A     | 1127 | CLA  | CAA-CBA-CGA-O1A |
| 25  | A     | 4004 | BCR  | C17-C18-C19-C20 |
| 22  | B     | 1241 | CLA  | C4-C3-C5-C6     |
| 22  | 6     | 619  | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1238 | CLA  | C16-C17-C18-C19 |
| 27  | A     | 5004 | NKP  | OAF-CAG-CAH-CAI |
| 22  | A     | 1117 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1203 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1104 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1105 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1112 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1203 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1207 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 1221 | CLA  | C14-C13-C15-C16 |
| 22  | L     | 1502 | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 604  | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 612  | CLA  | C6-C7-C8-C9     |
| 22  | 8     | 606  | CLA  | C11-C10-C8-C9   |
| 22  | 4     | 603  | CLA  | C11-C12-C13-C14 |
| 22  | 6     | 615  | CLA  | C11-C10-C8-C9   |
| 22  | 9     | 601  | CLA  | C6-C7-C8-C9     |
| 40  | Z     | 610  | CHL  | C6-C7-C8-C9     |
| 22  | A     | 1130 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 1228 | CLA  | C10-C11-C12-C13 |
| 26  | Z     | 801  | LHG  | C9-C10-C11-C12  |
| 22  | A     | 1138 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 609  | CLA  | C3-C5-C6-C7     |
| 22  | 4     | 607  | CLA  | C3-C5-C6-C7     |
| 40  | 7     | 610  | CHL  | C1A-C2A-CAA-CBA |
| 40  | 5     | 611  | CHL  | C1A-C2A-CAA-CBA |
| 40  | 2     | 610  | CHL  | C1A-C2A-CAA-CBA |
| 32  | A     | 5005 | DGA  | CA4-CA5-CA6-CA7 |
| 25  | B     | 4004 | BCR  | C9-C10-C11-C12  |
| 25  | K     | 4001 | BCR  | C9-C10-C11-C12  |
| 22  | B     | 1022 | CLA  | C4-C3-C5-C6     |
| 22  | Z     | 603  | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1205 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 1     | 608  | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 1110 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1133 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1134 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 1222 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 1403 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 616  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 608  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 615  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 609  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 603  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 609  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 609  | CLA  | C1A-C2A-CAA-CBA |
| 25  | A     | 4005 | BCR  | C16-C17-C18-C19 |
| 25  | B     | 4003 | BCR  | C20-C21-C22-C23 |
| 25  | 5     | 504  | BCR  | C16-C17-C18-C19 |
| 36  | F     | 4001 | RRX  | C12-C13-C14-C15 |
| 39  | 2     | 503  | LUT  | C32-C33-C34-C35 |
| 22  | A     | 1012 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1129 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1139 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1237 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1204 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1217 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1224 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1230 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1231 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1232 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1235 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1239 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1241 | CLA  | C2B-C3B-CAB-CBB |
| 22  | J     | 1901 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 1401 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 1403 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 601  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 611  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 612  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 613  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 616  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 611  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 612  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 601  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 4     | 603  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 612  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 605  | CLA  | C2B-C3B-CAB-CBB |
| 25  | A     | 4003 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 4001 | BCR  | C5-C6-C7-C8     |
| 25  | B     | 4001 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 4004 | BCR  | C23-C24-C25-C26 |
| 25  | B     | 4007 | BCR  | C1-C6-C7-C8     |
| 25  | G     | 4001 | BCR  | C5-C6-C7-C8     |
| 25  | G     | 4001 | BCR  | C23-C24-C25-C26 |
| 25  | K     | 4002 | BCR  | C1-C6-C7-C8     |
| 25  | K     | 4002 | BCR  | C5-C6-C7-C8     |
| 25  | L     | 4001 | BCR  | C1-C6-C7-C8     |
| 25  | L     | 4002 | BCR  | C23-C24-C25-C26 |
| 25  | 3     | 505  | BCR  | C23-C24-C25-C26 |
| 25  | 7     | 504  | BCR  | C23-C24-C25-C26 |
| 25  | 5     | 504  | BCR  | C23-C24-C25-C26 |
| 37  | 1     | 503  | C7Z  | C5-C6-C7-C8     |
| 39  | 1     | 501  | LUT  | C1-C6-C7-C8     |
| 39  | 7     | 501  | LUT  | C1-C6-C7-C8     |
| 39  | 2     | 501  | LUT  | C1-C6-C7-C8     |
| 22  | 1     | 602  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 602  | CLA  | CAA-CBA-CGA-O2A |
| 26  | 7     | 801  | LHG  | C30-C31-C32-C33 |
| 22  | 5     | 618  | CLA  | C3-C5-C6-C7     |
| 38  | 7     | 804  | SPH  | O1-C1-C2-N2     |
| 22  | 4     | 608  | CLA  | C4-C3-C5-C6     |
| 22  | 5     | 607  | CLA  | C4-C3-C5-C6     |
| 40  | Z     | 610  | CHL  | C4-C3-C5-C6     |
| 31  | J     | 5001 | LMG  | C11-C12-C13-C14 |
| 22  | B     | 1220 | CLA  | C2-C3-C5-C6     |
| 22  | 1     | 602  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1121 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1237 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | L     | 1502 | CLA  | C12-C13-C15-C16 |
| 22  | 3     | 601  | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 606  | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 604  | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 609  | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 609  | CLA  | C11-C10-C8-C7   |
| 23  | B     | 2002 | PQN  | C21-C22-C23-C25 |
| 40  | Z     | 609  | CHL  | C12-C13-C15-C16 |
| 22  | B     | 1236 | CLA  | C2A-CAA-CBA-CGA |
| 40  | Z     | 613  | CHL  | CAA-CBA-CGA-O1A |
| 40  | Z     | 613  | CHL  | CAA-CBA-CGA-O2A |
| 22  | 1     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 1     | 801  | LHG  | C13-C14-C15-C16 |
| 40  | 5     | 610  | CHL  | C13-C15-C16-C17 |
| 22  | A     | 1121 | CLA  | C16-C17-C18-C19 |
| 38  | K     | 5001 | SPH  | C11-C10-C9-C8   |
| 43  | 7     | 802  | 3PH  | C34-C35-C36-C37 |
| 22  | 2     | 604  | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1127 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 1206 | CLA  | C10-C11-C12-C13 |
| 25  | B     | 4005 | BCR  | C37-C22-C23-C24 |
| 25  | B     | 4007 | BCR  | C36-C18-C19-C20 |
| 22  | A     | 1138 | CLA  | C4-C3-C5-C6     |
| 23  | B     | 2002 | PQN  | C14-C13-C15-C16 |
| 40  | 9     | 610  | CHL  | C4-C3-C5-C6     |
| 22  | 2     | 612  | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1241 | CLA  | C2-C3-C5-C6     |
| 22  | 1     | 606  | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 1126 | CLA  | C10-C11-C12-C13 |
| 26  | A     | 5002 | LHG  | C11-C10-C9-C8   |
| 22  | A     | 1106 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1237 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 1222 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 607  | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1013 | CLA  | C5-C6-C7-C8     |
| 25  | 6     | 504  | BCR  | C15-C16-C17-C18 |
| 22  | 5     | 609  | CLA  | C15-C16-C17-C18 |
| 26  | 5     | 801  | LHG  | C29-C30-C31-C32 |
| 22  | L     | 1503 | CLA  | CBA-CGA-O2A-C1  |
| 41  | 2     | 803  | SQD  | C11-C12-C13-C14 |
| 22  | 8     | 609  | CLA  | C4-C3-C5-C6     |
| 22  | B     | 1240 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 5     | 618  | CLA  | C2-C3-C5-C6     |
| 22  | 6     | 619  | CLA  | C2-C3-C5-C6     |
| 40  | Z     | 610  | CHL  | C2-C3-C5-C6     |
| 43  | 7     | 802  | 3PH  | C37-C38-C39-C3A |
| 22  | B     | 1221 | CLA  | C15-C16-C17-C18 |
| 22  | 7     | 612  | CLA  | O1A-CGA-O2A-C1  |
| 26  | 4     | 801  | LHG  | C16-C17-C18-C19 |
| 45  | 8     | 803  | LPX  | C14-C15-C16-C17 |
| 26  | 6     | 801  | LHG  | C4-C5-C6-O8     |
| 31  | A     | 5003 | LMG  | O1-C7-C8-C9     |
| 22  | A     | 1107 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 1134 | CLA  | C2A-CAA-CBA-CGA |
| 40  | 2     | 609  | CHL  | C2A-CAA-CBA-CGA |
| 22  | B     | 1240 | CLA  | C5-C6-C7-C8     |
| 22  | 2     | 603  | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1208 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1123 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 1136 | CLA  | C13-C15-C16-C17 |
| 22  | 1     | 606  | CLA  | C4-C3-C5-C6     |
| 25  | L     | 4002 | BCR  | C9-C10-C11-C12  |
| 40  | 1     | 610  | CHL  | CAA-CBA-CGA-O2A |
| 22  | K     | 1404 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1119 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1212 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1215 | CLA  | C4B-C3B-CAB-CBB |
| 22  | J     | 1901 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 607  | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 606  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 605  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 612  | CLA  | CBA-CGA-O2A-C1  |
| 26  | 4     | 801  | LHG  | C26-C27-C28-C29 |
| 21  | A     | 1011 | CL0  | CHA-CBD-CGD-O1D |
| 21  | A     | 1011 | CL0  | CHA-CBD-CGD-O2D |
| 40  | 8     | 613  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 8     | 613  | CHL  | CHA-CBD-CGD-O2D |
| 40  | 5     | 610  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 5     | 610  | CHL  | CHA-CBD-CGD-O2D |
| 40  | 5     | 611  | CHL  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 40  | 5     | 611  | CHL  | CHA-CBD-CGD-O2D |
| 40  | 6     | 611  | CHL  | CHA-CBD-CGD-O1D |
| 40  | 6     | 611  | CHL  | CHA-CBD-CGD-O2D |
| 22  | 7     | 615  | CLA  | CAA-CBA-CGA-O2A |
| 23  | A     | 2001 | PQN  | C26-C27-C28-C30 |
| 22  | A     | 1120 | CLA  | C4-C3-C5-C6     |
| 22  | L     | 1502 | CLA  | C4-C3-C5-C6     |
| 22  | 7     | 606  | CLA  | C4-C3-C5-C6     |
| 22  | 6     | 607  | CLA  | C4-C3-C5-C6     |
| 26  | 7     | 801  | LHG  | O7-C5-C6-O8     |
| 22  | A     | 1103 | CLA  | C5-C6-C7-C8     |
| 25  | 7     | 503  | BCR  | C7-C8-C9-C34    |
| 22  | A     | 1106 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1122 | CLA  | C11-C10-C8-C7   |
| 26  | 9     | 801  | LHG  | C26-C27-C28-C29 |
| 22  | 9     | 608  | CLA  | CAA-CBA-CGA-O1A |
| 26  | B     | 5006 | LHG  | C27-C28-C29-C30 |
| 32  | A     | 5005 | DGA  | CBB-CCB-CDB-CEB |
| 28  | B     | 6101 | LMT  | C5'-C4'-O1B-C1B |
| 22  | A     | 1105 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 1113 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 1140 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1206 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 612  | CLA  | C14-C13-C15-C16 |
| 22  | 3     | 601  | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 603  | CLA  | C6-C7-C8-C9     |
| 28  | B     | 6101 | LMT  | C4B-C5B-C6B-O6B |
| 22  | 4     | 602  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 9     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 38  | 7     | 803  | SPH  | C4-C5-C6-C7     |
| 40  | 8     | 610  | CHL  | C2A-CAA-CBA-CGA |
| 22  | L     | 1503 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 5     | 801  | LHG  | C7-C8-C9-C10    |
| 22  | B     | 1238 | CLA  | C4-C3-C5-C6     |
| 22  | 3     | 601  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 601  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 604  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 605  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 9     | 604  | CLA  | C3A-C2A-CAA-CBA |
| 40  | 2     | 609  | CHL  | CAA-CBA-CGA-O2A |
| 22  | A     | 1110 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1138 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 4     | 608  | CLA  | C2-C3-C5-C6     |
| 22  | 5     | 604  | CLA  | C10-C11-C12-C13 |
| 27  | A     | 5004 | NKP  | CAQ-CAR-CAS-CAT |
| 26  | 7     | 801  | LHG  | C26-C27-C28-C29 |
| 26  | 8     | 801  | LHG  | C7-C8-C9-C10    |
| 22  | Z     | 602  | CLA  | O1A-CGA-O2A-C1  |
| 40  | 8     | 613  | CHL  | C10-C11-C12-C13 |
| 22  | 1     | 604  | CLA  | C11-C12-C13-C15 |
| 28  | B     | 5005 | LMT  | O5'-C1'-O1'-C1  |
| 26  | 8     | 801  | LHG  | C9-C10-C11-C12  |
| 32  | A     | 5005 | DGA  | CEA-CFA-CGA-CHA |
| 22  | B     | 1235 | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 1124 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1230 | CLA  | C2-C3-C5-C6     |
| 22  | 7     | 609  | CLA  | C2-C3-C5-C6     |
| 25  | 3     | 506  | BCR  | C19-C20-C21-C22 |
| 25  | 6     | 503  | BCR  | C13-C14-C15-C16 |
| 39  | 5     | 501  | LUT  | C29-C30-C31-C32 |
| 22  | B     | 1234 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 1127 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 1240 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1240 | CLA  | C15-C16-C17-C18 |
| 26  | 6     | 801  | LHG  | C26-C27-C28-C29 |
| 22  | 7     | 609  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1125 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 605  | CLA  | C3-C5-C6-C7     |
| 44  | 7     | 805  | PLM  | CC-CD-CE-CF     |
| 22  | A     | 1138 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1220 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 1238 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 612  | CLA  | C6-C7-C8-C9     |
| 22  | A     | 1137 | CLA  | CAA-CBA-CGA-O2A |
| 22  | G     | 1601 | CLA  | CAA-CBA-CGA-O2A |
| 22  | L     | 1502 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 605  | CLA  | CAA-CBA-CGA-O2A |
| 26  | Z     | 801  | LHG  | O6-C4-C5-C6     |
| 25  | 3     | 504  | BCR  | C11-C12-C13-C14 |
| 25  | 3     | 504  | BCR  | C17-C18-C19-C20 |
| 28  | 9     | 803  | LMT  | C9-C10-C11-C12  |
| 22  | 1     | 601  | CLA  | C5-C6-C7-C8     |
| 22  | 2     | 604  | CLA  | CAA-CBA-CGA-O2A |
| 23  | B     | 2002 | PQN  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 2     | 602  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1110 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 1115 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1222 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 612  | CLA  | C12-C13-C15-C16 |
| 22  | Z     | 607  | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 601  | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 615  | CLA  | C11-C10-C8-C7   |
| 40  | Z     | 610  | CHL  | C11-C10-C8-C7   |
| 40  | Z     | 609  | CHL  | C11-C12-C13-C15 |
| 43  | 6     | 802  | 3PH  | C32-C33-C34-C35 |
| 22  | A     | 1108 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1119 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1124 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1126 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1133 | CLA  | C2B-C3B-CAB-CBB |
| 22  | A     | 1141 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1023 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1203 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1215 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1219 | CLA  | C2B-C3B-CAB-CBB |
| 22  | B     | 1220 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 1404 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 602  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 605  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 613  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 605  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 608  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 604  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 606  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 8     | 607  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 615  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 601  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 618  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 601  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 612  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 601  | CLA  | C2B-C3B-CAB-CBB |
| 22  | 2     | 603  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | A     | 4001 | BCR  | C23-C24-C25-C26 |
| 25  | A     | 4001 | BCR  | C23-C24-C25-C30 |
| 25  | B     | 4007 | BCR  | C5-C6-C7-C8     |
| 25  | K     | 4001 | BCR  | C5-C6-C7-C8     |
| 25  | L     | 4001 | BCR  | C5-C6-C7-C8     |
| 25  | 3     | 503  | BCR  | C23-C24-C25-C26 |
| 25  | 3     | 506  | BCR  | C1-C6-C7-C8     |
| 25  | 3     | 506  | BCR  | C5-C6-C7-C8     |
| 25  | 6     | 503  | BCR  | C23-C24-C25-C26 |
| 37  | J     | 4002 | C7Z  | C5-C6-C7-C8     |
| 39  | Z     | 501  | LUT  | C1-C6-C7-C8     |
| 39  | Z     | 501  | LUT  | C5-C6-C7-C8     |
| 39  | 3     | 502  | LUT  | C1-C6-C7-C8     |
| 39  | 7     | 501  | LUT  | C5-C6-C7-C8     |
| 39  | 8     | 501  | LUT  | C5-C6-C7-C8     |
| 39  | 2     | 501  | LUT  | C5-C6-C7-C8     |
| 22  | B     | 1207 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 611  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 2     | 607  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1139 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 605  | CLA  | C2-C1-O2A-CGA   |
| 32  | A     | 5005 | DGA  | CB6-CB7-CB8-CB9 |
| 26  | B     | 5001 | LHG  | C2-C3-O3-P      |
| 26  | 9     | 801  | LHG  | C5-C4-O6-P      |
| 22  | A     | 1104 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 602  | CLA  | CAA-CBA-CGA-O2A |
| 33  | B     | 5003 | DGD  | O1G-C1A-C2A-C3A |
| 22  | A     | 1106 | CLA  | C13-C15-C16-C17 |
| 22  | 9     | 601  | CLA  | C8-C10-C11-C12  |
| 22  | K     | 1402 | CLA  | C4-C3-C5-C6     |
| 22  | 6     | 615  | CLA  | CAA-CBA-CGA-O2A |
| 32  | A     | 5005 | DGA  | OG1-CA1-CA2-CA3 |
| 22  | 3     | 601  | CLA  | C8-C10-C11-C12  |
| 26  | 1     | 801  | LHG  | O2-C2-C3-O3     |
| 22  | A     | 1122 | CLA  | CBD-CGD-O2D-CED |
| 40  | 1     | 610  | CHL  | C2C-C3C-CAC-CBC |
| 32  | A     | 5005 | DGA  | CB2-CB1-OG2-CG2 |
| 22  | B     | 1216 | CLA  | CAA-CBA-CGA-O2A |
| 27  | A     | 5004 | NKP  | CAO-CAP-CAQ-CAR |
| 22  | A     | 1131 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1136 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 1206 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 3     | 610  | CLA  | CAA-CBA-CGA-O2A |
| 26  | 6     | 801  | LHG  | O8-C23-C24-C25  |
| 26  | 9     | 801  | LHG  | O8-C23-C24-C25  |
| 40  | 8     | 613  | CHL  | CAA-CBA-CGA-O2A |
| 40  | 6     | 611  | CHL  | CAA-CBA-CGA-O2A |
| 25  | K     | 4002 | BCR  | C9-C10-C11-C12  |
| 41  | 2     | 803  | SQD  | C4-C5-C6-S      |
| 22  | 1     | 603  | CLA  | CAA-CBA-CGA-O2A |
| 26  | Z     | 801  | LHG  | O7-C7-C8-C9     |
| 22  | B     | 1226 | CLA  | C13-C15-C16-C17 |
| 22  | 5     | 607  | CLA  | C2-C3-C5-C6     |
| 26  | A     | 5002 | LHG  | C27-C28-C29-C30 |
| 22  | 6     | 602  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 1131 | CLA  | CAA-CBA-CGA-O2A |
| 22  | L     | 1503 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 612  | CLA  | CAA-CBA-CGA-O2A |
| 26  | A     | 5002 | LHG  | C24-C25-C26-C27 |
| 22  | 3     | 606  | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 619  | CLA  | C6-C7-C8-C9     |
| 23  | B     | 2002 | PQN  | C19-C18-C20-C21 |
| 22  | B     | 1236 | CLA  | C10-C11-C12-C13 |
| 32  | A     | 5005 | DGA  | OG1-CG1-CG2-CG3 |
| 22  | B     | 1238 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 1108 | CLA  | C4B-C3B-CAB-CBB |
| 22  | A     | 1128 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 1130 | CLA  | C4B-C3B-CAB-CBB |
| 22  | B     | 1210 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 604  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 616  | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 601  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 615  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 618  | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 605  | CLA  | C1A-C2A-CAA-CBA |
| 43  | 8     | 806  | 3PH  | C32-C33-C34-C35 |
| 22  | A     | 1104 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 1121 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1125 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1134 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1237 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 603  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 607  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 9     | 607  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 40  | 4     | 611  | CHL  | CAA-CBA-CGA-O2A |
| 26  | 6     | 801  | LHG  | C17-C18-C19-C20 |
| 26  | B     | 5002 | LHG  | O7-C5-C6-O8     |
| 26  | 9     | 801  | LHG  | O7-C5-C6-O8     |
| 25  | A     | 4001 | BCR  | C21-C22-C23-C24 |
| 25  | A     | 4003 | BCR  | C17-C18-C19-C20 |
| 25  | B     | 4005 | BCR  | C7-C8-C9-C10    |
| 25  | 3     | 506  | BCR  | C11-C12-C13-C14 |
| 25  | 7     | 503  | BCR  | C7-C8-C9-C10    |
| 25  | 5     | 503  | BCR  | C7-C8-C9-C10    |
| 25  | 5     | 503  | BCR  | C17-C18-C19-C20 |
| 25  | G     | 4001 | BCR  | C19-C20-C21-C22 |
| 37  | J     | 4002 | C7Z  | C13-C14-C15-C35 |
| 26  | 2     | 801  | LHG  | C27-C28-C29-C30 |
| 38  | K     | 5001 | SPH  | C13-C14-C15-C16 |
| 22  | K     | 1404 | CLA  | C6-C7-C8-C10    |
| 26  | Z     | 801  | LHG  | C31-C32-C33-C34 |
| 22  | A     | 1108 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1128 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1241 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 609  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 609  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 2     | 605  | CLA  | C2A-CAA-CBA-CGA |
| 26  | B     | 5006 | LHG  | C9-C10-C11-C12  |
| 22  | 5     | 605  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 6     | 601  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 6     | 603  | CLA  | CAA-CBA-CGA-O2A |
| 26  | 5     | 801  | LHG  | O7-C7-C8-C9     |
| 31  | J     | 5001 | LMG  | O8-C28-C29-C30  |
| 32  | A     | 5005 | DGA  | CA3-CA4-CA5-CA6 |
| 22  | A     | 1135 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 1130 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 1223 | CLA  | C15-C16-C17-C18 |
| 40  | 5     | 610  | CHL  | C2-C1-O2A-CGA   |
| 40  | 6     | 613  | CHL  | C2-C1-O2A-CGA   |
| 22  | B     | 1212 | CLA  | CAA-CBA-CGA-O2A |
| 41  | 1     | 802  | SQD  | C25-C26-C27-C28 |
| 22  | A     | 1105 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1121 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1123 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1124 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1128 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 1131 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 1140 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 1140 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1219 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 1236 | CLA  | C12-C13-C15-C16 |
| 22  | 1     | 601  | CLA  | C11-C10-C8-C7   |
| 22  | 8     | 605  | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 603  | CLA  | C6-C7-C8-C10    |
| 22  | B     | 1228 | CLA  | C16-C17-C18-C19 |
| 26  | 8     | 801  | LHG  | O7-C7-C8-C9     |
| 22  | 1     | 604  | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 1210 | CLA  | C5-C6-C7-C8     |
| 22  | 4     | 603  | CLA  | C5-C6-C7-C8     |
| 41  | 1     | 802  | SQD  | C29-C30-C31-C32 |
| 22  | A     | 1137 | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 1130 | CLA  | C8-C10-C11-C12  |
| 26  | 9     | 801  | LHG  | C27-C28-C29-C30 |
| 22  | A     | 1121 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1210 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1213 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 1217 | CLA  | C4-C3-C5-C6     |
| 22  | F     | 1301 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 604  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 606  | CLA  | C3A-C2A-CAA-CBA |
| 22  | 9     | 601  | CLA  | C3A-C2A-CAA-CBA |
| 32  | A     | 5005 | DGA  | OA1-CA1-CA2-CA3 |
| 22  | A     | 1140 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 606  | CLA  | C8-C10-C11-C12  |
| 22  | Z     | 605  | CLA  | C13-C15-C16-C17 |
| 35  | B     | 5004 | T7X  | C26-C27-C28-C29 |
| 22  | B     | 1022 | CLA  | C2-C3-C5-C6     |
| 33  | B     | 5003 | DGD  | CFA-CGA-CHA-CIA |
| 26  | A     | 5002 | LHG  | C9-C10-C11-C12  |
| 22  | B     | 1206 | CLA  | CAA-CBA-CGA-O1A |
| 22  | K     | 1402 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 5     | 612  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 607  | CLA  | CAA-CBA-CGA-O2A |
| 22  | G     | 1601 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Z     | 602  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 615  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 4     | 604  | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | A     | 1124 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 1219 | CLA  | C11-C10-C8-C9   |
| 22  | L     | 1502 | CLA  | C14-C13-C15-C16 |
| 22  | 4     | 605  | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 607  | CLA  | C6-C7-C8-C9     |
| 40  | Z     | 610  | CHL  | C11-C10-C8-C9   |
| 22  | 9     | 606  | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 603  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 2     | 607  | CLA  | CAA-CBA-CGA-O1A |
| 26  | 4     | 802  | LHG  | C10-C11-C12-C13 |
| 22  | A     | 1108 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1216 | CLA  | CAA-CBA-CGA-O1A |
| 22  | L     | 1502 | CLA  | CAA-CBA-CGA-O1A |
| 22  | L     | 1503 | CLA  | CAA-CBA-CGA-O1A |
| 31  | J     | 5001 | LMG  | O10-C28-C29-C30 |
| 39  | Z     | 501  | LUT  | C21-C26-C27-C28 |
| 39  | 3     | 501  | LUT  | C21-C26-C27-C28 |
| 39  | 7     | 501  | LUT  | C21-C26-C27-C28 |
| 39  | 9     | 501  | LUT  | C21-C26-C27-C28 |
| 41  | 2     | 803  | SQD  | O5-C5-C6-S      |
| 22  | 2     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1131 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 4     | 605  | CLA  | CAA-CBA-CGA-O1A |
| 26  | 5     | 801  | LHG  | O9-C7-C8-C9     |
| 26  | 6     | 801  | LHG  | O10-C23-C24-C25 |
| 40  | 6     | 611  | CHL  | CAA-CBA-CGA-O1A |
| 22  | 7     | 606  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1134 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1207 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 1     | 603  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 3     | 610  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 7     | 609  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 5     | 605  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 607  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 3     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1104 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 605  | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1110 | CLA  | C15-C16-C17-C18 |
| 43  | 7     | 802  | 3PH  | C3C-C3D-C3E-C3F |
| 22  | A     | 1128 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1237 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 603  | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 26  | 5     | 801  | LHG  | O10-C23-C24-C25 |
| 28  | 9     | 803  | LMT  | O5B-C1B-O1B-C4' |
| 22  | A     | 1127 | CLA  | C15-C16-C17-C18 |
| 22  | F     | 1301 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 1113 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1211 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 1     | 613  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 1     | 606  | CLA  | C2-C3-C5-C6     |
| 22  | Z     | 608  | CLA  | CAA-CBA-CGA-O1A |
| 40  | 8     | 613  | CHL  | CAA-CBA-CGA-O1A |
| 22  | A     | 1124 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1205 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 1211 | CLA  | CAD-CBD-CGD-O2D |
| 22  | G     | 1602 | CLA  | CAD-CBD-CGD-O2D |
| 22  | 6     | 619  | CLA  | CAD-CBD-CGD-O2D |
| 40  | 6     | 613  | CHL  | CAD-CBD-CGD-O2D |
| 22  | B     | 1204 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 40  | Z     | 609  | CHL  | CAA-CBA-CGA-O2A |
| 22  | 4     | 609  | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 1107 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 1241 | CLA  | C2-C1-O2A-CGA   |
| 22  | K     | 1402 | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 601  | CLA  | C2-C1-O2A-CGA   |
| 26  | Z     | 801  | LHG  | O9-C7-C8-C9     |
| 26  | 8     | 801  | LHG  | O9-C7-C8-C9     |
| 22  | Z     | 607  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 607  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 618  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 6     | 604  | CLA  | CAA-CBA-CGA-O2A |
| 31  | J     | 5001 | LMG  | O7-C10-C11-C12  |
| 22  | 1     | 604  | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 612  | CLA  | C11-C12-C13-C15 |
| 33  | B     | 5003 | DGD  | C2B-C3B-C4B-C5B |
| 22  | 5     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 607  | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 1103 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 1135 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 7     | 605  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 608  | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 607  | CLA  | CAA-CBA-CGA-O2A |
| 26  | 7     | 801  | LHG  | O8-C23-C24-C25  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 27  | A     | 5004 | NKP  | OAJ-CAK-CAL-CAM |
| 40  | 2     | 610  | CHL  | CAA-CBA-CGA-O2A |
| 22  | 2     | 608  | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1212 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 606  | CLA  | CAA-CBA-CGA-O1A |
| 26  | 9     | 801  | LHG  | O10-C23-C24-C25 |
| 26  | Z     | 801  | LHG  | C26-C27-C28-C29 |
| 22  | B     | 1021 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1203 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 1219 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 603  | CLA  | CAA-CBA-CGA-O2A |
| 30  | A     | 5007 | DAO  | C1-C2-C3-C4     |
| 22  | A     | 1121 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 1236 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 7     | 606  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 8     | 609  | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 601  | CLA  | CAA-CBA-CGA-O1A |
| 27  | A     | 5004 | NKP  | OAE-CAK-CAL-CAM |
| 43  | 8     | 806  | 3PH  | C36-C37-C38-C39 |

There are no ring outliers.

290 monomers are involved in 585 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | B     | 1226 | CLA  | 3       | 0            |
| 40  | 9     | 610  | CHL  | 1       | 0            |
| 22  | 3     | 605  | CLA  | 3       | 0            |
| 25  | G     | 4001 | BCR  | 1       | 0            |
| 22  | 5     | 606  | CLA  | 1       | 0            |
| 28  | 9     | 803  | LMT  | 3       | 0            |
| 22  | B     | 1222 | CLA  | 4       | 0            |
| 22  | 1     | 615  | CLA  | 3       | 0            |
| 22  | B     | 1221 | CLA  | 3       | 0            |
| 22  | 7     | 616  | CLA  | 3       | 0            |
| 22  | B     | 1225 | CLA  | 3       | 0            |
| 22  | A     | 1119 | CLA  | 3       | 0            |
| 22  | 8     | 607  | CLA  | 4       | 0            |
| 22  | A     | 1115 | CLA  | 4       | 0            |
| 39  | 2     | 502  | LUT  | 4       | 0            |
| 22  | 1     | 607  | CLA  | 2       | 0            |
| 25  | 3     | 504  | BCR  | 3       | 0            |
| 22  | 4     | 609  | CLA  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | 9     | 606  | CLA  | 1       | 0            |
| 22  | 9     | 601  | CLA  | 3       | 0            |
| 22  | 3     | 601  | CLA  | 3       | 0            |
| 22  | 5     | 622  | CLA  | 1       | 0            |
| 22  | A     | 1109 | CLA  | 3       | 0            |
| 22  | B     | 1229 | CLA  | 2       | 0            |
| 25  | B     | 4001 | BCR  | 2       | 0            |
| 25  | B     | 4007 | BCR  | 3       | 0            |
| 40  | 2     | 613  | CHL  | 1       | 0            |
| 22  | L     | 1502 | CLA  | 1       | 0            |
| 26  | 4     | 801  | LHG  | 1       | 0            |
| 40  | 1     | 609  | CHL  | 1       | 0            |
| 22  | 5     | 618  | CLA  | 5       | 0            |
| 22  | B     | 1232 | CLA  | 1       | 0            |
| 22  | A     | 1120 | CLA  | 2       | 0            |
| 22  | A     | 1013 | CLA  | 5       | 0            |
| 40  | Z     | 613  | CHL  | 4       | 0            |
| 22  | 2     | 604  | CLA  | 2       | 0            |
| 26  | B     | 5001 | LHG  | 1       | 0            |
| 22  | 8     | 612  | CLA  | 1       | 0            |
| 22  | 5     | 607  | CLA  | 3       | 0            |
| 39  | Z     | 503  | LUT  | 3       | 0            |
| 22  | B     | 1203 | CLA  | 3       | 0            |
| 22  | 3     | 603  | CLA  | 3       | 0            |
| 22  | A     | 1106 | CLA  | 2       | 0            |
| 22  | A     | 1128 | CLA  | 5       | 0            |
| 22  | B     | 1213 | CLA  | 4       | 0            |
| 25  | 7     | 503  | BCR  | 3       | 0            |
| 22  | A     | 1123 | CLA  | 1       | 0            |
| 25  | 3     | 503  | BCR  | 1       | 0            |
| 25  | 6     | 503  | BCR  | 3       | 0            |
| 22  | A     | 1114 | CLA  | 4       | 0            |
| 39  | 2     | 501  | LUT  | 1       | 0            |
| 22  | 8     | 603  | CLA  | 1       | 0            |
| 32  | 9     | 802  | DGA  | 4       | 0            |
| 22  | 6     | 612  | CLA  | 3       | 0            |
| 22  | B     | 1021 | CLA  | 6       | 0            |
| 22  | B     | 1220 | CLA  | 5       | 0            |
| 22  | 9     | 602  | CLA  | 1       | 0            |
| 40  | 1     | 610  | CHL  | 1       | 0            |
| 22  | 3     | 606  | CLA  | 4       | 0            |
| 40  | 8     | 613  | CHL  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | A     | 4003 | BCR  | 3       | 0            |
| 28  | 1     | 803  | LMT  | 2       | 0            |
| 22  | A     | 1139 | CLA  | 2       | 0            |
| 22  | B     | 1214 | CLA  | 6       | 0            |
| 22  | B     | 1205 | CLA  | 3       | 0            |
| 22  | 6     | 607  | CLA  | 1       | 0            |
| 39  | 1     | 502  | LUT  | 4       | 0            |
| 45  | 8     | 803  | LPX  | 1       | 0            |
| 22  | 5     | 612  | CLA  | 1       | 0            |
| 22  | 6     | 605  | CLA  | 2       | 0            |
| 22  | Z     | 605  | CLA  | 4       | 0            |
| 24  | C     | 3003 | SF4  | 1       | 0            |
| 22  | 7     | 612  | CLA  | 1       | 0            |
| 22  | 4     | 604  | CLA  | 4       | 0            |
| 22  | B     | 1236 | CLA  | 6       | 0            |
| 22  | A     | 1107 | CLA  | 3       | 0            |
| 22  | A     | 1129 | CLA  | 2       | 0            |
| 40  | 5     | 617  | CHL  | 1       | 0            |
| 41  | 1     | 802  | SQD  | 1       | 0            |
| 22  | B     | 1215 | CLA  | 3       | 0            |
| 22  | B     | 1235 | CLA  | 3       | 0            |
| 22  | A     | 1118 | CLA  | 3       | 0            |
| 28  | 8     | 805  | LMT  | 1       | 0            |
| 22  | A     | 1103 | CLA  | 4       | 0            |
| 22  | 4     | 606  | CLA  | 1       | 0            |
| 26  | A     | 5001 | LHG  | 3       | 0            |
| 22  | 6     | 603  | CLA  | 3       | 0            |
| 25  | A     | 4001 | BCR  | 1       | 0            |
| 25  | A     | 4002 | BCR  | 4       | 0            |
| 26  | 7     | 801  | LHG  | 2       | 0            |
| 22  | A     | 1116 | CLA  | 6       | 0            |
| 22  | 1     | 605  | CLA  | 1       | 0            |
| 26  | 6     | 801  | LHG  | 4       | 0            |
| 25  | A     | 4005 | BCR  | 5       | 0            |
| 25  | A     | 4004 | BCR  | 2       | 0            |
| 38  | 7     | 803  | SPH  | 1       | 0            |
| 22  | K     | 1401 | CLA  | 4       | 0            |
| 25  | L     | 4001 | BCR  | 1       | 0            |
| 23  | A     | 2001 | PQN  | 1       | 0            |
| 22  | A     | 1136 | CLA  | 2       | 0            |
| 39  | 4     | 502  | LUT  | 6       | 0            |
| 22  | 6     | 609  | CLA  | 7       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | A     | 1124 | CLA  | 5       | 0            |
| 22  | A     | 1134 | CLA  | 1       | 0            |
| 40  | 2     | 609  | CHL  | 3       | 0            |
| 22  | 2     | 601  | CLA  | 1       | 0            |
| 39  | Z     | 501  | LUT  | 1       | 0            |
| 22  | 7     | 603  | CLA  | 5       | 0            |
| 25  | 4     | 503  | BCR  | 2       | 0            |
| 22  | 9     | 605  | CLA  | 3       | 0            |
| 22  | J     | 1901 | CLA  | 3       | 0            |
| 39  | 3     | 501  | LUT  | 2       | 0            |
| 22  | 2     | 603  | CLA  | 3       | 0            |
| 22  | 7     | 602  | CLA  | 2       | 0            |
| 22  | 6     | 604  | CLA  | 2       | 0            |
| 22  | B     | 1218 | CLA  | 1       | 0            |
| 25  | B     | 4006 | BCR  | 2       | 0            |
| 32  | A     | 5005 | DGA  | 5       | 0            |
| 22  | B     | 1212 | CLA  | 2       | 0            |
| 22  | 7     | 601  | CLA  | 4       | 0            |
| 40  | 4     | 617  | CHL  | 1       | 0            |
| 22  | B     | 1238 | CLA  | 4       | 0            |
| 39  | 2     | 503  | LUT  | 1       | 0            |
| 25  | I     | 4001 | BCR  | 3       | 0            |
| 22  | B     | 1204 | CLA  | 1       | 0            |
| 39  | 9     | 501  | LUT  | 4       | 0            |
| 39  | Z     | 502  | LUT  | 4       | 0            |
| 22  | 8     | 605  | CLA  | 3       | 0            |
| 22  | Z     | 604  | CLA  | 4       | 0            |
| 25  | B     | 4002 | BCR  | 3       | 0            |
| 22  | 6     | 606  | CLA  | 1       | 0            |
| 22  | 2     | 605  | CLA  | 1       | 0            |
| 22  | 1     | 602  | CLA  | 1       | 0            |
| 22  | Z     | 601  | CLA  | 3       | 0            |
| 22  | B     | 1216 | CLA  | 4       | 0            |
| 22  | B     | 1202 | CLA  | 2       | 0            |
| 40  | 2     | 610  | CHL  | 2       | 0            |
| 22  | 3     | 604  | CLA  | 4       | 0            |
| 22  | 3     | 607  | CLA  | 1       | 0            |
| 22  | 2     | 602  | CLA  | 1       | 0            |
| 22  | 8     | 609  | CLA  | 2       | 0            |
| 22  | A     | 1125 | CLA  | 3       | 0            |
| 25  | 8     | 503  | BCR  | 1       | 0            |
| 22  | 5     | 615  | CLA  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | 5     | 601  | CLA  | 3       | 0            |
| 22  | A     | 1012 | CLA  | 7       | 0            |
| 40  | 7     | 610  | CHL  | 3       | 0            |
| 26  | Z     | 801  | LHG  | 1       | 0            |
| 39  | 6     | 501  | LUT  | 3       | 0            |
| 25  | 7     | 504  | BCR  | 1       | 0            |
| 39  | 7     | 501  | LUT  | 2       | 0            |
| 22  | 3     | 608  | CLA  | 1       | 0            |
| 31  | J     | 5001 | LMG  | 1       | 0            |
| 25  | 6     | 504  | BCR  | 1       | 0            |
| 25  | B     | 4003 | BCR  | 3       | 0            |
| 22  | 3     | 613  | CLA  | 3       | 0            |
| 39  | 9     | 502  | LUT  | 2       | 0            |
| 22  | A     | 1127 | CLA  | 6       | 0            |
| 22  | 8     | 604  | CLA  | 1       | 0            |
| 22  | Z     | 611  | CLA  | 2       | 0            |
| 22  | 8     | 601  | CLA  | 6       | 0            |
| 40  | 4     | 613  | CHL  | 1       | 0            |
| 22  | 1     | 601  | CLA  | 4       | 0            |
| 22  | B     | 1239 | CLA  | 2       | 0            |
| 22  | 5     | 605  | CLA  | 2       | 0            |
| 22  | 1     | 611  | CLA  | 3       | 0            |
| 36  | F     | 4001 | RRX  | 1       | 0            |
| 39  | 5     | 502  | LUT  | 4       | 0            |
| 40  | 9     | 613  | CHL  | 1       | 0            |
| 22  | F     | 1302 | CLA  | 2       | 0            |
| 22  | 3     | 618  | CLA  | 3       | 0            |
| 40  | 3     | 611  | CHL  | 3       | 0            |
| 22  | 1     | 603  | CLA  | 3       | 0            |
| 22  | B     | 1240 | CLA  | 8       | 0            |
| 22  | B     | 1207 | CLA  | 2       | 0            |
| 22  | 5     | 609  | CLA  | 3       | 0            |
| 39  | 8     | 501  | LUT  | 4       | 0            |
| 22  | 9     | 604  | CLA  | 4       | 0            |
| 40  | 4     | 610  | CHL  | 3       | 0            |
| 22  | 9     | 612  | CLA  | 2       | 0            |
| 28  | A     | 5006 | LMT  | 1       | 0            |
| 22  | B     | 1241 | CLA  | 1       | 0            |
| 22  | 4     | 608  | CLA  | 1       | 0            |
| 22  | 5     | 603  | CLA  | 3       | 0            |
| 22  | Z     | 607  | CLA  | 2       | 0            |
| 22  | 7     | 607  | CLA  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | B     | 1228 | CLA  | 1       | 0            |
| 22  | 5     | 604  | CLA  | 2       | 0            |
| 22  | B     | 1234 | CLA  | 4       | 0            |
| 22  | 5     | 613  | CLA  | 2       | 0            |
| 22  | A     | 1132 | CLA  | 1       | 0            |
| 22  | Z     | 606  | CLA  | 2       | 0            |
| 22  | 6     | 619  | CLA  | 3       | 0            |
| 22  | 8     | 602  | CLA  | 3       | 0            |
| 22  | B     | 1023 | CLA  | 6       | 0            |
| 22  | 7     | 606  | CLA  | 2       | 0            |
| 22  | A     | 1113 | CLA  | 1       | 0            |
| 26  | 2     | 801  | LHG  | 2       | 0            |
| 22  | B     | 1217 | CLA  | 2       | 0            |
| 22  | A     | 1108 | CLA  | 2       | 0            |
| 25  | 5     | 503  | BCR  | 4       | 0            |
| 26  | B     | 5006 | LHG  | 1       | 0            |
| 22  | 7     | 611  | CLA  | 1       | 0            |
| 25  | B     | 4004 | BCR  | 4       | 0            |
| 22  | A     | 1121 | CLA  | 2       | 0            |
| 39  | 5     | 501  | LUT  | 4       | 0            |
| 38  | K     | 5001 | SPH  | 1       | 0            |
| 22  | B     | 1227 | CLA  | 2       | 0            |
| 40  | Z     | 609  | CHL  | 3       | 0            |
| 28  | B     | 5005 | LMT  | 3       | 0            |
| 22  | B     | 1206 | CLA  | 2       | 0            |
| 25  | 3     | 506  | BCR  | 2       | 0            |
| 22  | B     | 1022 | CLA  | 1       | 0            |
| 22  | A     | 1131 | CLA  | 1       | 0            |
| 22  | 7     | 615  | CLA  | 1       | 0            |
| 33  | B     | 5003 | DGD  | 4       | 0            |
| 22  | 4     | 601  | CLA  | 4       | 0            |
| 26  | A     | 5002 | LHG  | 4       | 0            |
| 39  | 1     | 501  | LUT  | 2       | 0            |
| 22  | 1     | 606  | CLA  | 1       | 0            |
| 22  | A     | 1104 | CLA  | 4       | 0            |
| 22  | F     | 1301 | CLA  | 3       | 0            |
| 22  | 3     | 612  | CLA  | 5       | 0            |
| 22  | 8     | 611  | CLA  | 1       | 0            |
| 22  | A     | 1126 | CLA  | 9       | 0            |
| 22  | 5     | 602  | CLA  | 2       | 0            |
| 25  | K     | 4001 | BCR  | 2       | 0            |
| 39  | 7     | 502  | LUT  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | A     | 1117 | CLA  | 4       | 0            |
| 28  | B     | 6101 | LMT  | 2       | 0            |
| 22  | B     | 1208 | CLA  | 3       | 0            |
| 22  | A     | 1122 | CLA  | 3       | 0            |
| 39  | 3     | 502  | LUT  | 5       | 0            |
| 39  | 6     | 502  | LUT  | 1       | 0            |
| 22  | A     | 1112 | CLA  | 2       | 0            |
| 22  | 6     | 601  | CLA  | 4       | 0            |
| 22  | K     | 1402 | CLA  | 2       | 0            |
| 22  | 7     | 609  | CLA  | 2       | 0            |
| 40  | Z     | 610  | CHL  | 5       | 0            |
| 21  | A     | 1011 | CL0  | 5       | 0            |
| 25  | J     | 4001 | BCR  | 4       | 0            |
| 25  | 3     | 505  | BCR  | 3       | 0            |
| 39  | 8     | 502  | LUT  | 2       | 0            |
| 22  | A     | 1111 | CLA  | 6       | 0            |
| 22  | B     | 1231 | CLA  | 2       | 0            |
| 40  | 6     | 610  | CHL  | 2       | 0            |
| 43  | 7     | 802  | 3PH  | 1       | 0            |
| 22  | 4     | 612  | CLA  | 3       | 0            |
| 22  | 4     | 605  | CLA  | 2       | 0            |
| 22  | B     | 1224 | CLA  | 3       | 0            |
| 22  | A     | 1137 | CLA  | 4       | 0            |
| 40  | 6     | 617  | CHL  | 1       | 0            |
| 22  | 7     | 613  | CLA  | 3       | 0            |
| 22  | 8     | 606  | CLA  | 4       | 0            |
| 22  | 6     | 615  | CLA  | 2       | 0            |
| 25  | B     | 4005 | BCR  | 2       | 0            |
| 31  | A     | 5003 | LMG  | 1       | 0            |
| 22  | 1     | 604  | CLA  | 2       | 0            |
| 38  | 7     | 804  | SPH  | 1       | 0            |
| 22  | 8     | 608  | CLA  | 4       | 0            |
| 28  | 4     | 803  | LMT  | 1       | 0            |
| 22  | A     | 1133 | CLA  | 5       | 0            |
| 22  | 2     | 607  | CLA  | 3       | 0            |
| 25  | 5     | 504  | BCR  | 2       | 0            |
| 22  | B     | 1209 | CLA  | 5       | 0            |
| 22  | A     | 1140 | CLA  | 1       | 0            |
| 22  | B     | 1230 | CLA  | 5       | 0            |
| 22  | A     | 1101 | CLA  | 2       | 0            |
| 22  | 3     | 616  | CLA  | 1       | 0            |
| 22  | A     | 1138 | CLA  | 5       | 0            |

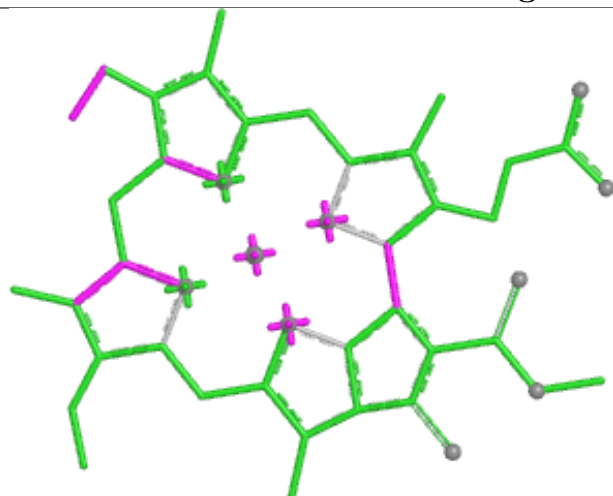
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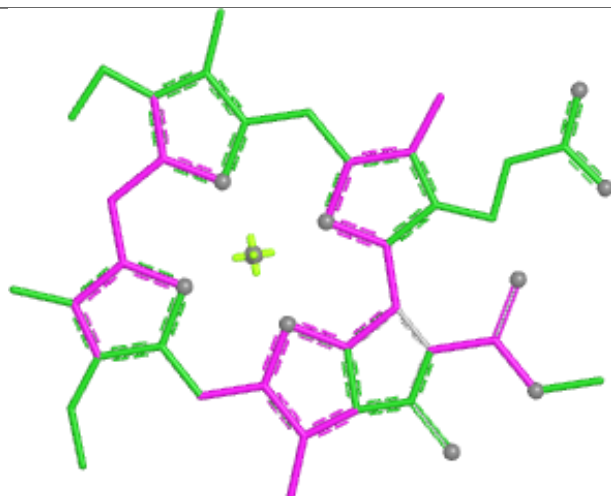
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | K     | 4002 | BCR  | 3       | 0            |
| 26  | 1     | 801  | LHG  | 1       | 0            |
| 22  | A     | 1130 | CLA  | 3       | 0            |
| 41  | 2     | 803  | SQD  | 1       | 0            |
| 39  | 4     | 501  | LUT  | 5       | 0            |
| 22  | 3     | 610  | CLA  | 1       | 0            |
| 22  | A     | 1105 | CLA  | 2       | 0            |
| 25  | L     | 4002 | BCR  | 2       | 0            |
| 22  | K     | 1404 | CLA  | 1       | 0            |
| 22  | 6     | 608  | CLA  | 2       | 0            |
| 22  | B     | 1210 | CLA  | 4       | 0            |
| 22  | 7     | 604  | CLA  | 1       | 0            |
| 22  | B     | 1237 | CLA  | 3       | 0            |
| 22  | 1     | 608  | CLA  | 4       | 0            |
| 40  | 5     | 610  | CHL  | 6       | 0            |
| 22  | A     | 1110 | CLA  | 2       | 0            |
| 22  | 9     | 603  | CLA  | 2       | 0            |
| 22  | B     | 1211 | CLA  | 1       | 0            |
| 22  | 1     | 613  | CLA  | 2       | 0            |
| 22  | 4     | 602  | CLA  | 1       | 0            |

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

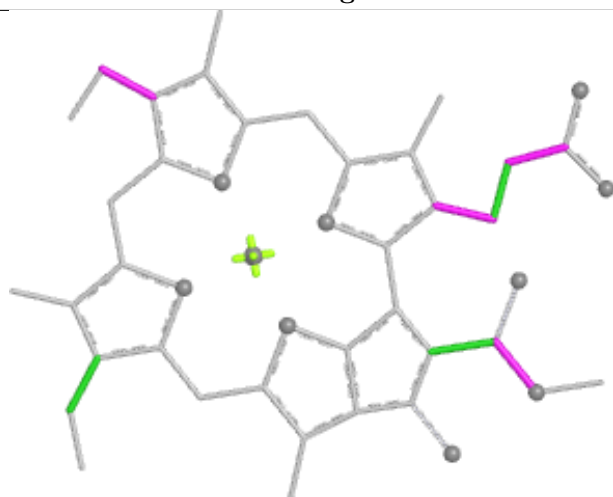
## Ligand CLA 5 608



Bond lengths



Bond angles

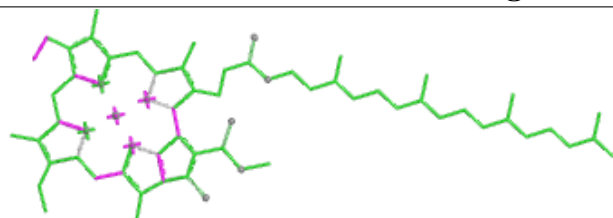


Torsions

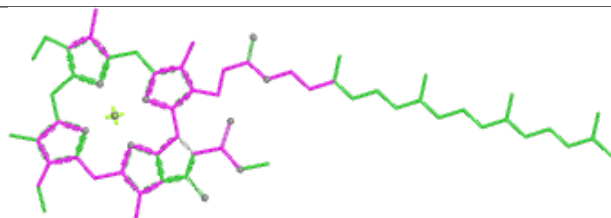


Rings

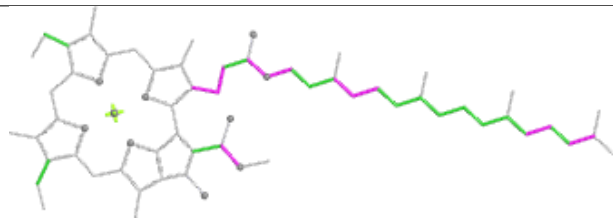
## Ligand CLA B 1226



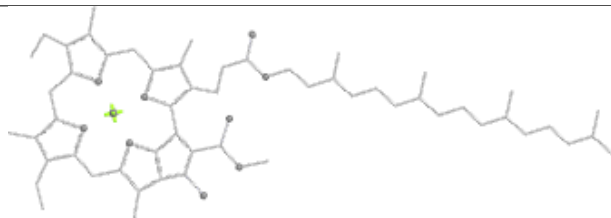
Bond lengths



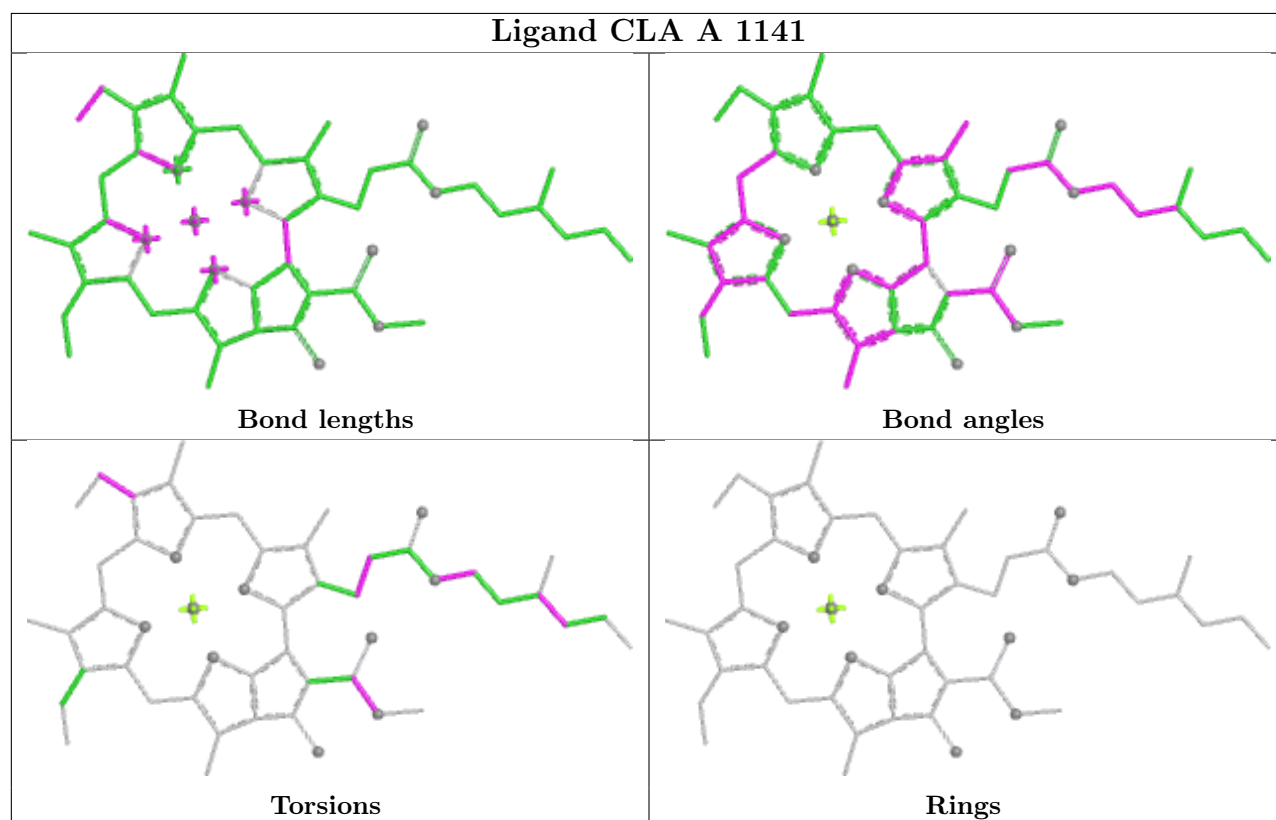
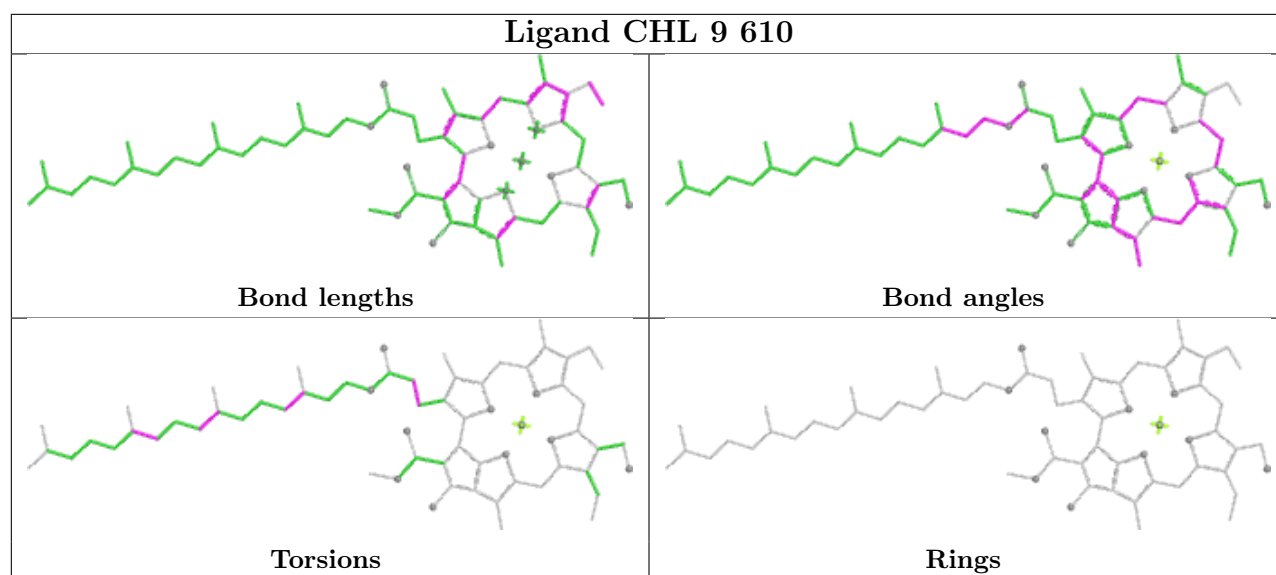
Bond angles

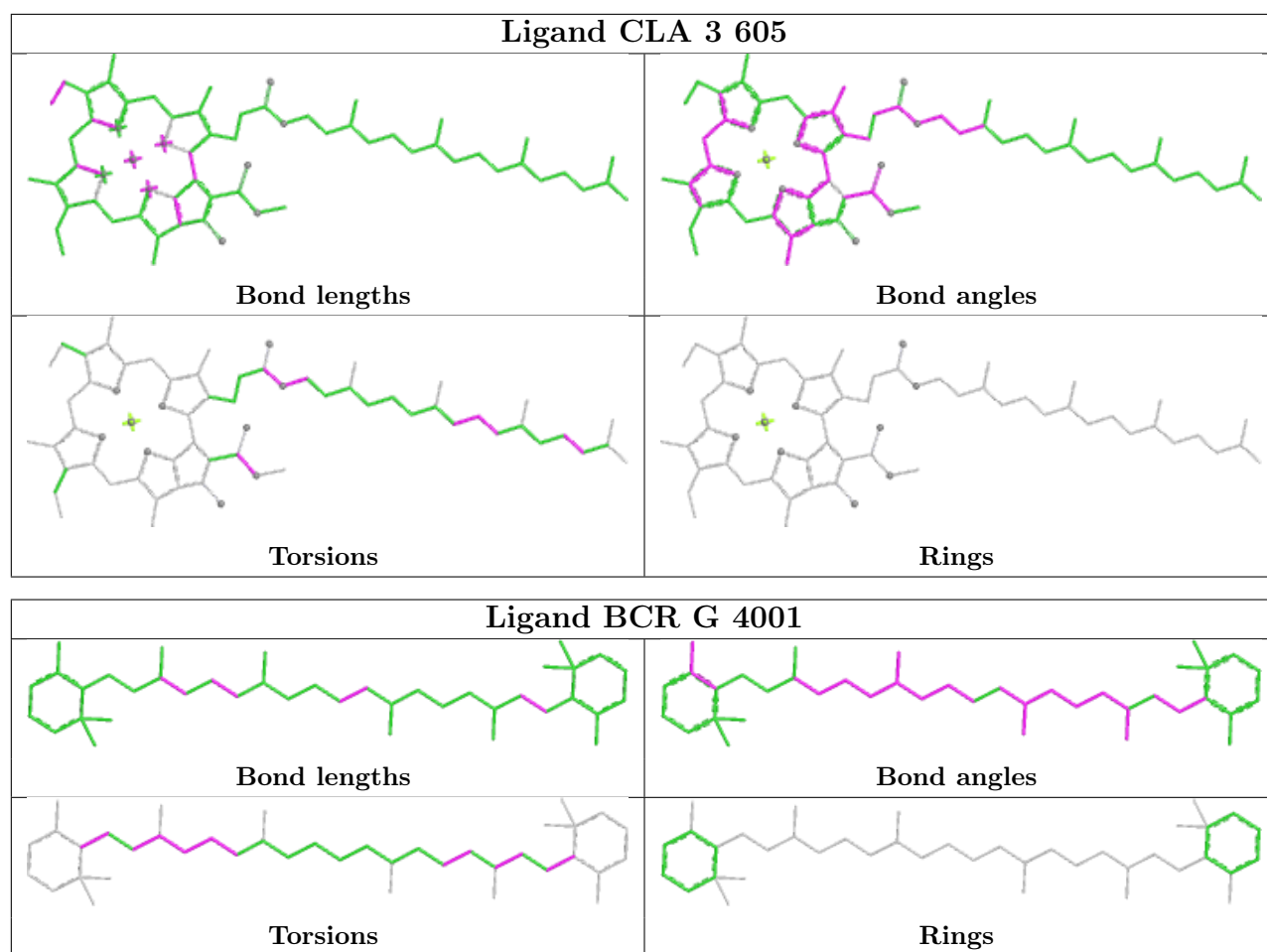


Torsions

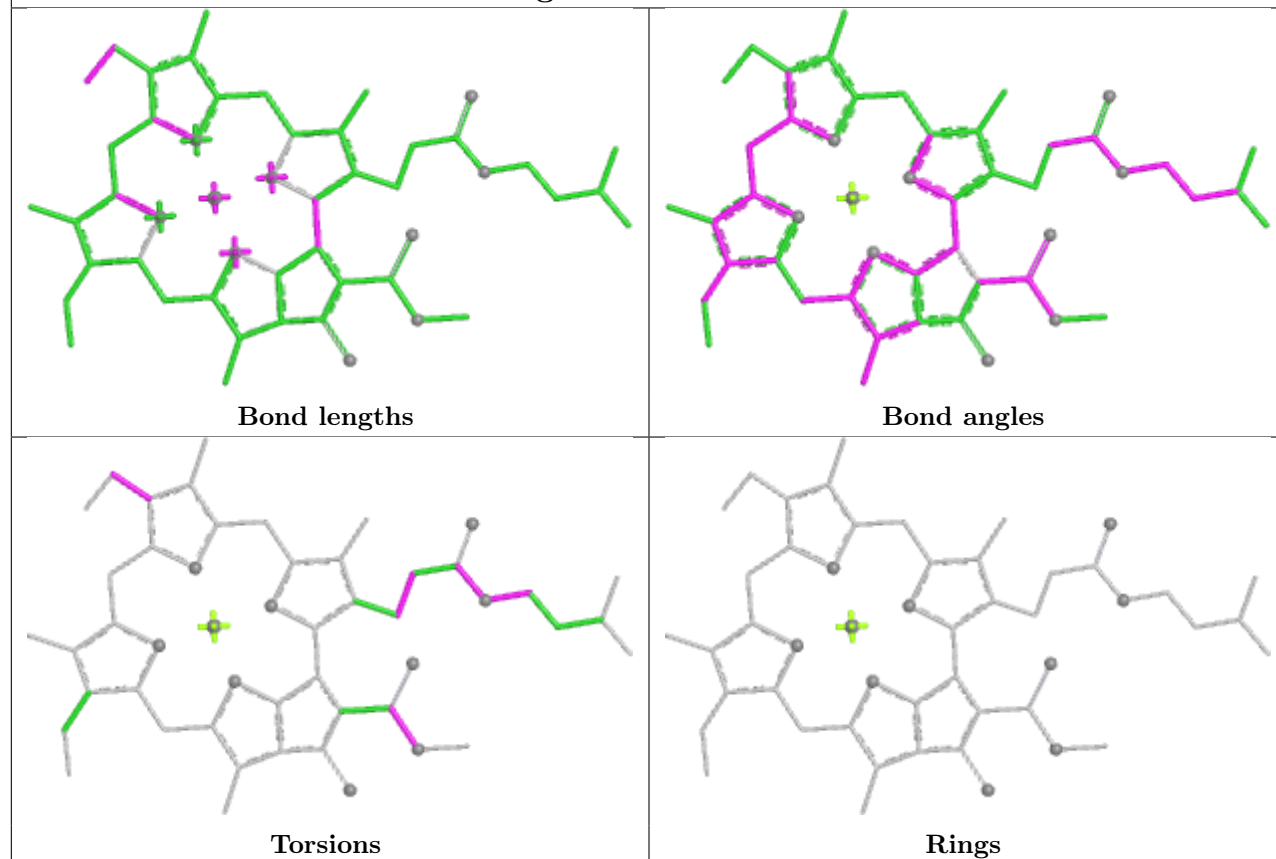


Rings

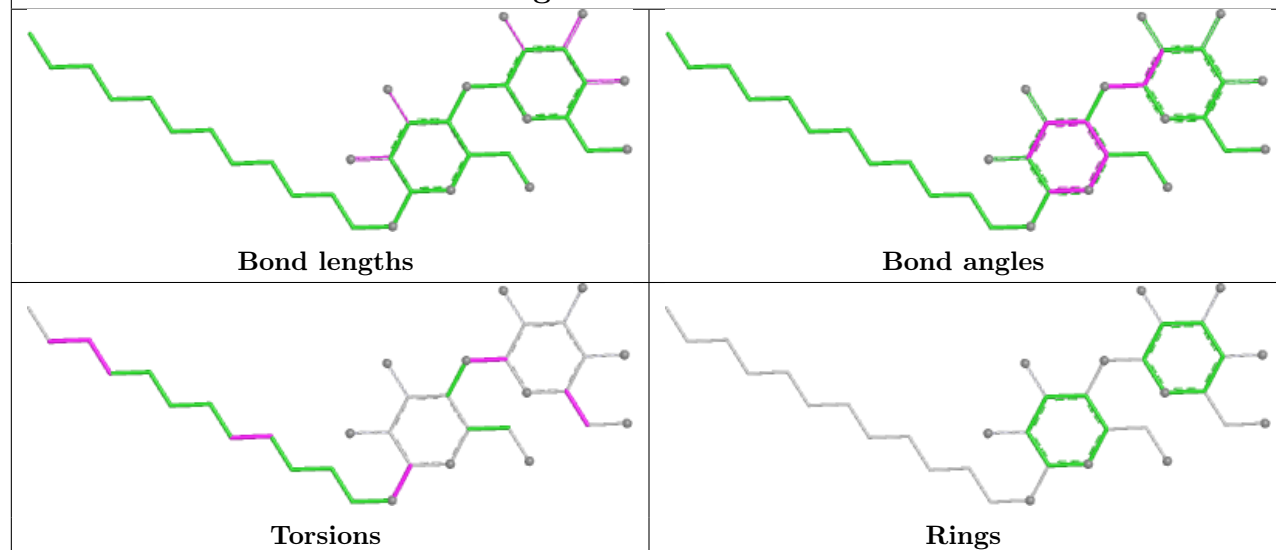




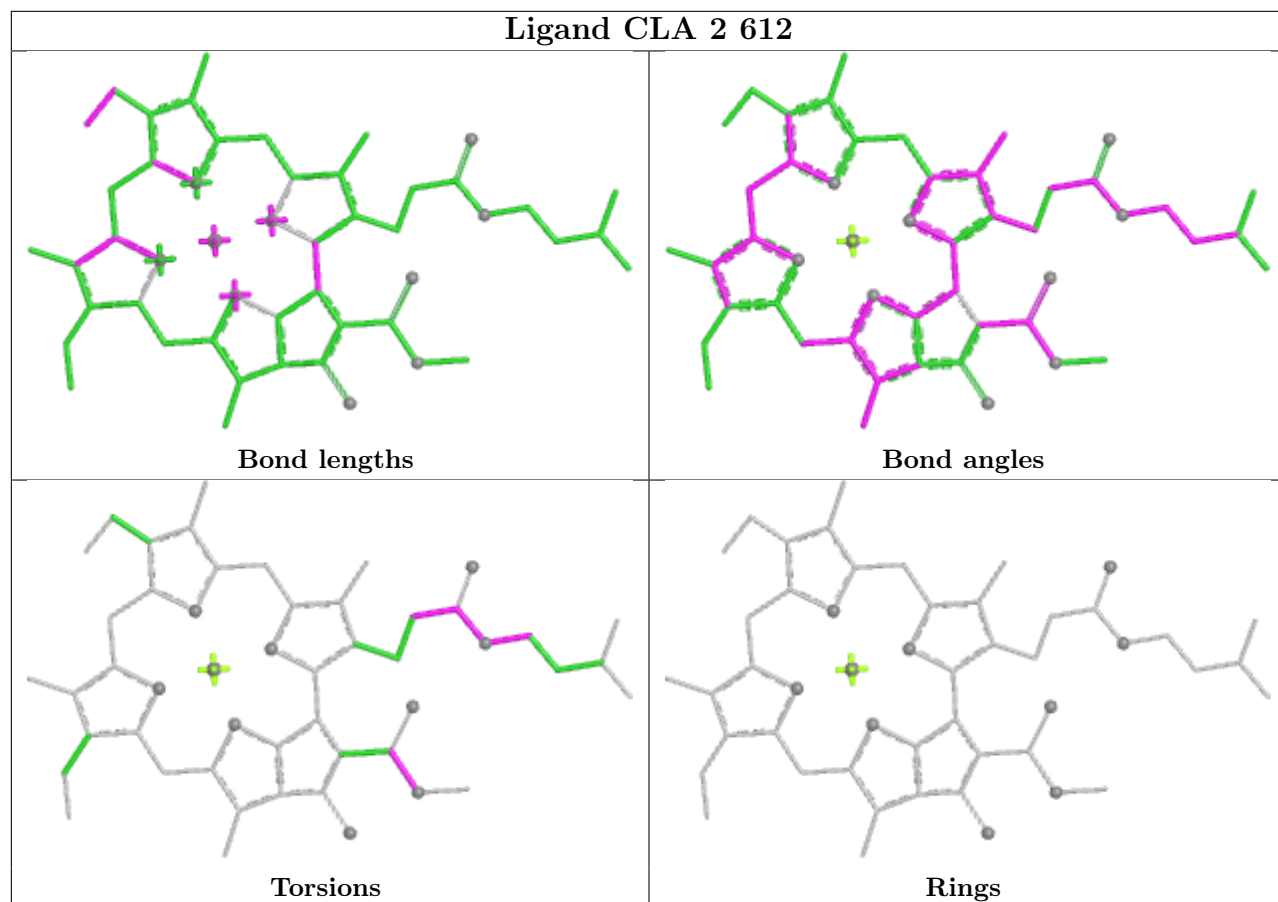
## Ligand CLA 5 606



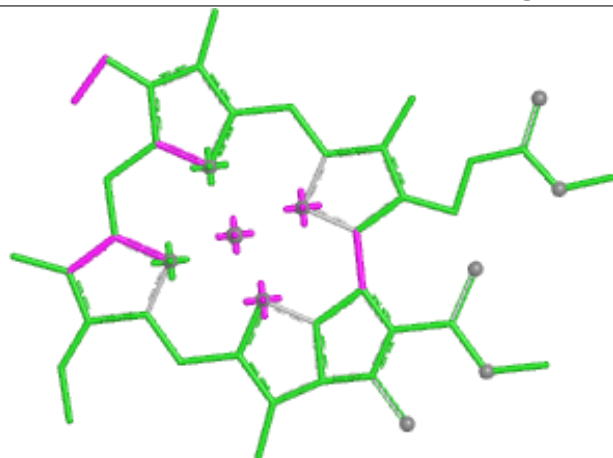
## Ligand LMT 9 803



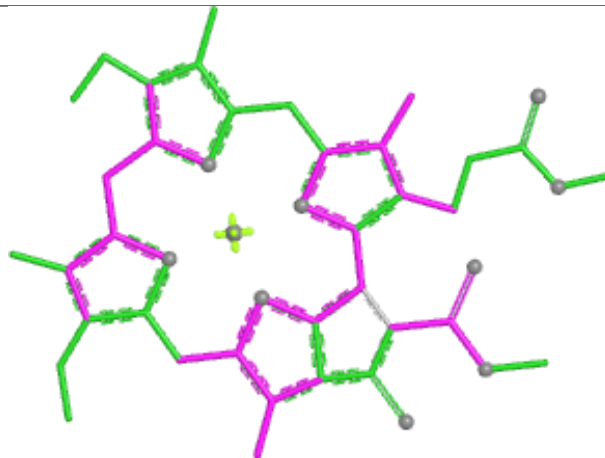
## Ligand CLA 2 612



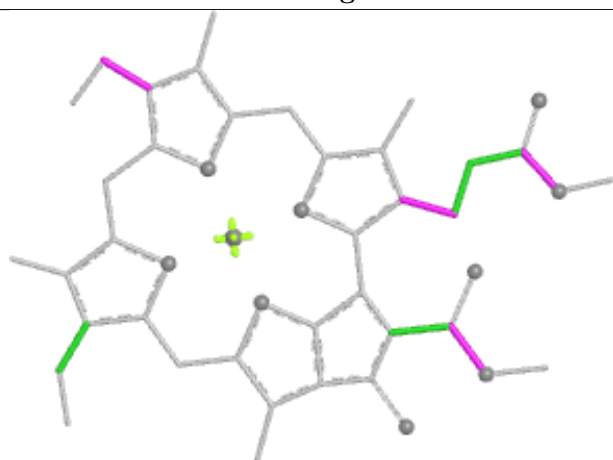
## Ligand CLA 6 618



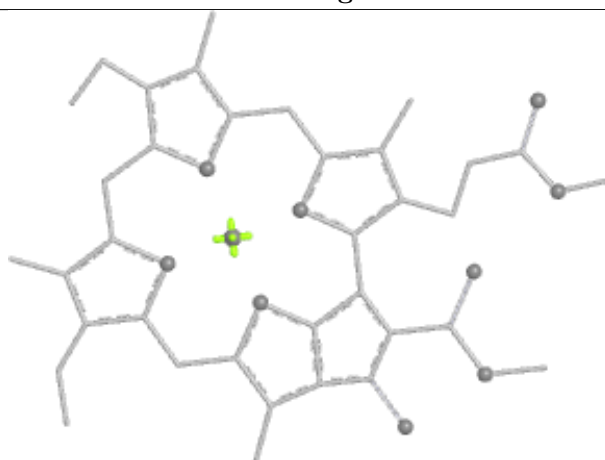
Bond lengths



Bond angles

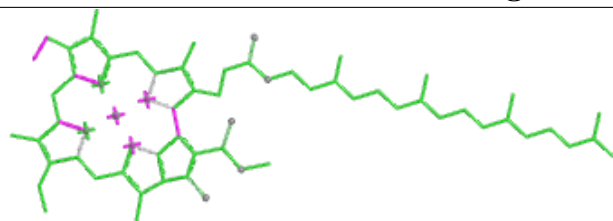


Torsions

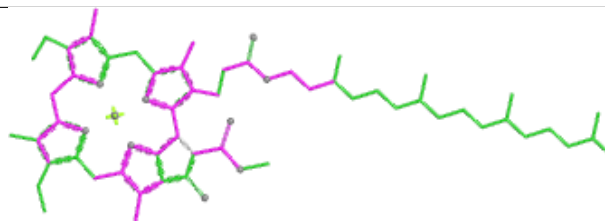


Rings

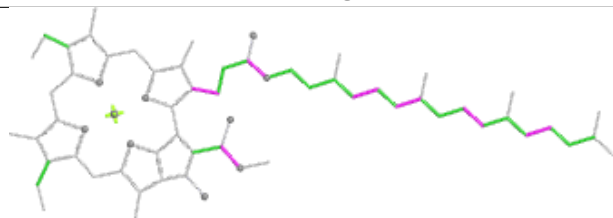
## Ligand CLA B 1222



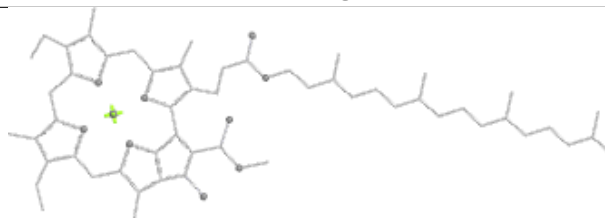
Bond lengths



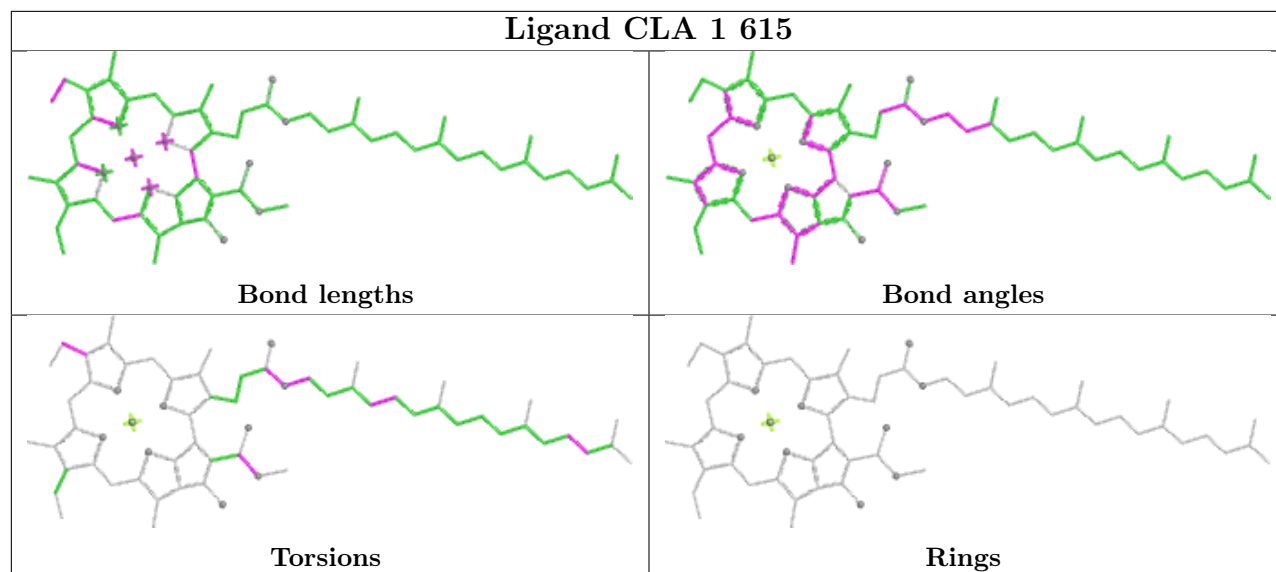
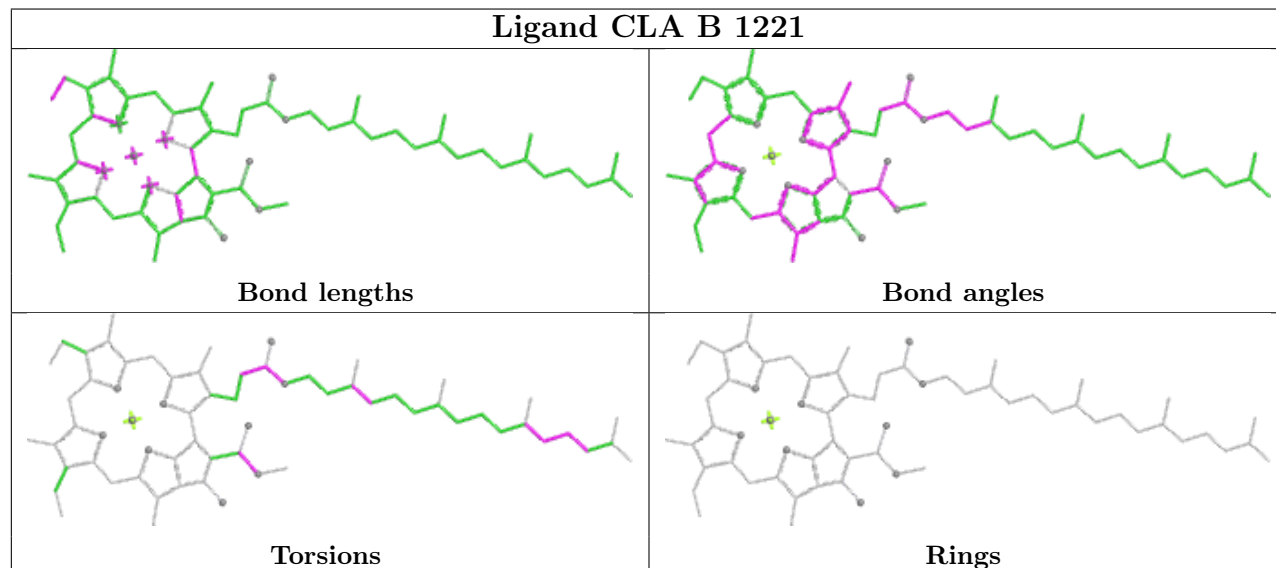
Bond angles



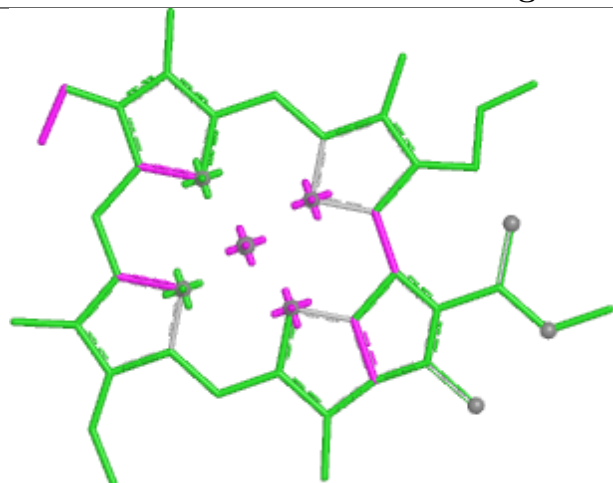
Torsions



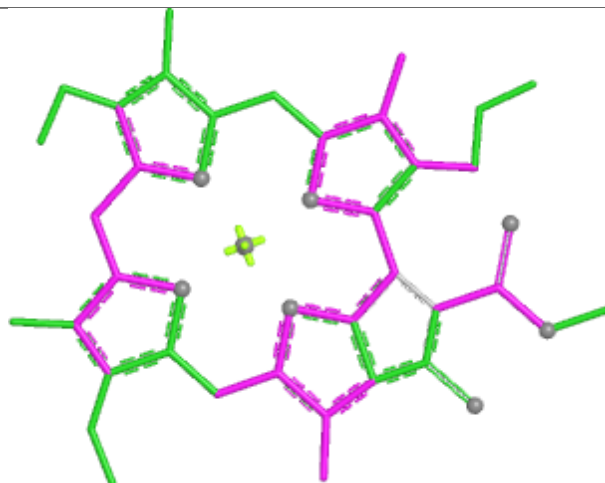
Rings

**Ligand CLA 1 615****Ligand CLA B 1221**

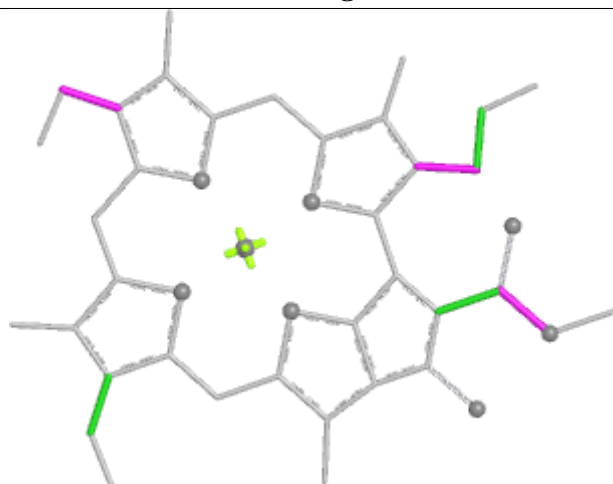
## Ligand CLA 7 608



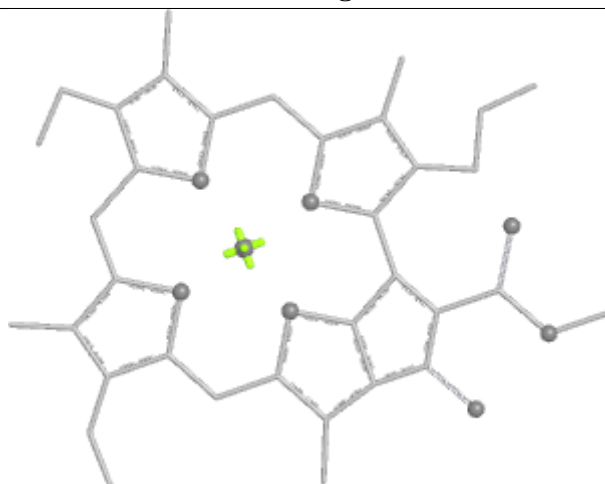
Bond lengths



Bond angles

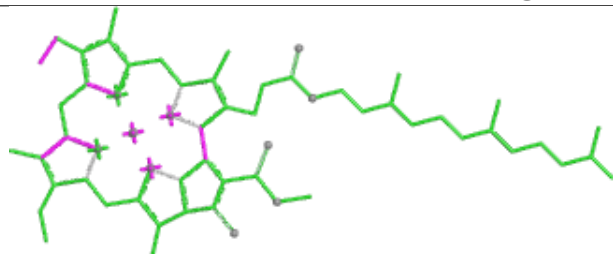


Torsions

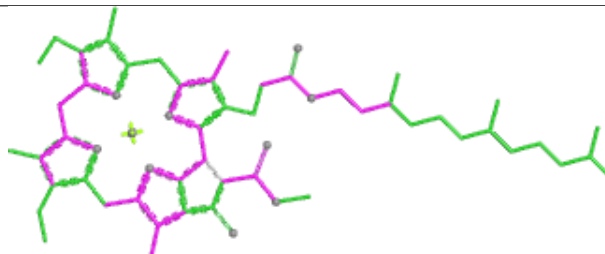


Rings

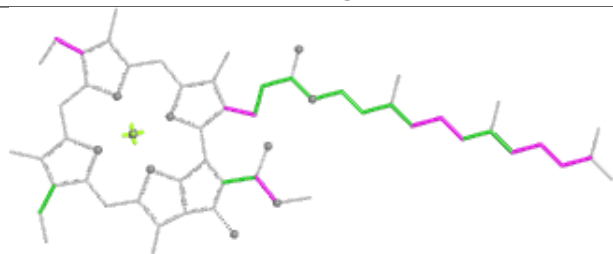
## Ligand CLA 7 616



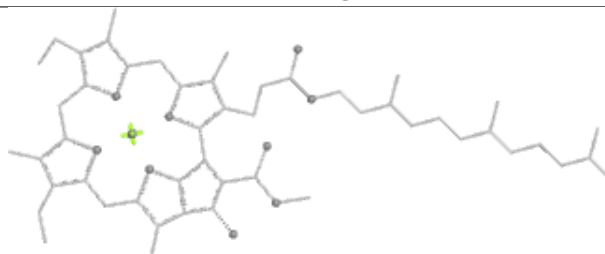
Bond lengths



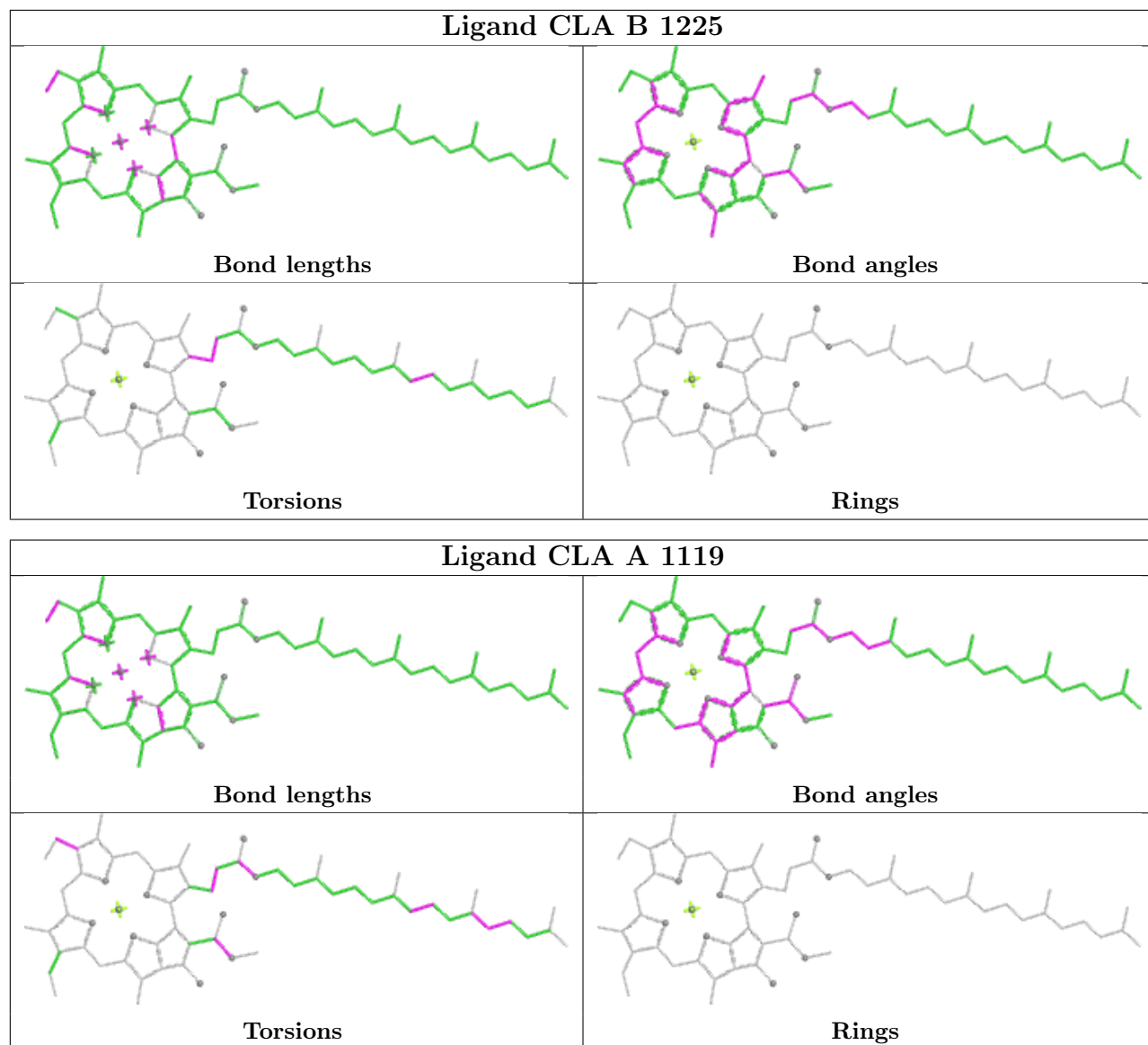
Bond angles



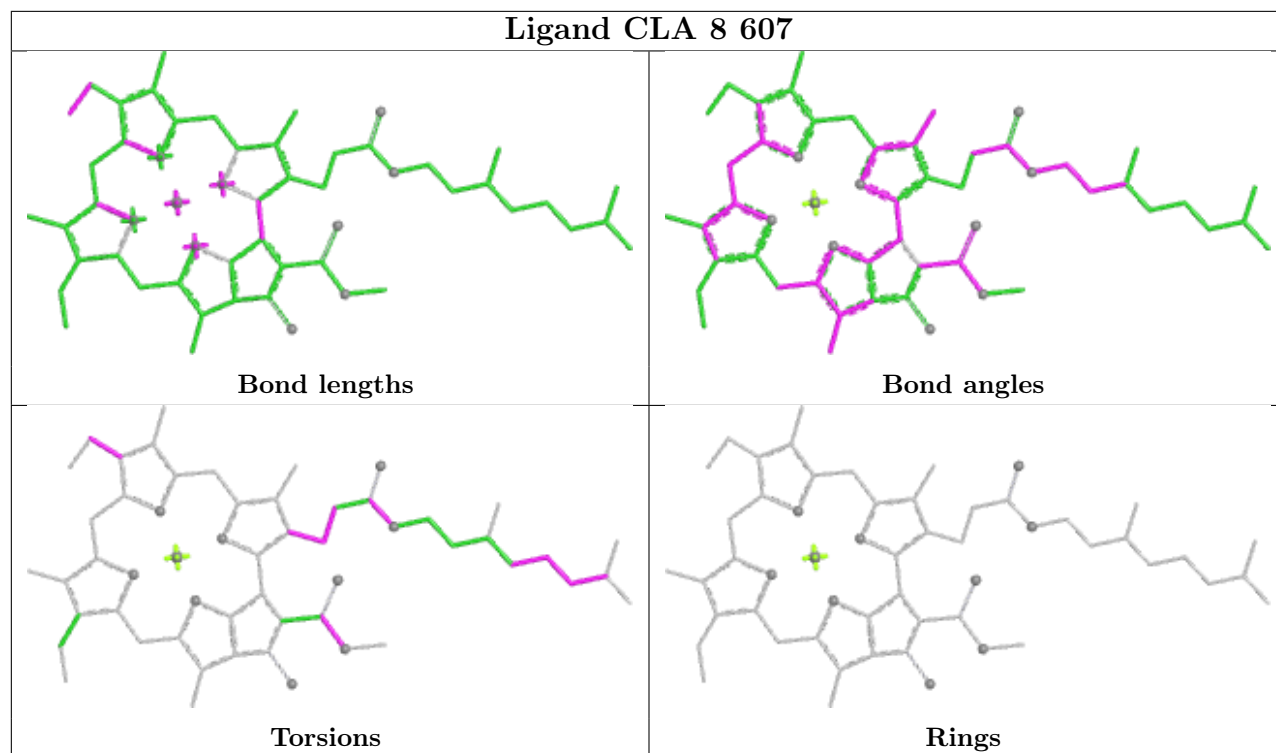
Torsions



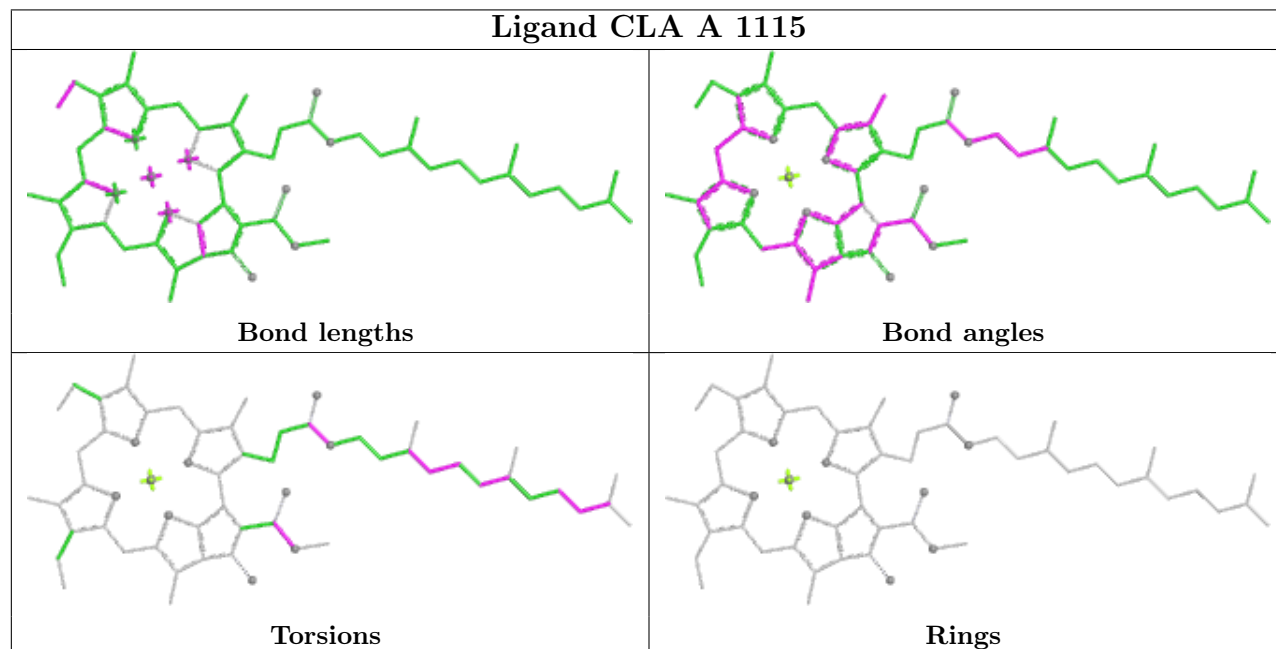
Rings



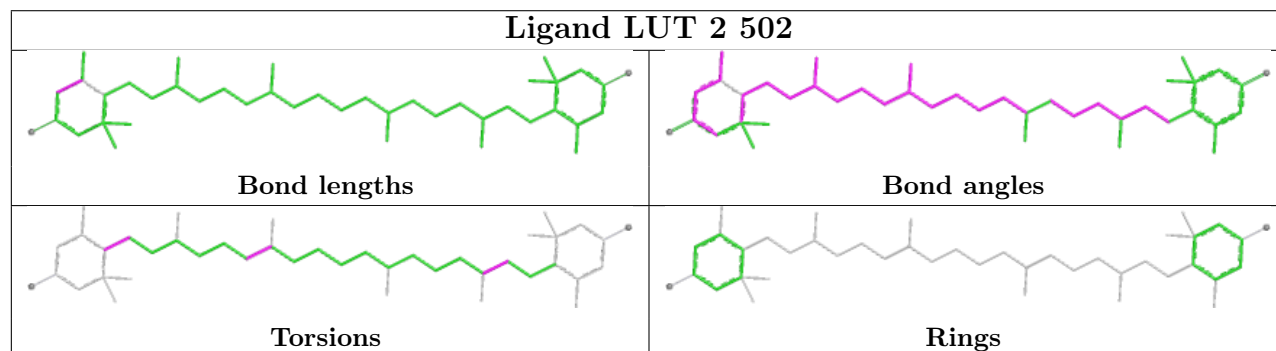
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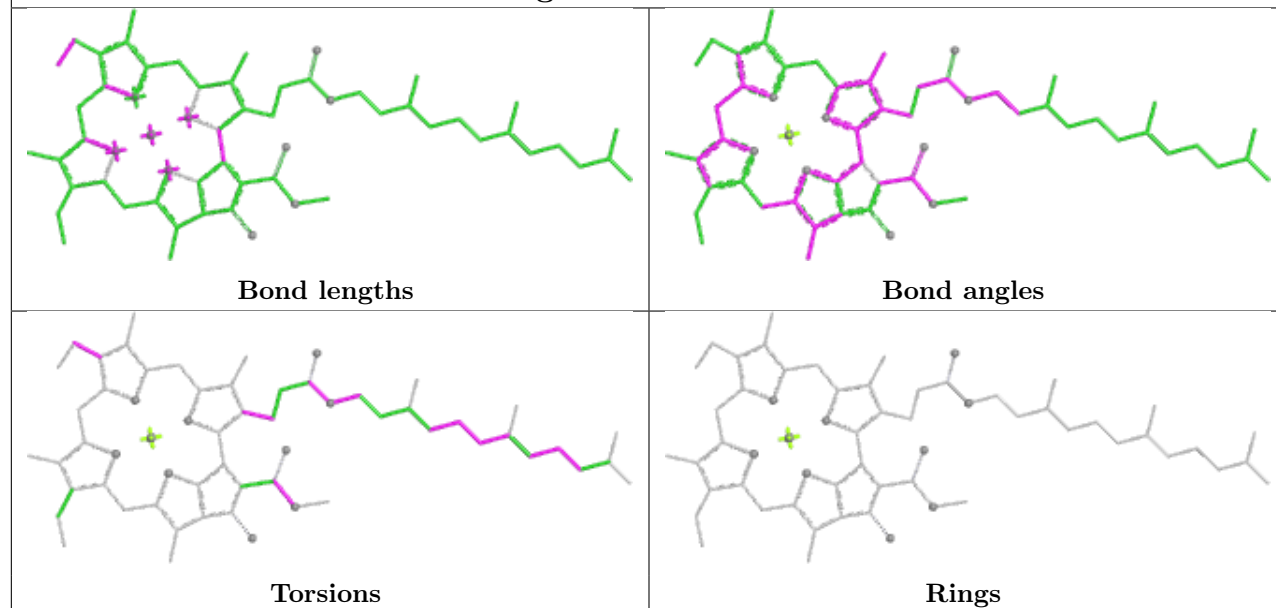
## Ligand CLA A 1115



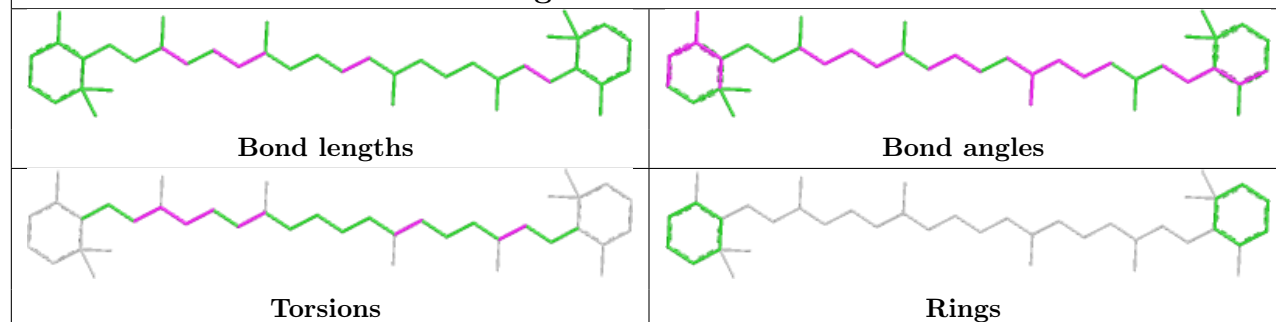
## Ligand LUT 2 502



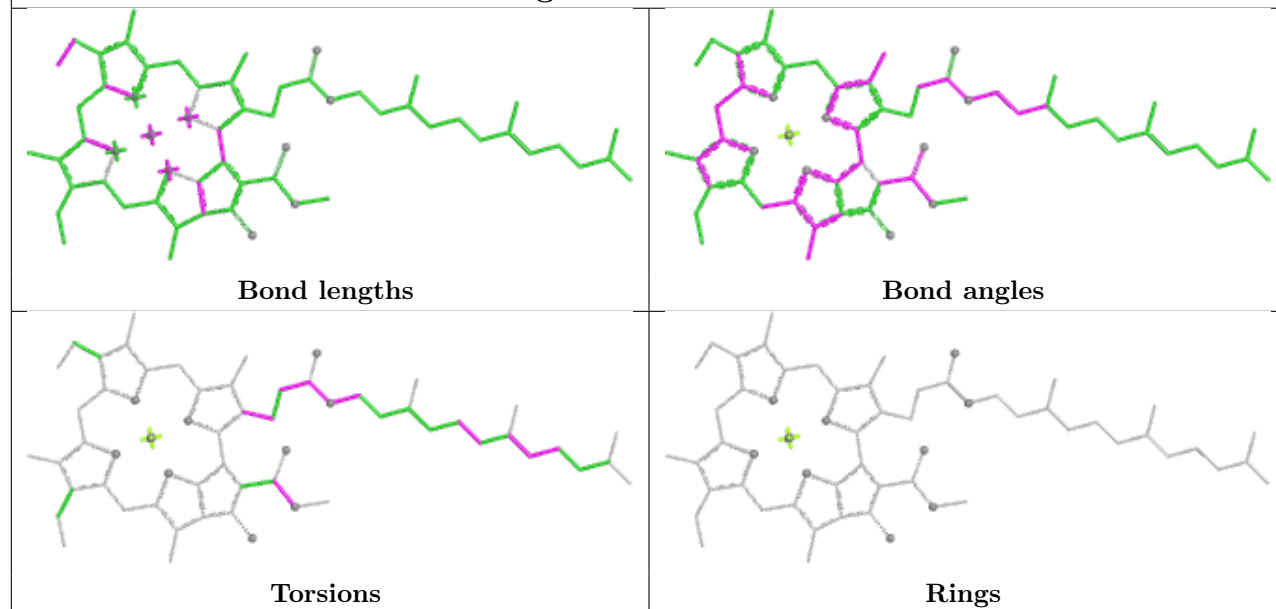
## Ligand CLA 1 607



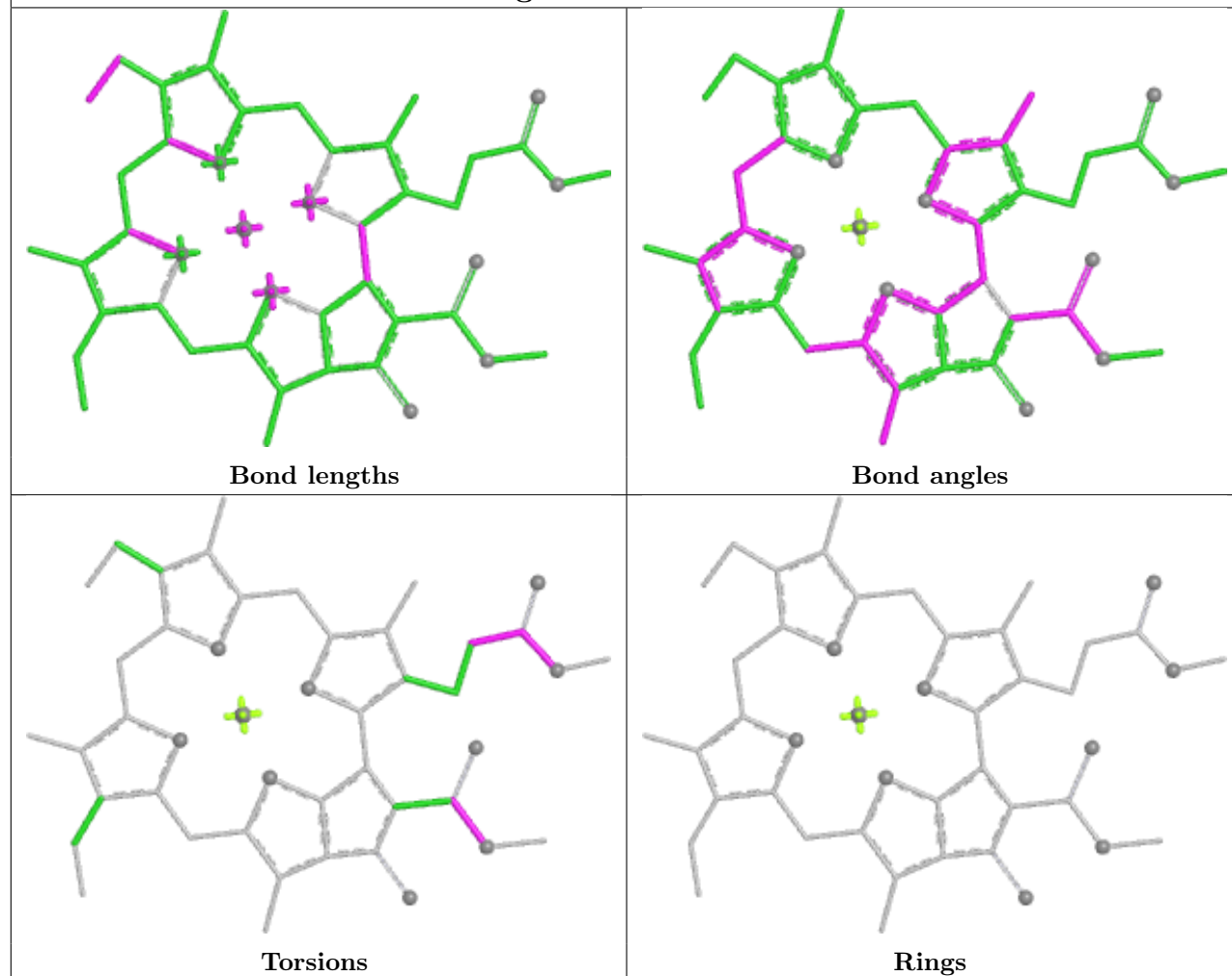
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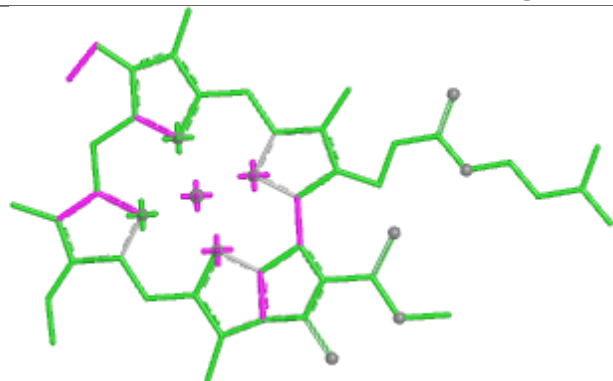
## Ligand CLA 4 609



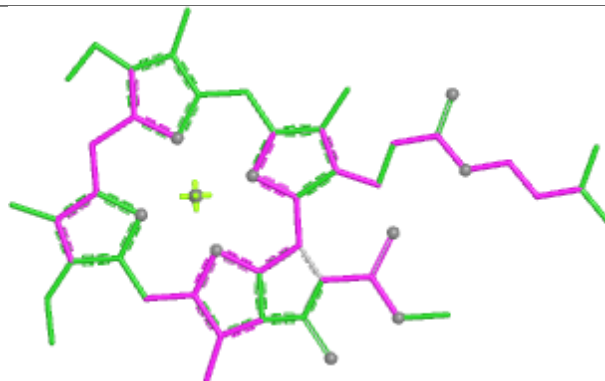
## Ligand CLA Z 602



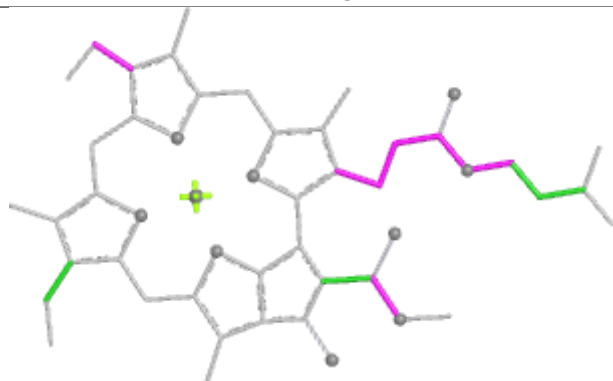
## Ligand CLA 9 606



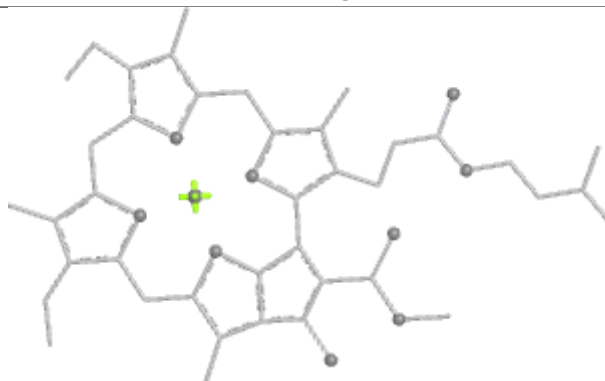
Bond lengths



Bond angles

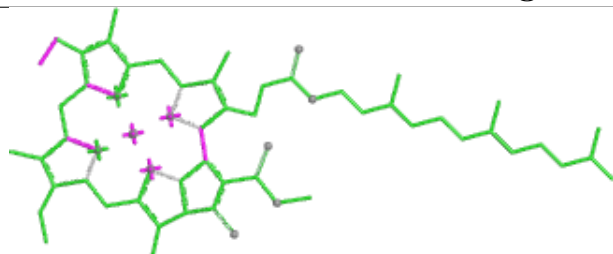


Torsions

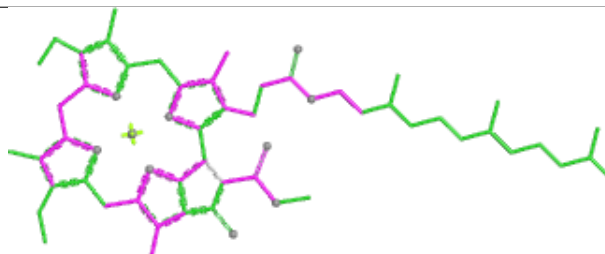


Rings

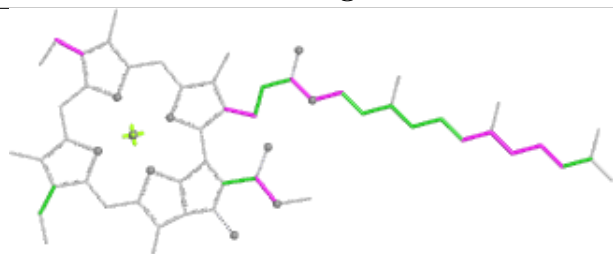
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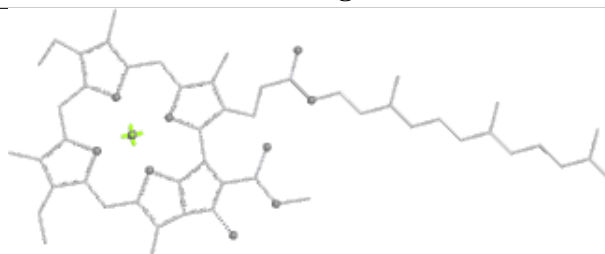
Bond lengths



Bond angles

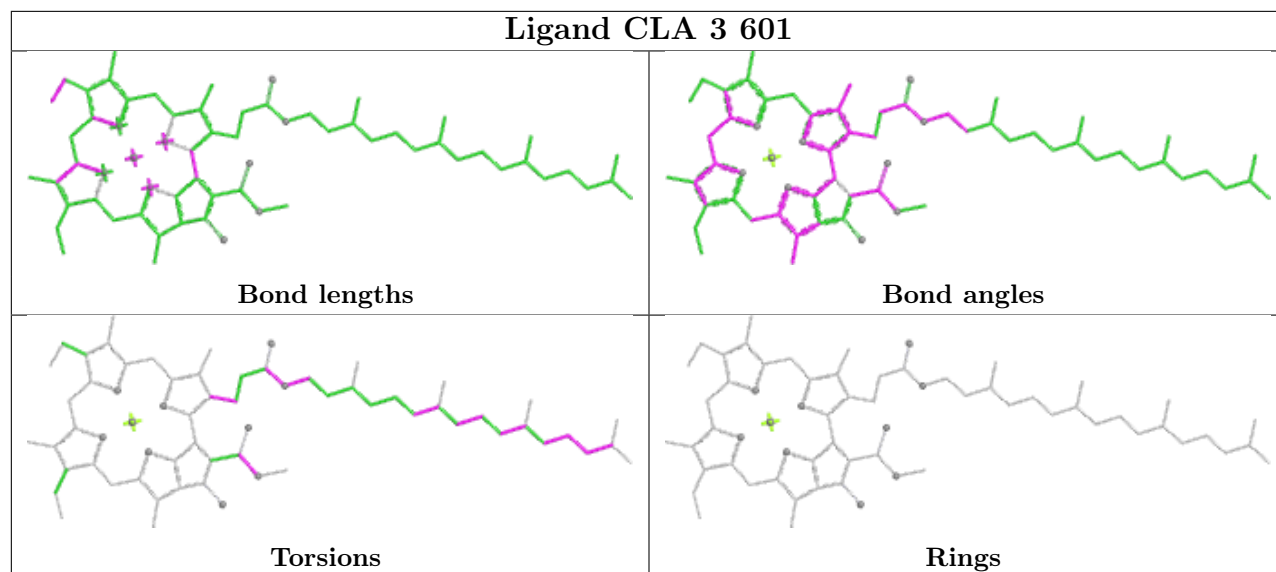


Torsions

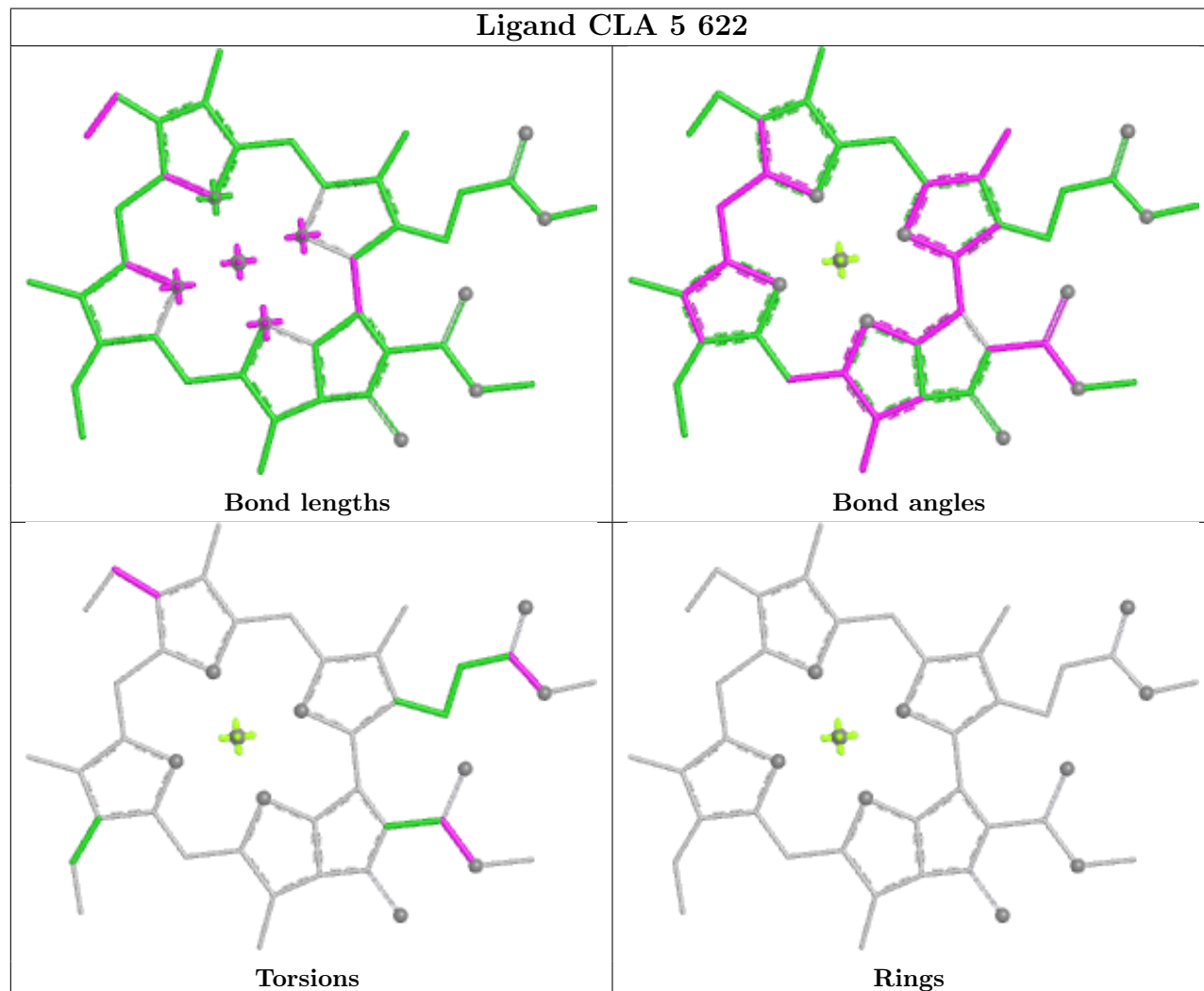


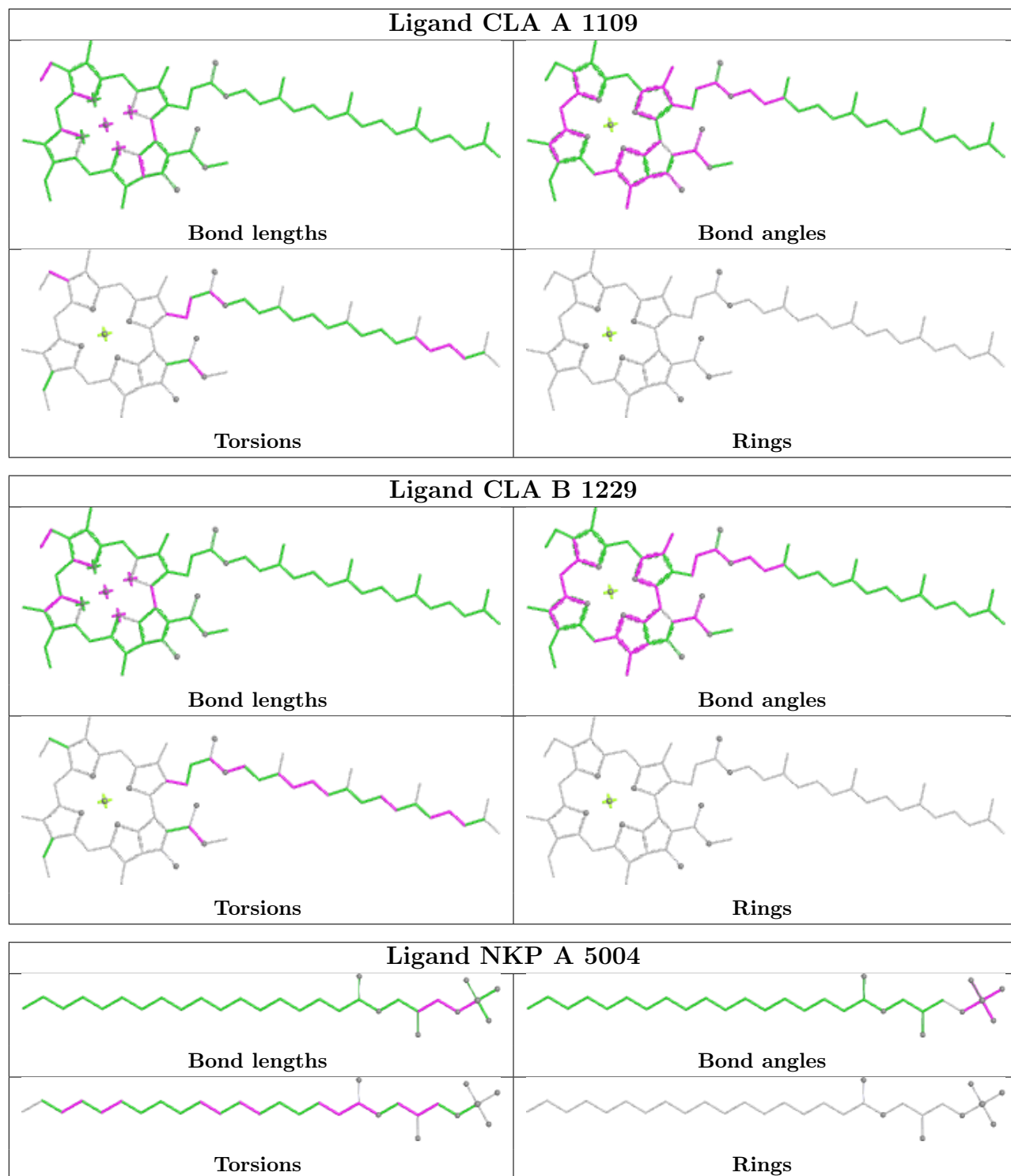
Rings

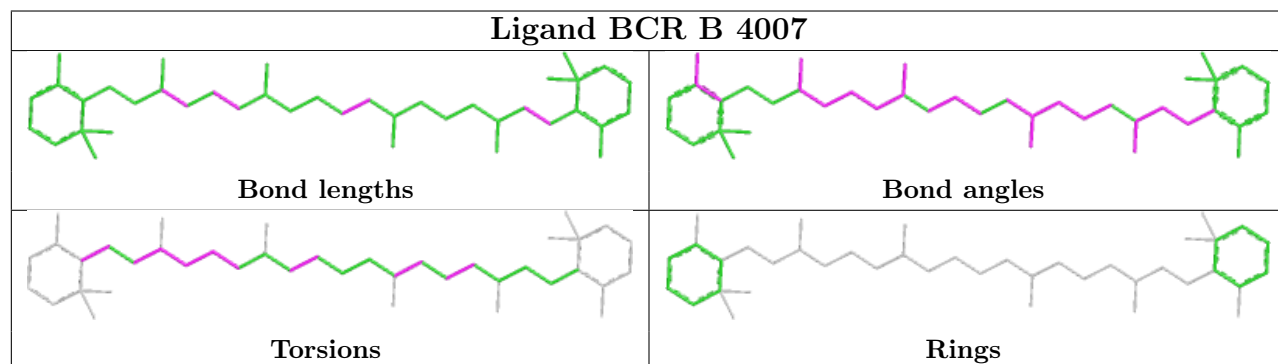
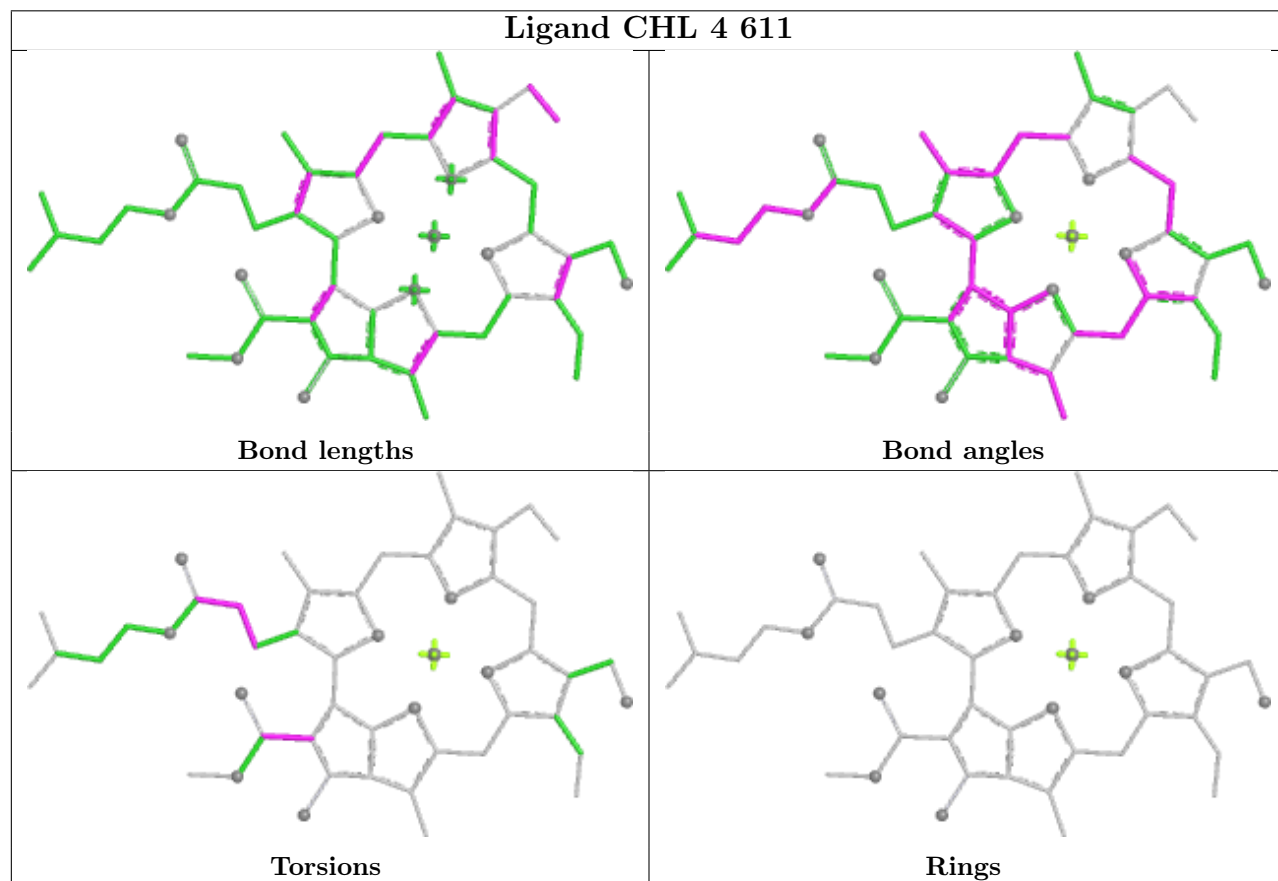
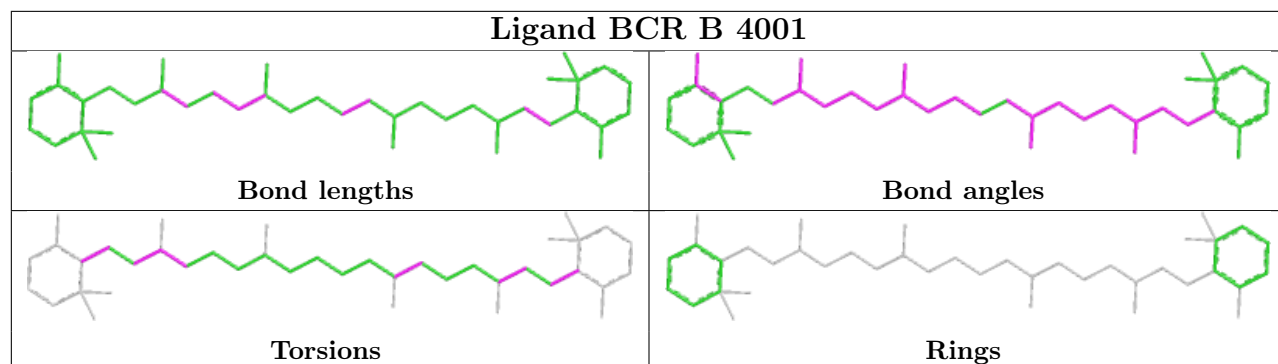
## Ligand CLA 3 601



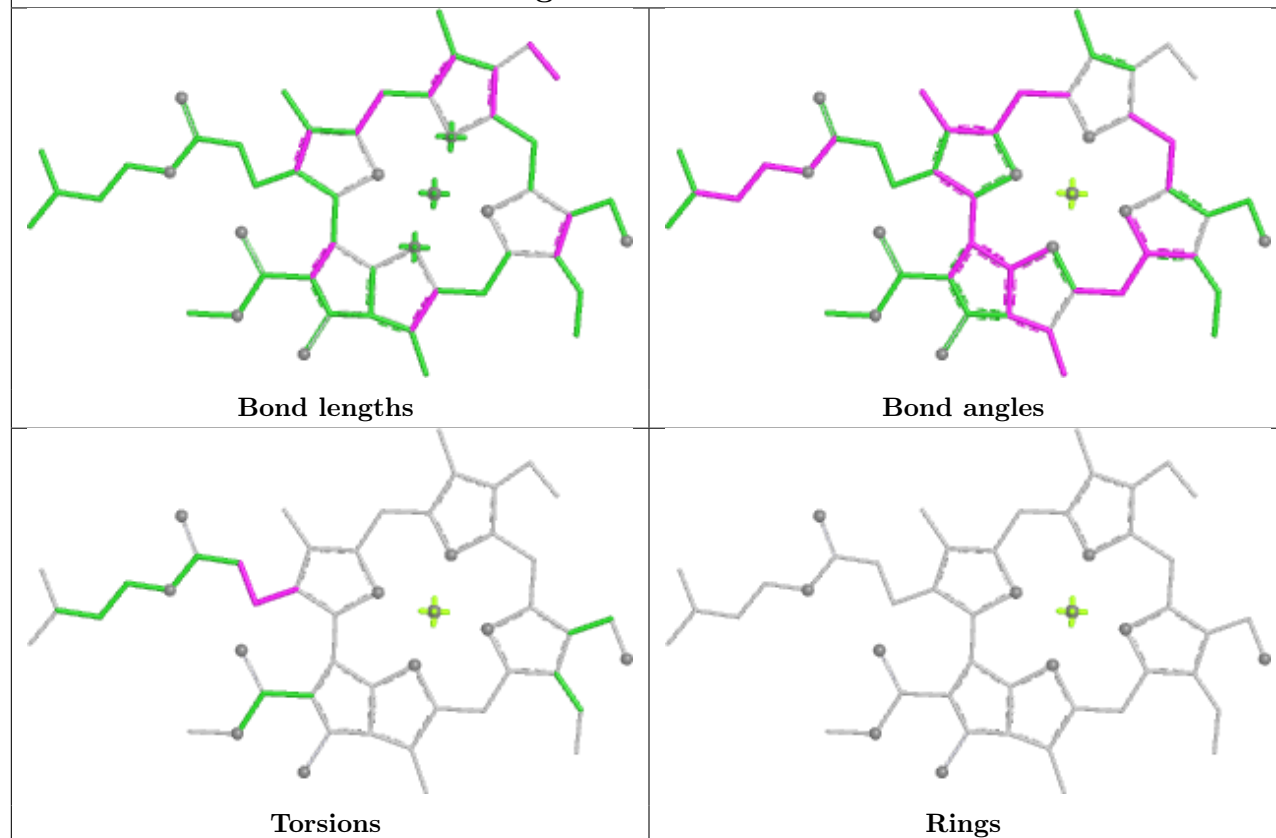
## Ligand CLA 5 622



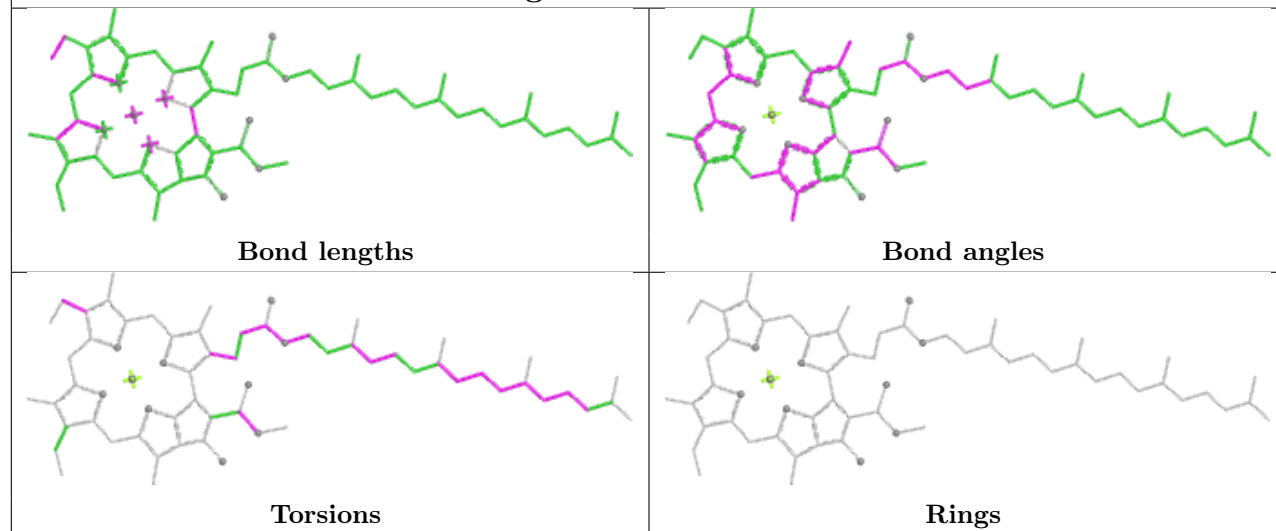


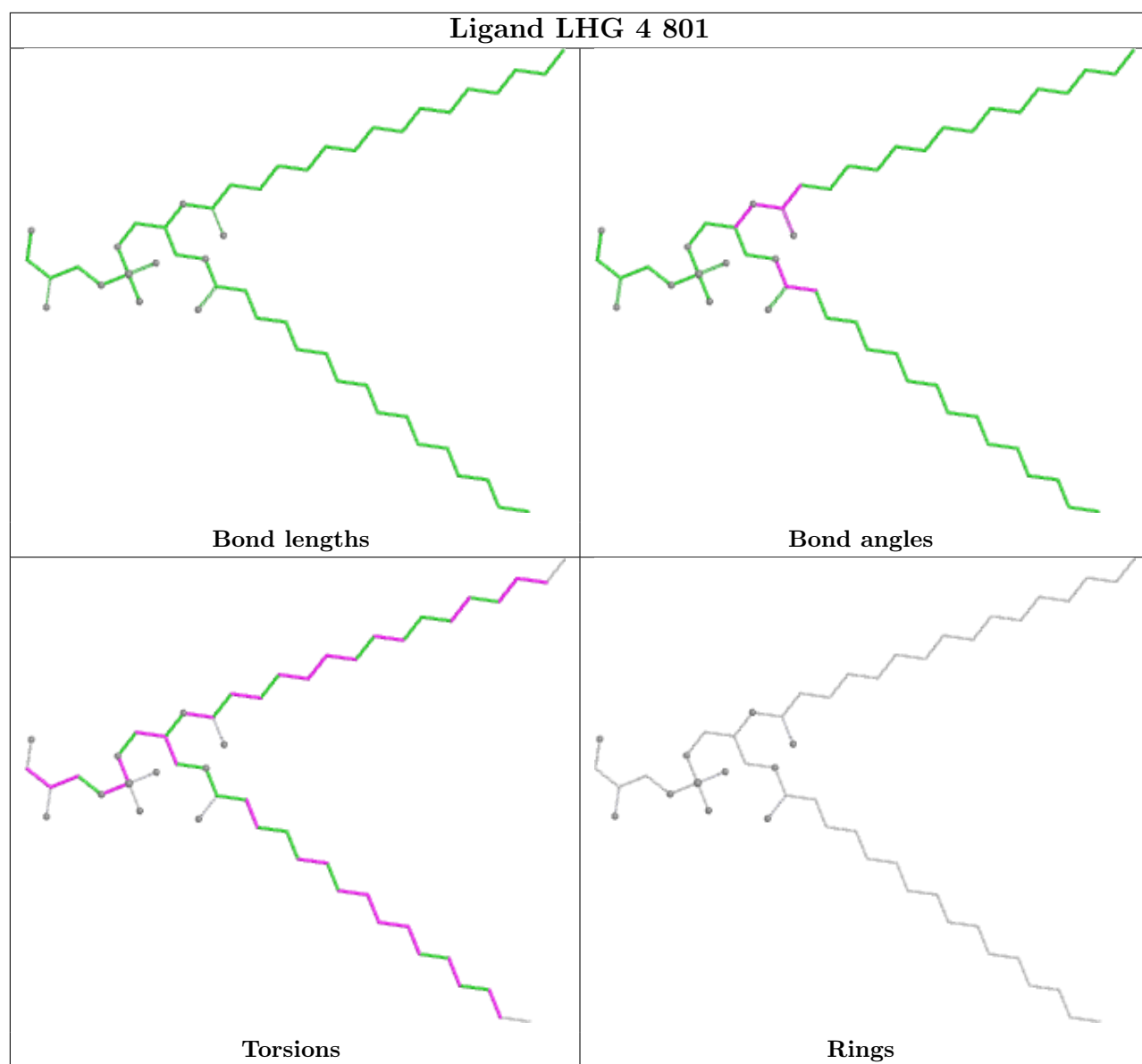


## Ligand CHL 2 613

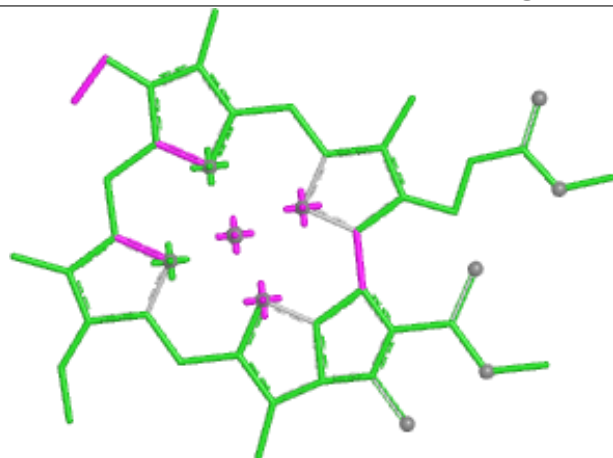


## Ligand CLA L 1502

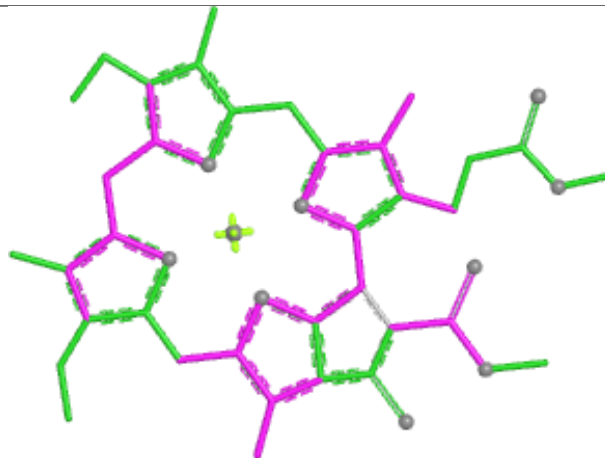




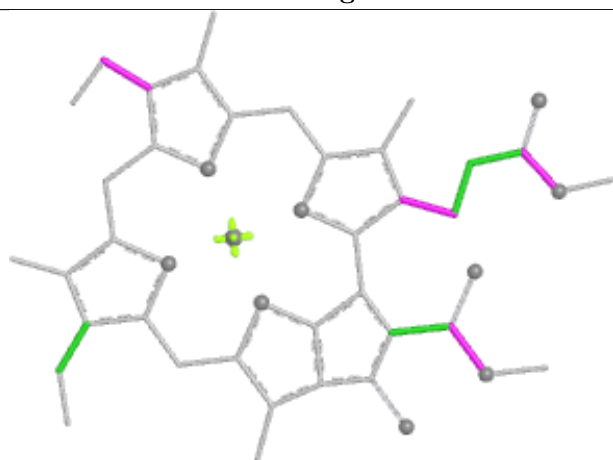
## Ligand CLA 8 615



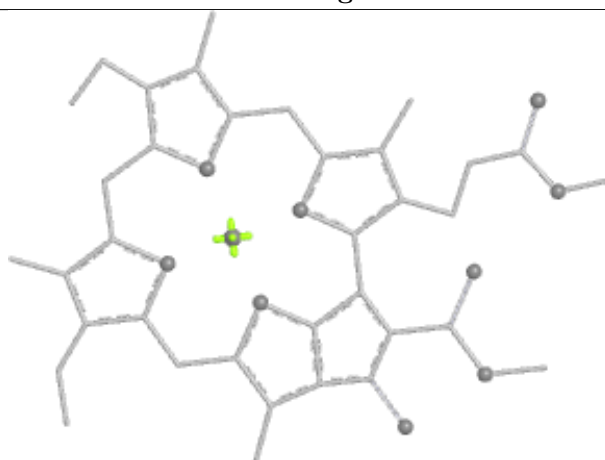
Bond lengths



Bond angles

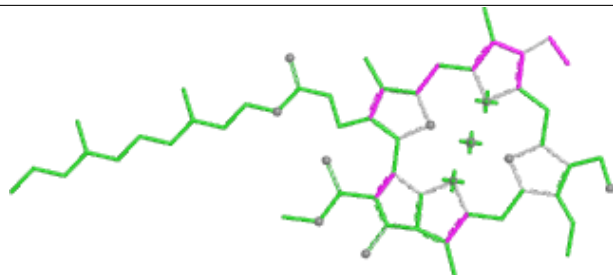


Torsions

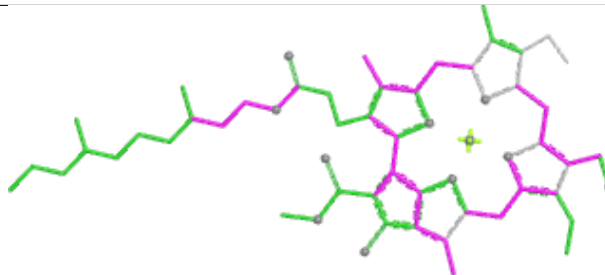


Rings

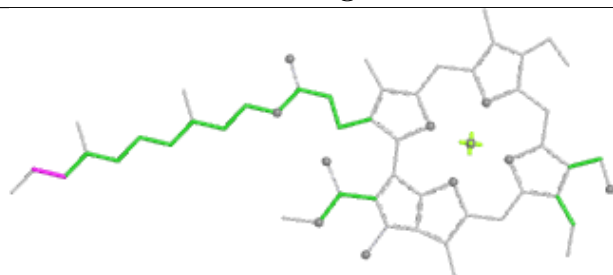
## Ligand CHL 1 609



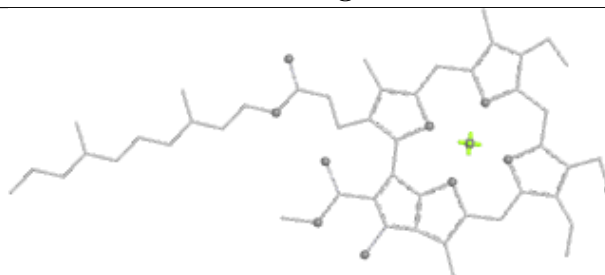
Bond lengths



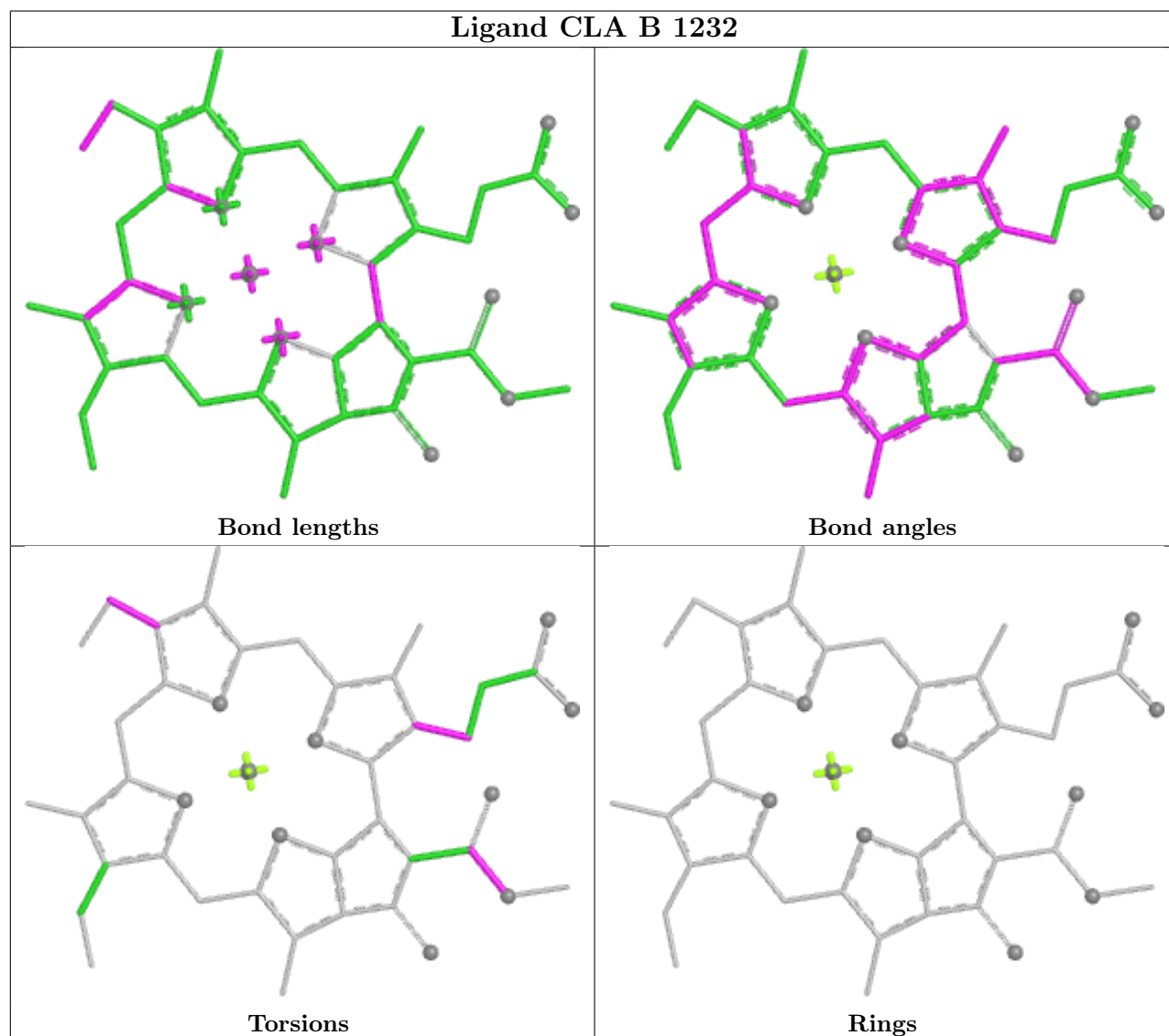
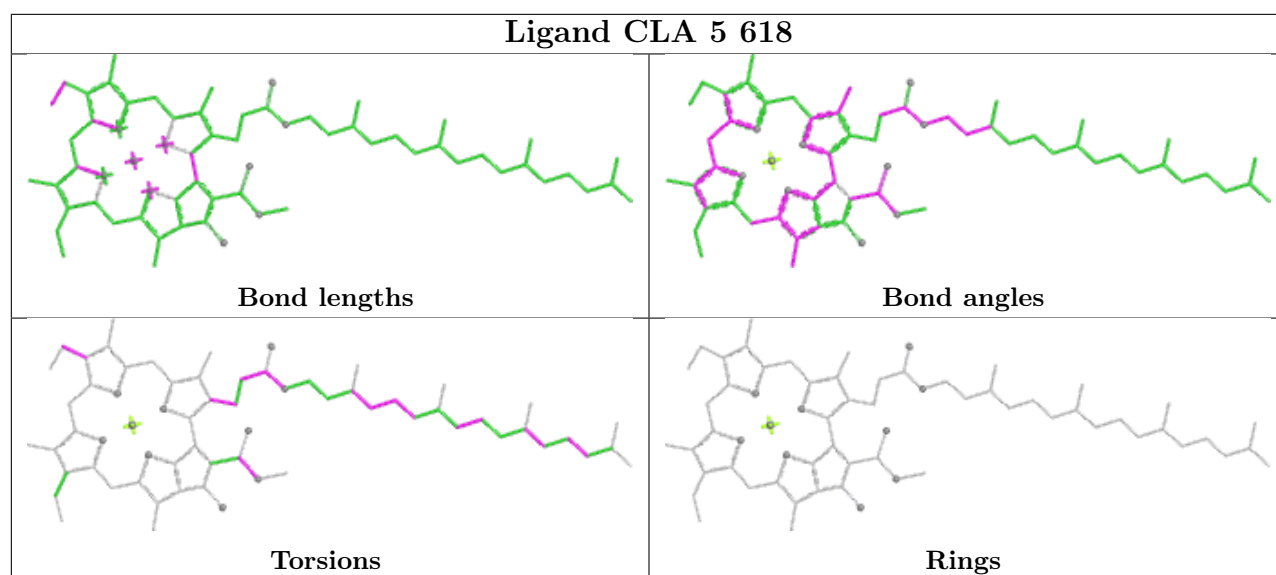
Bond angles

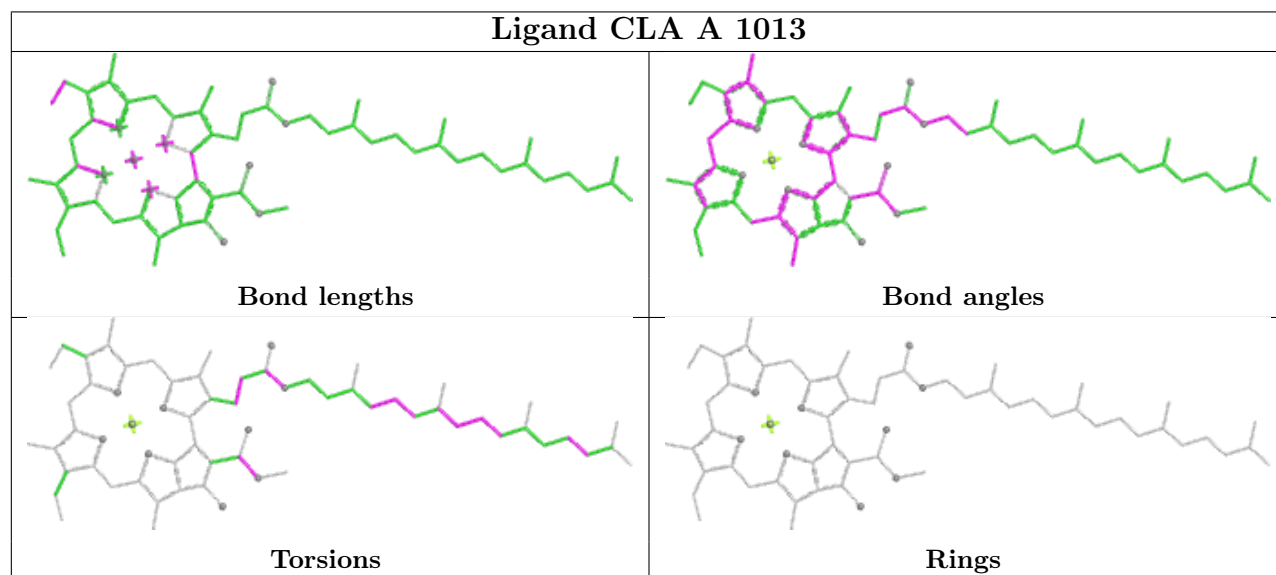
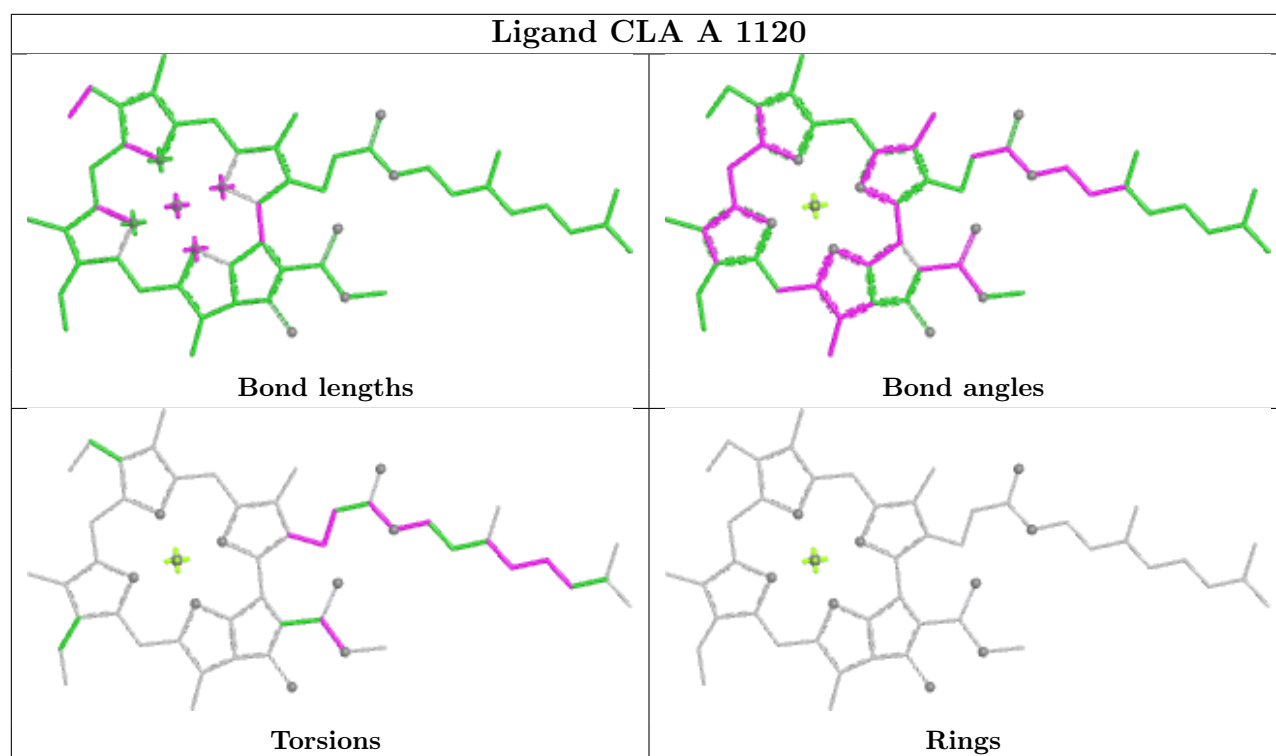


Torsions

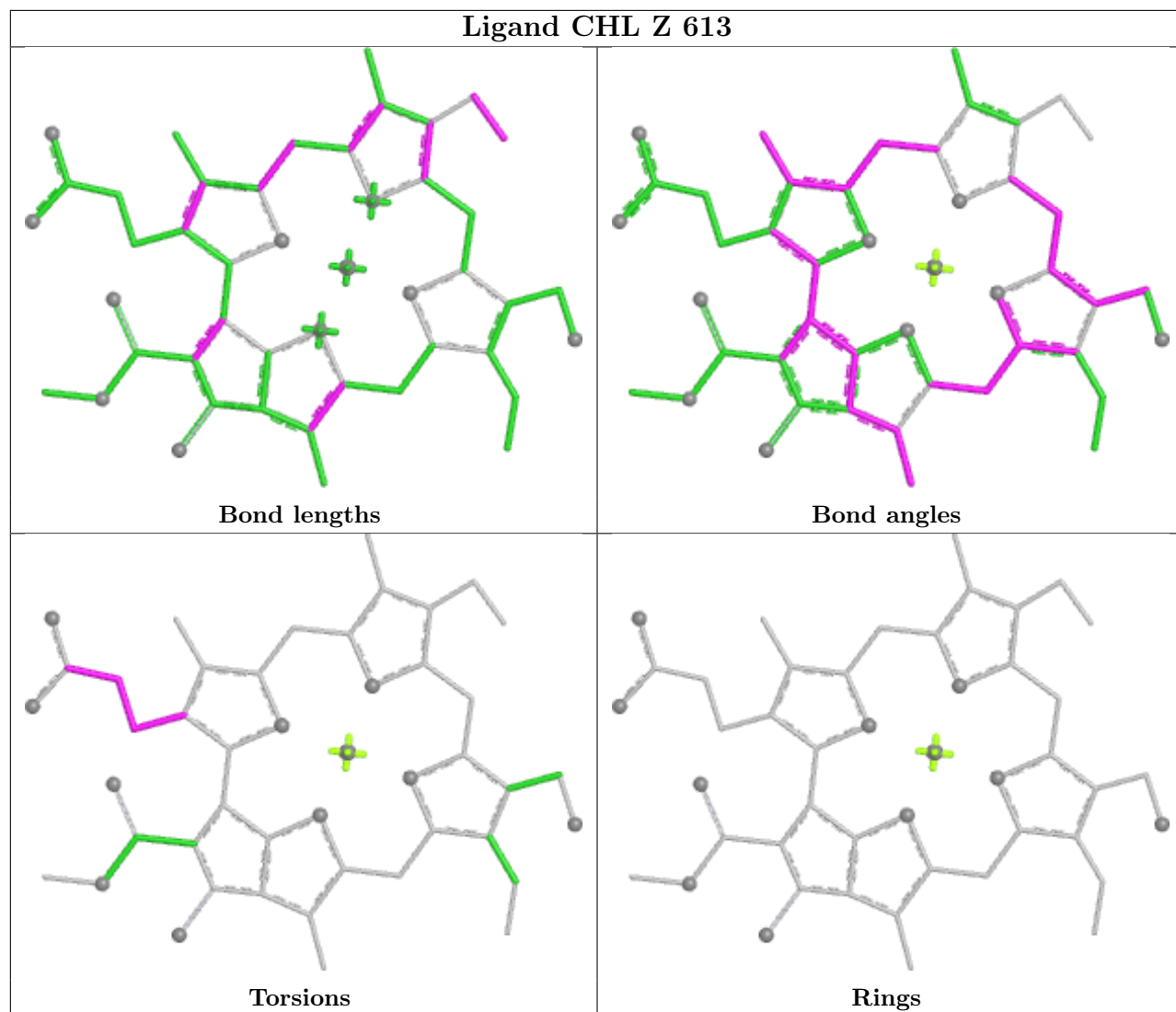


Rings

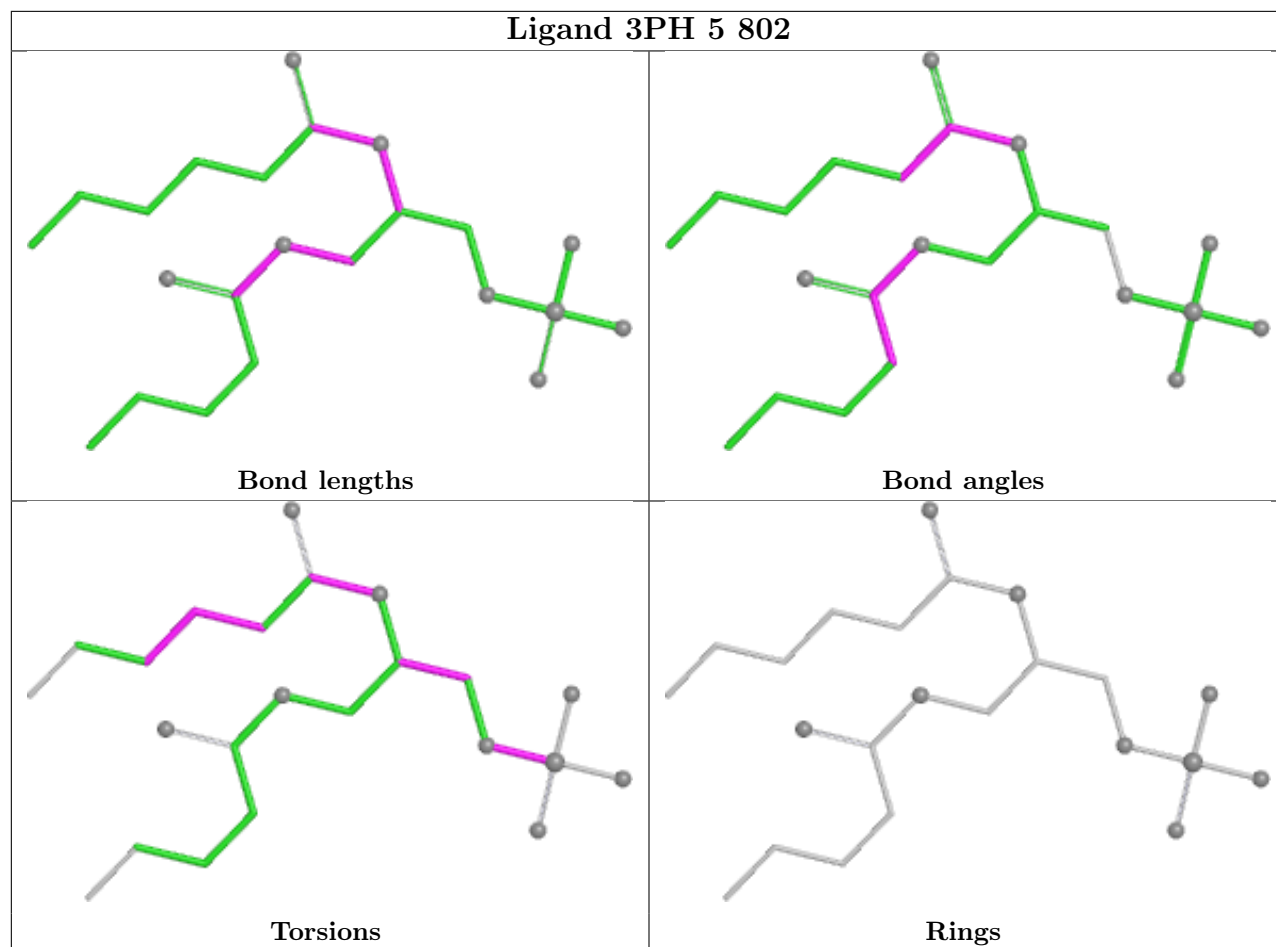




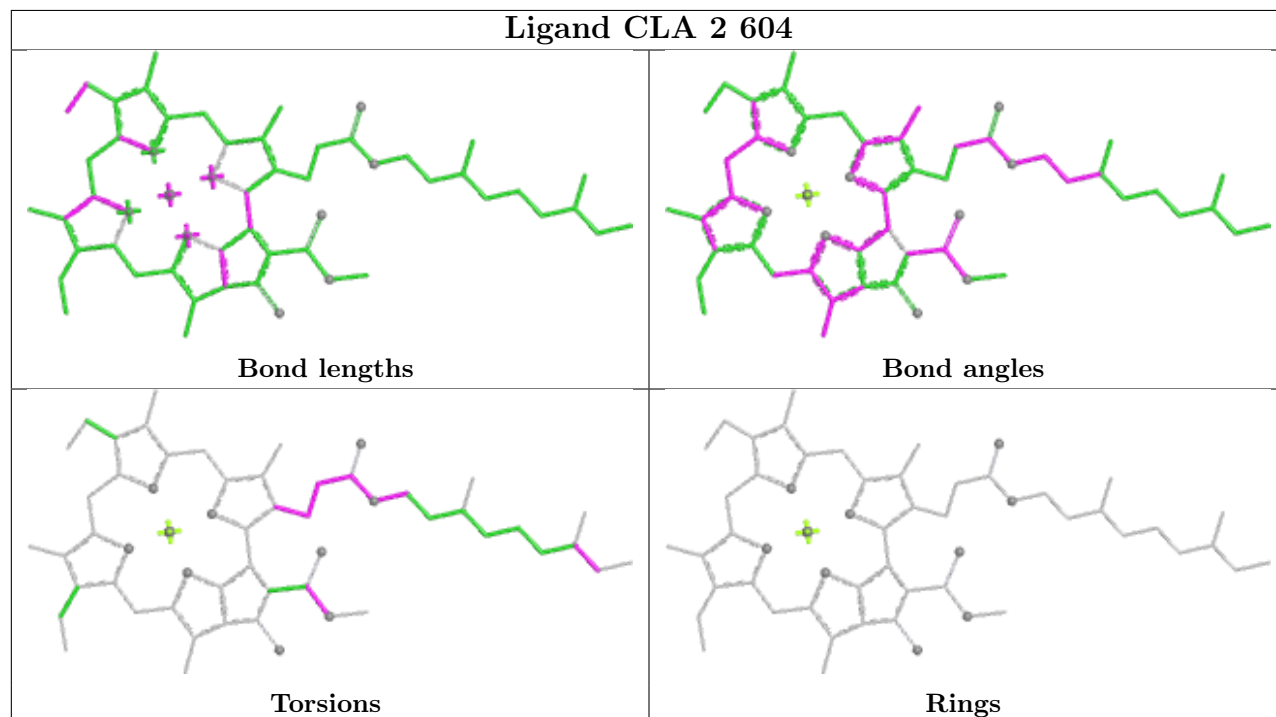
## Ligand CHL Z 613

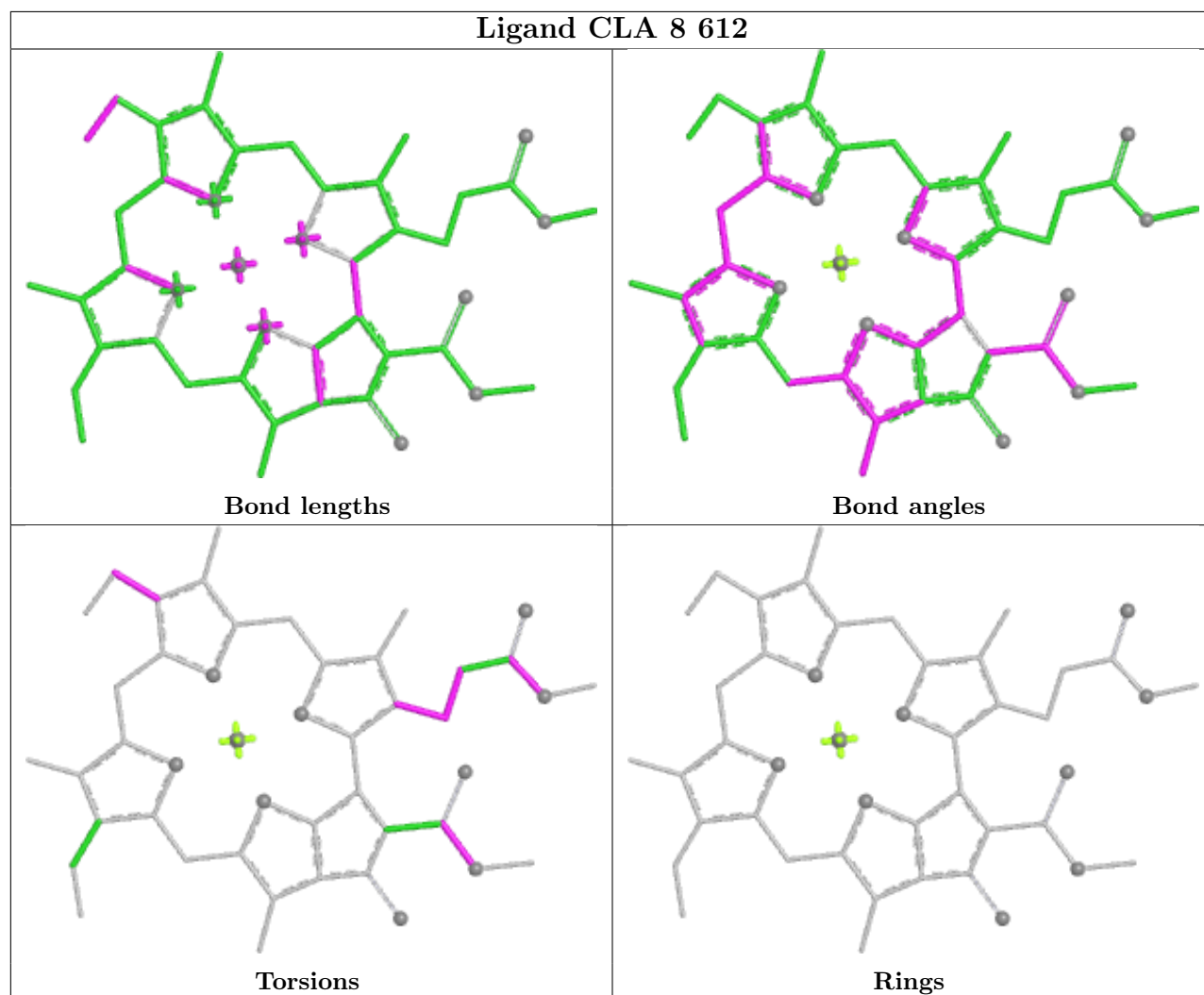
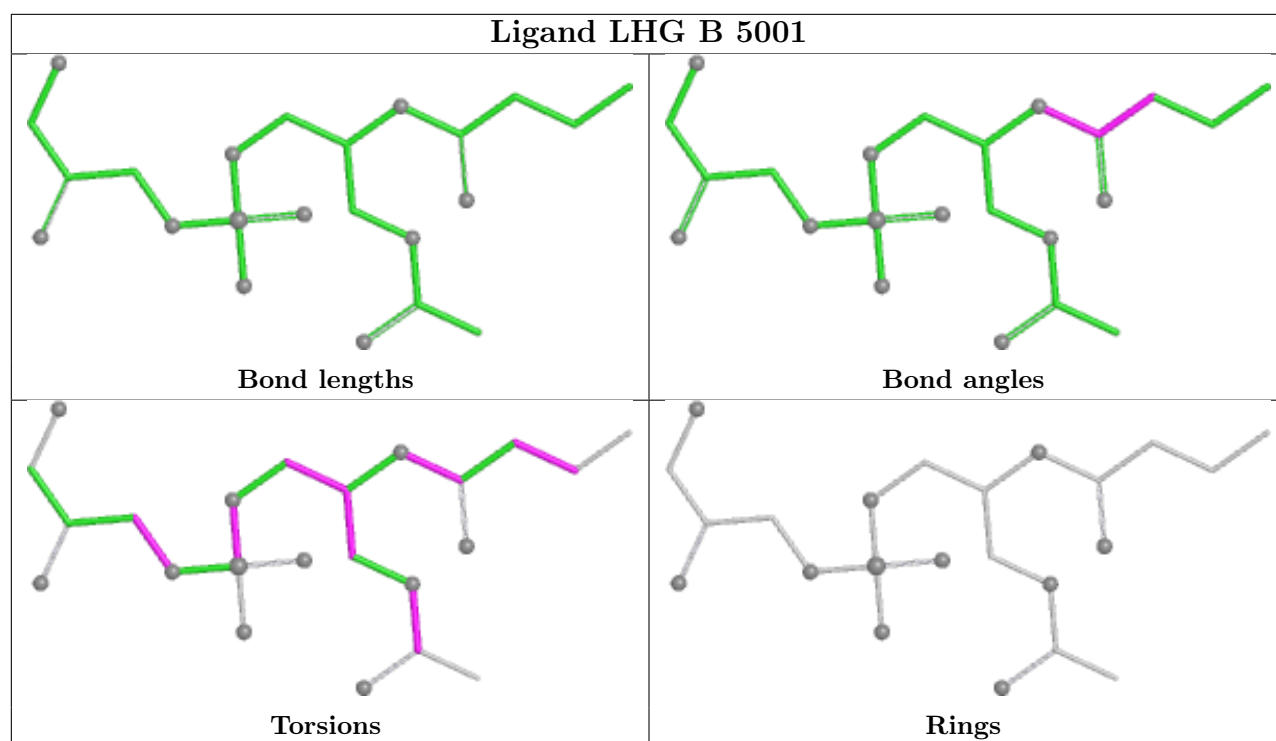


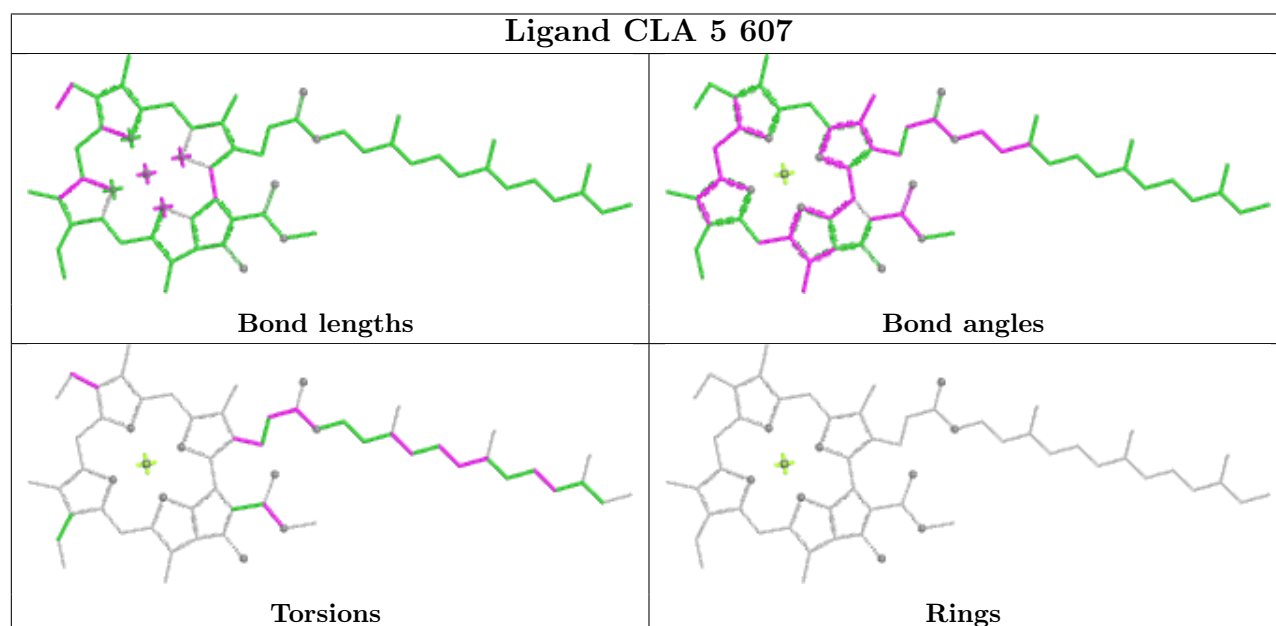
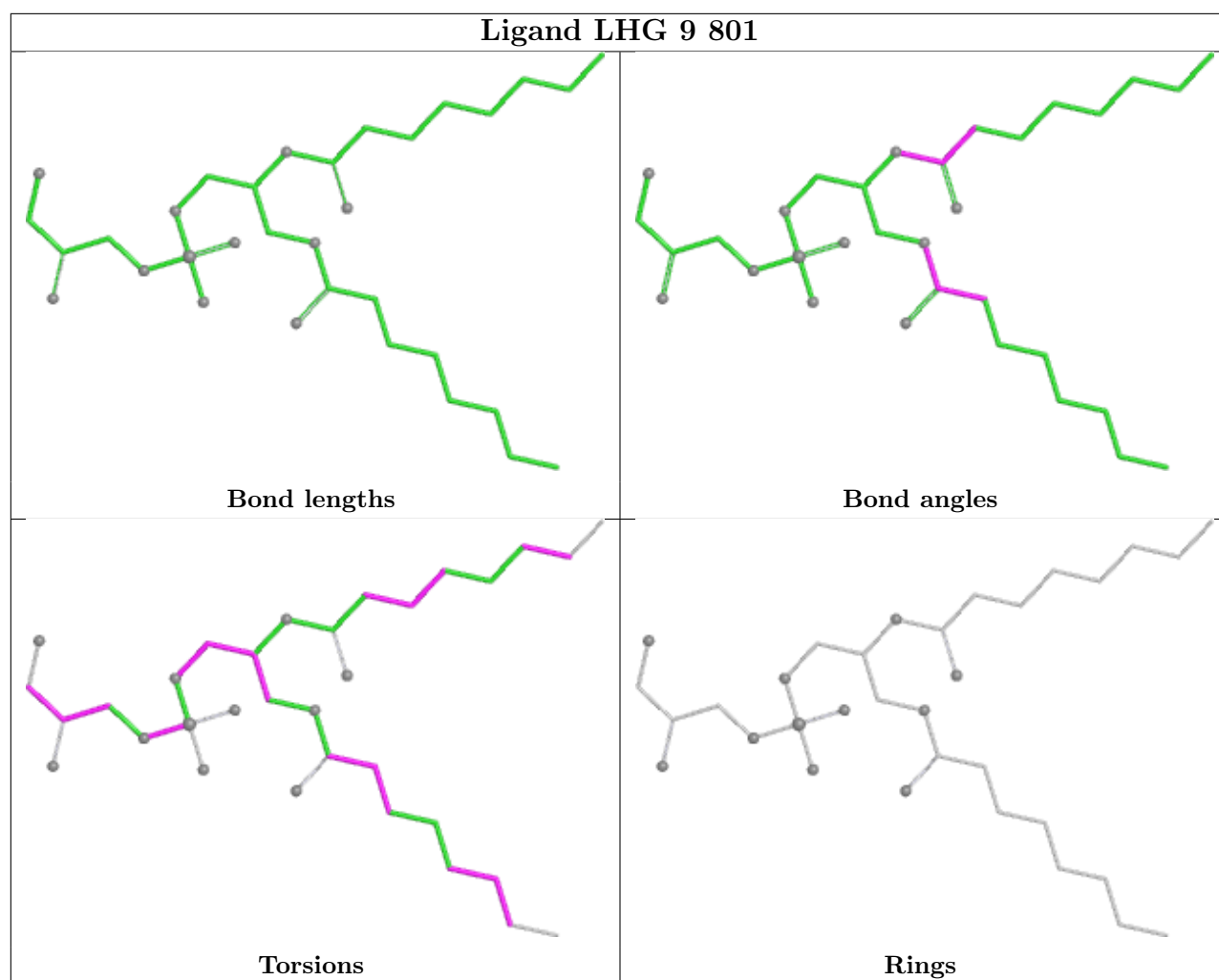
## Ligand 3PH 5 802



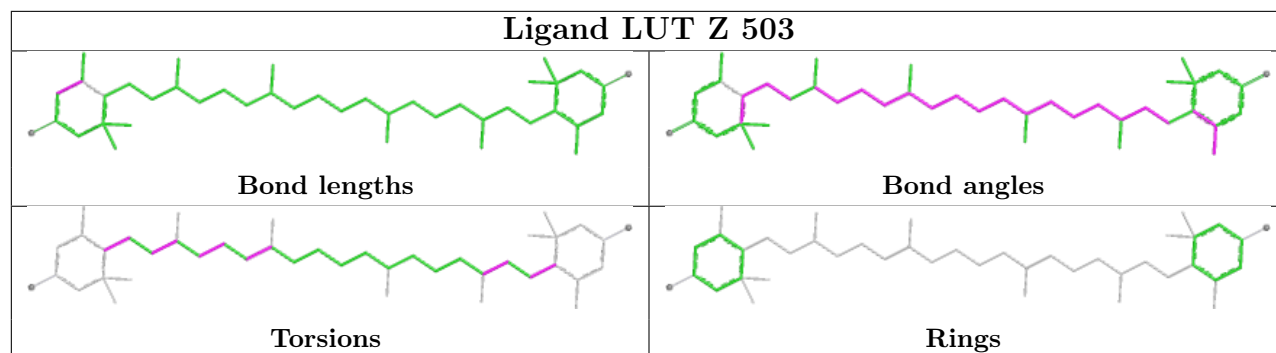
## Ligand CLA 2 604



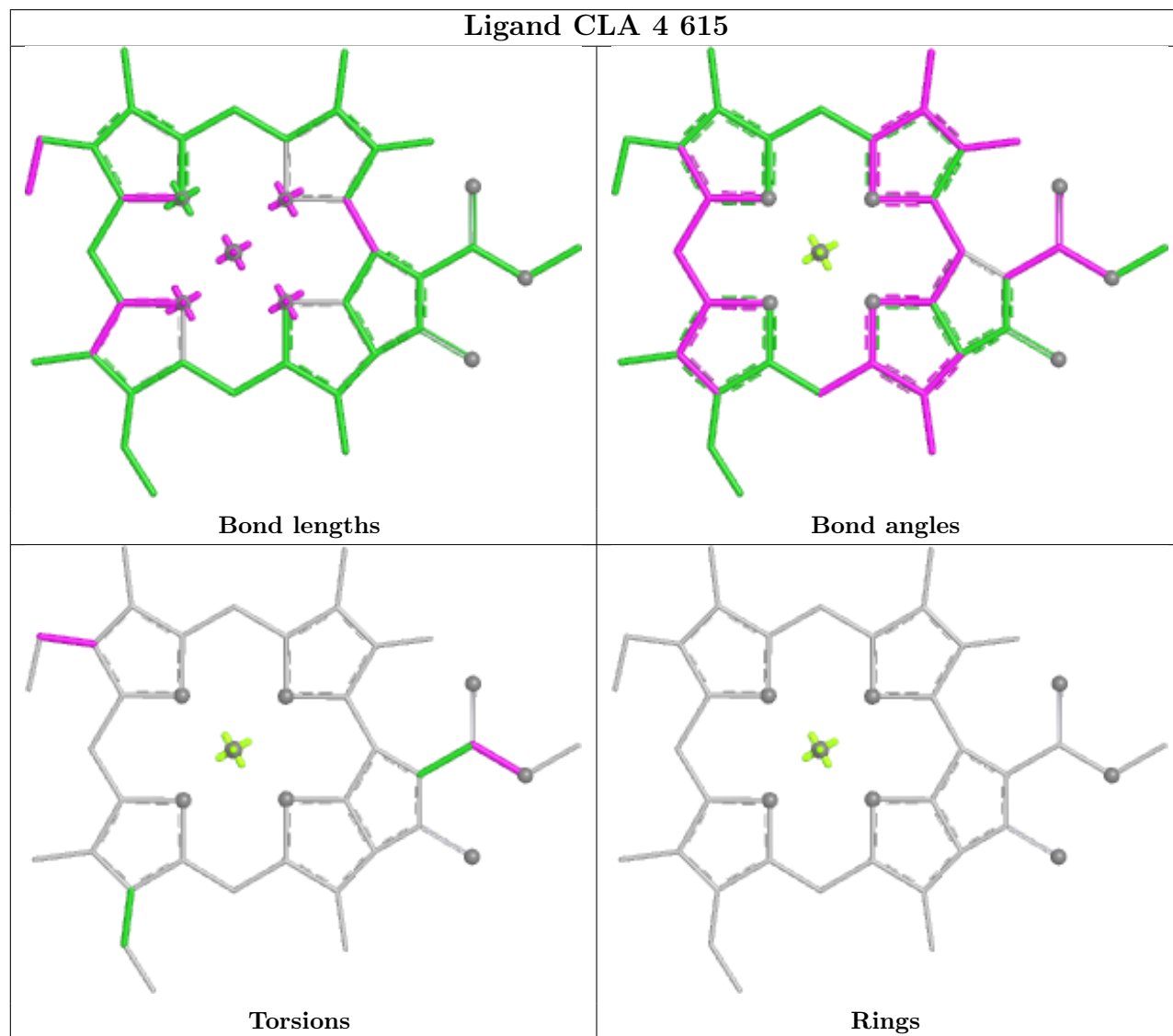


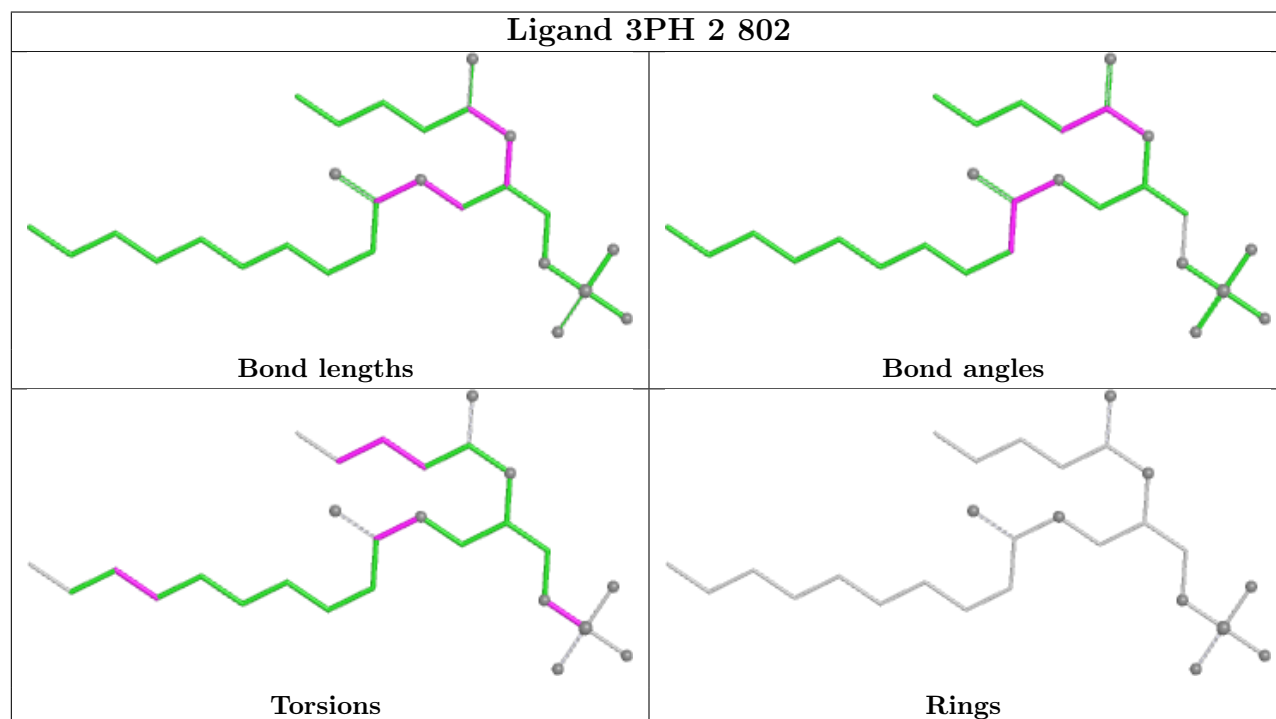
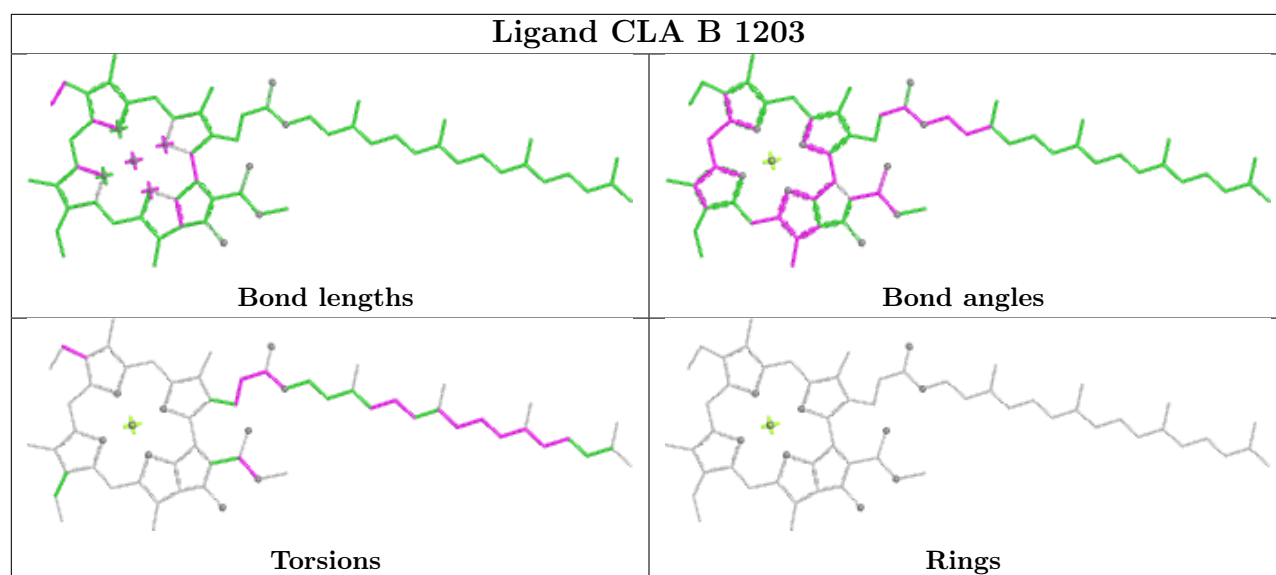


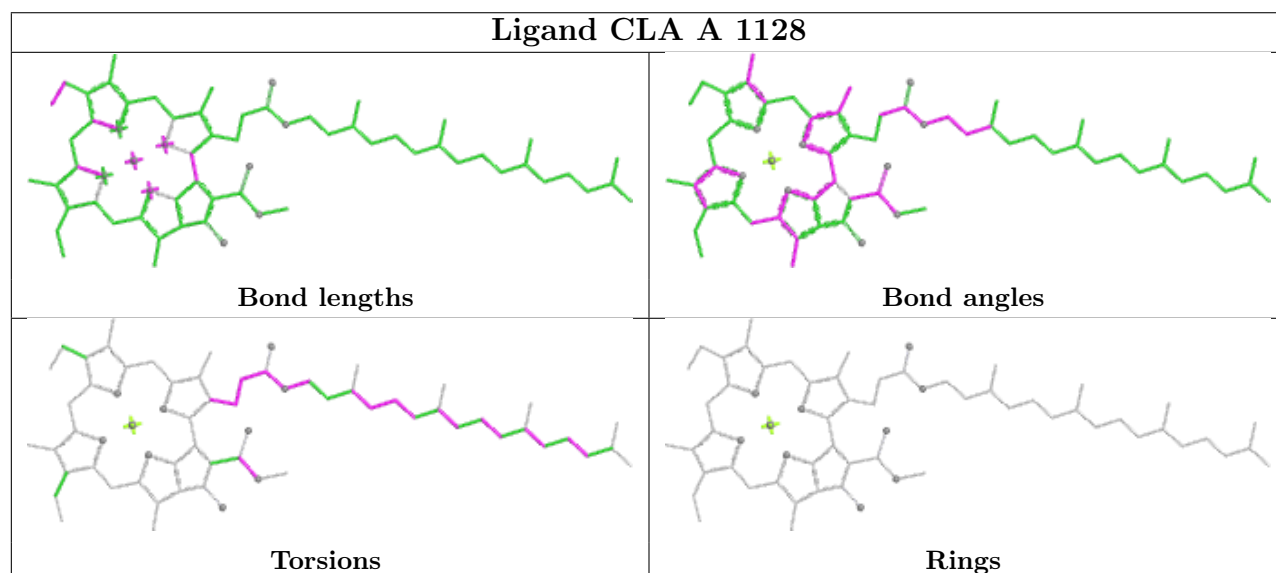
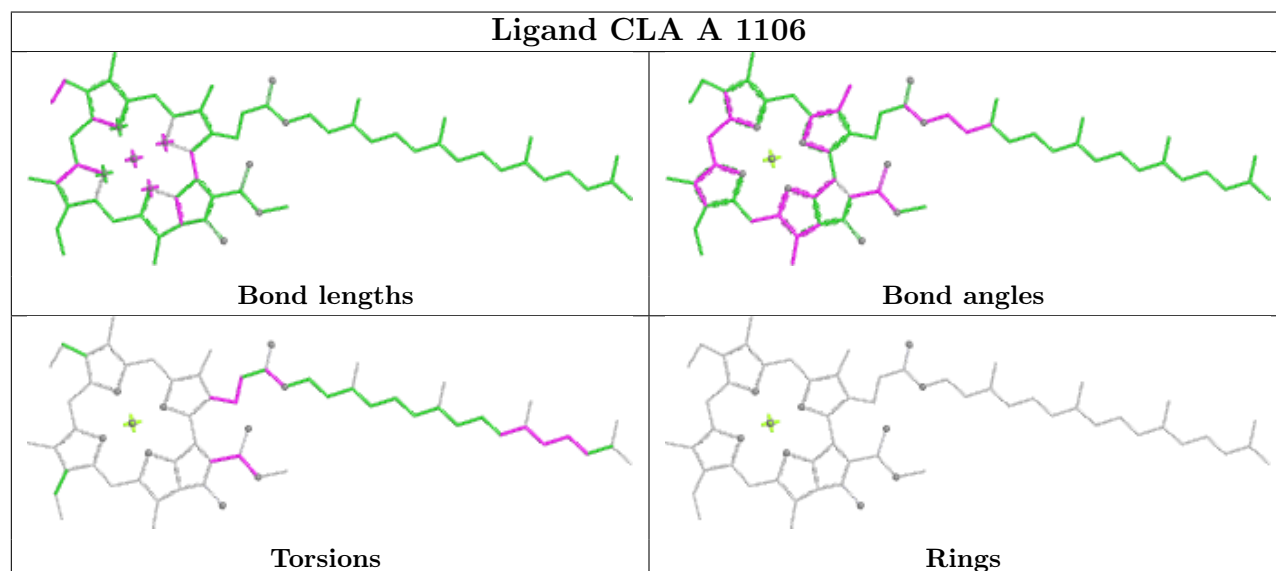
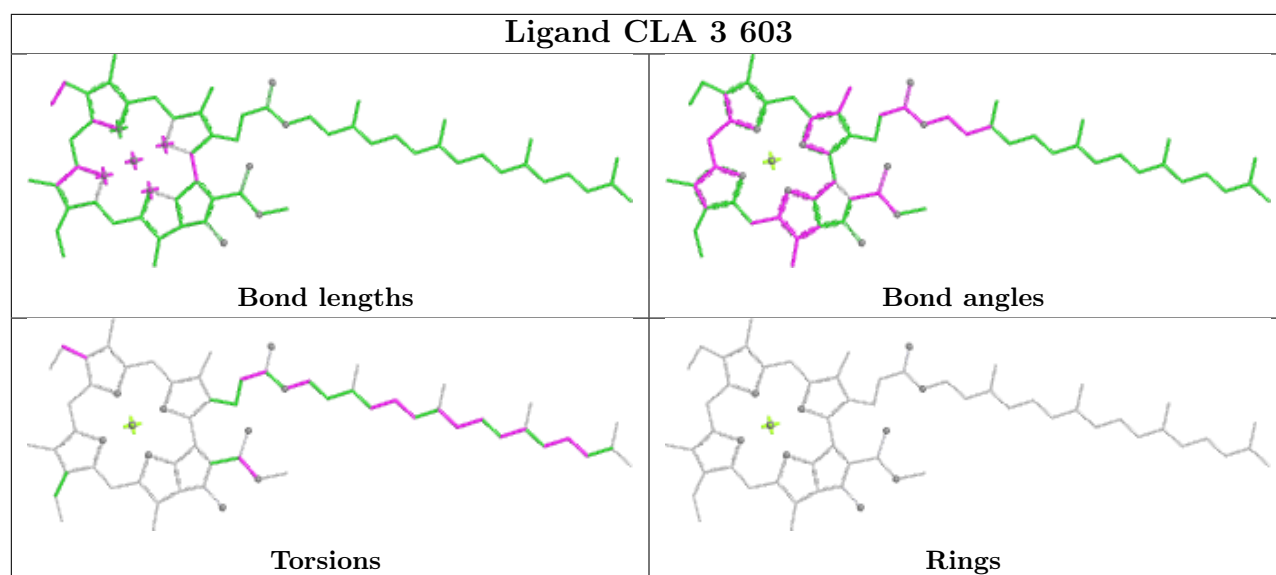
## Ligand LUT Z 503

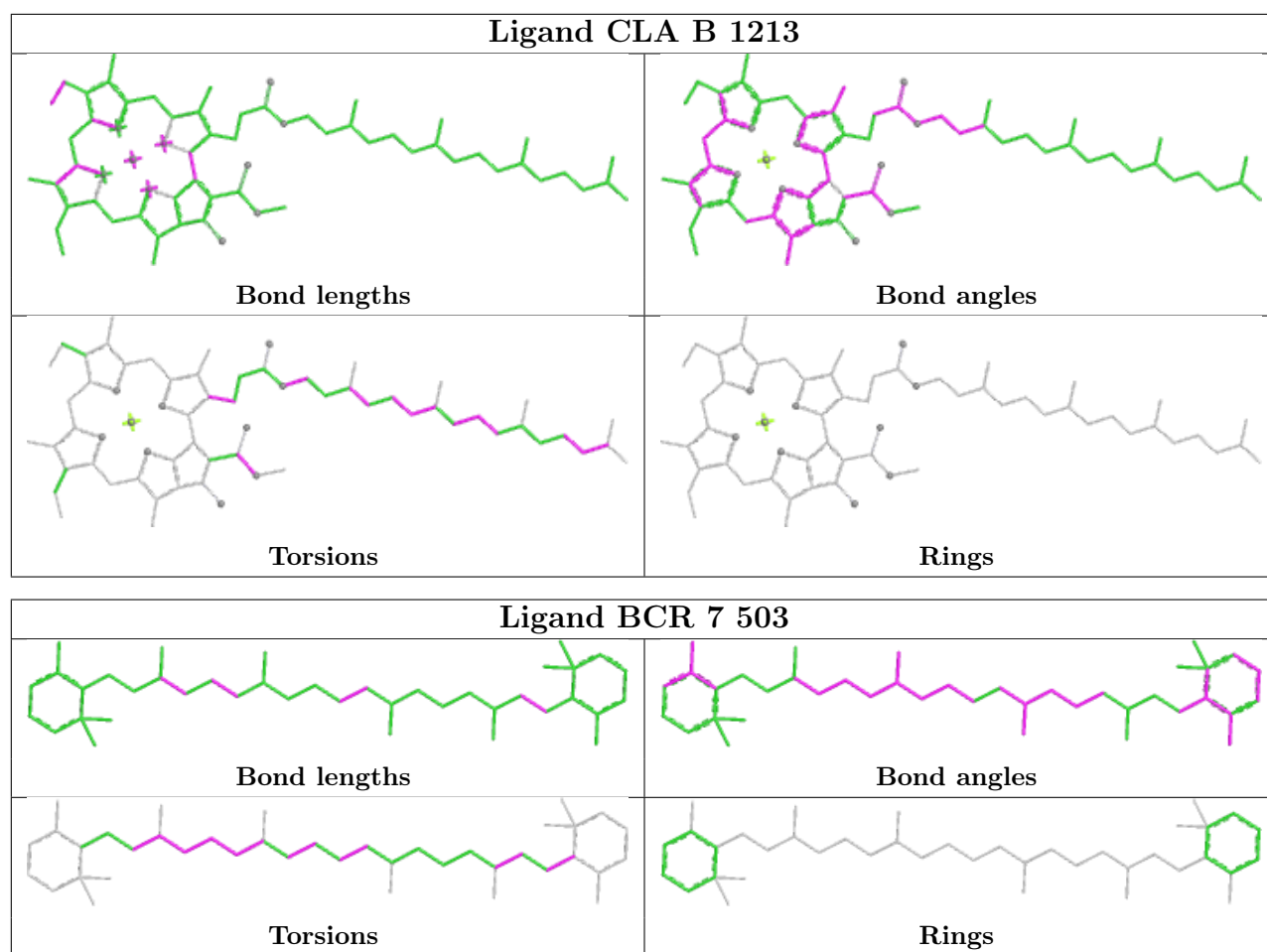


## Ligand CLA 4 615

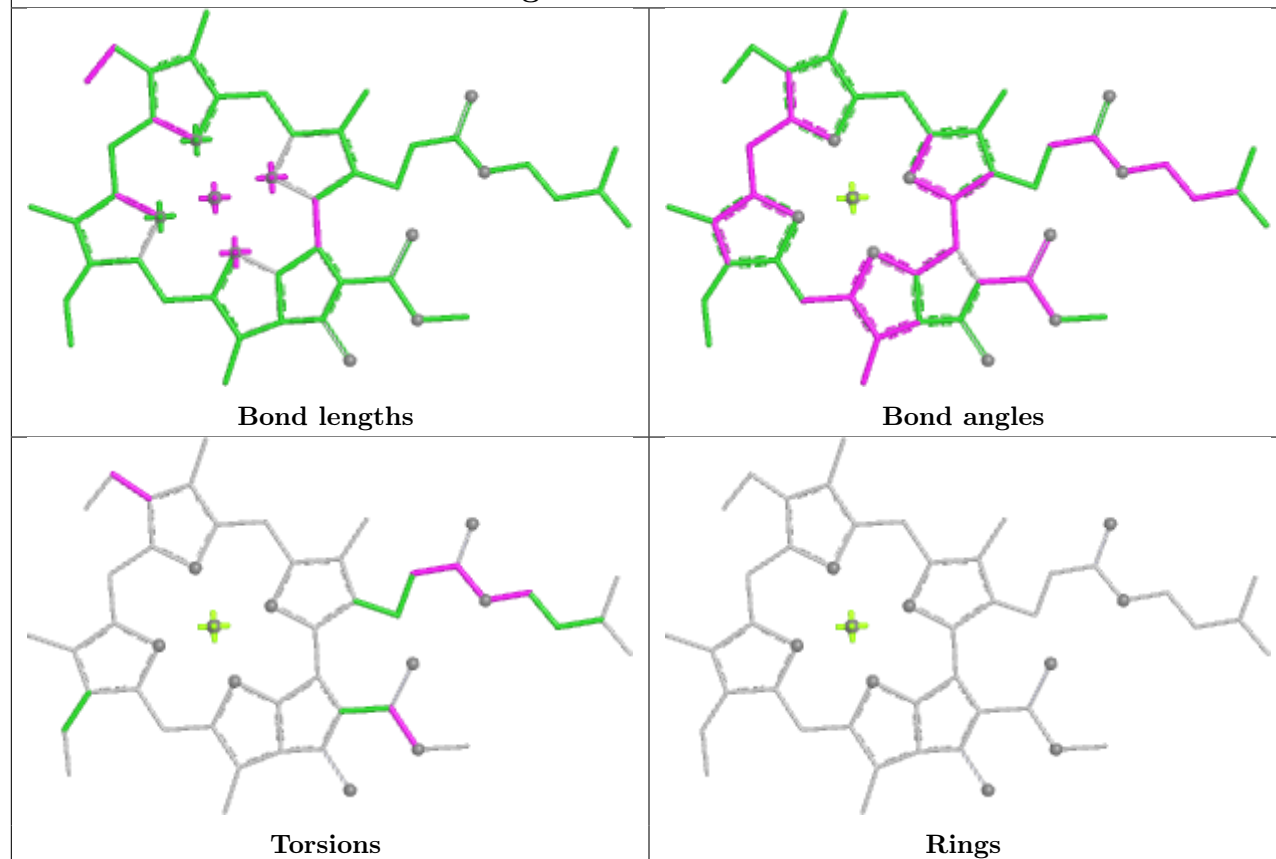




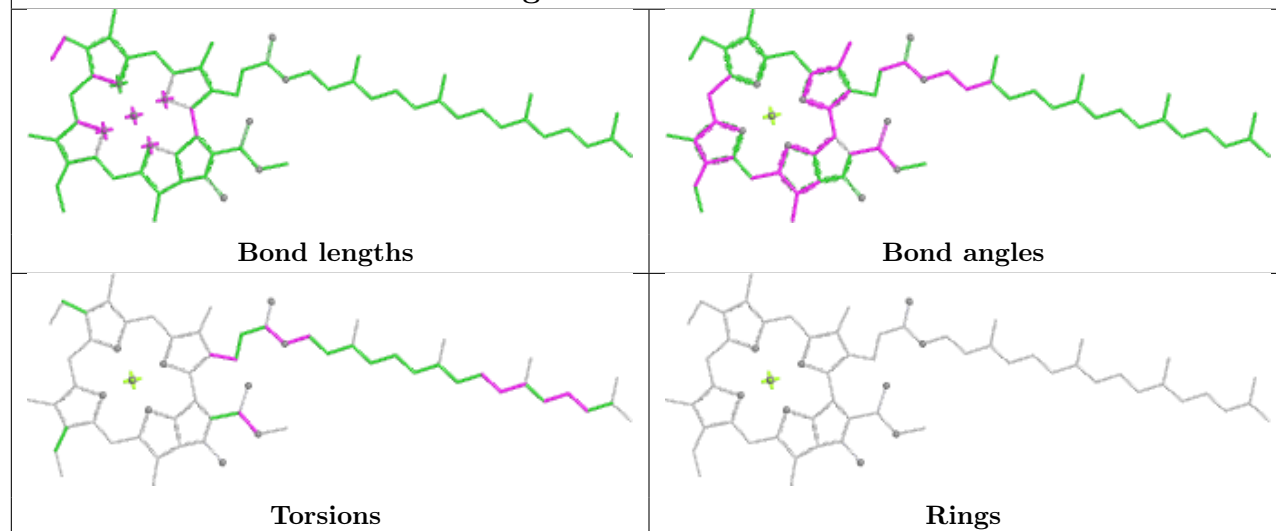


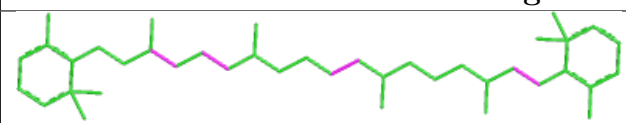
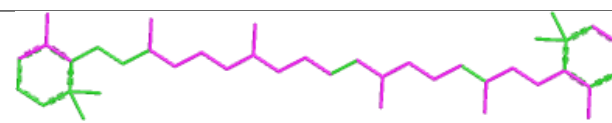
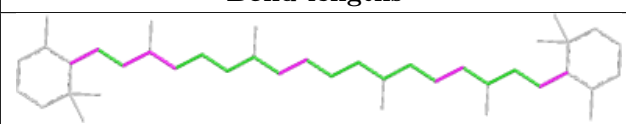
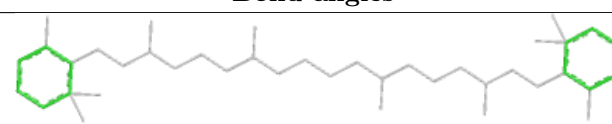


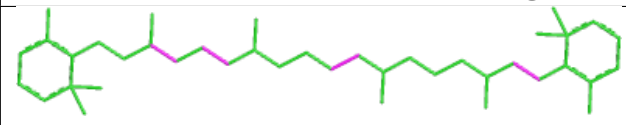
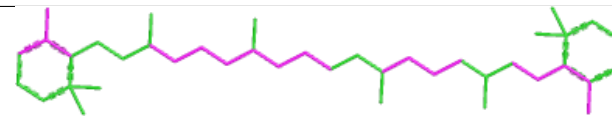
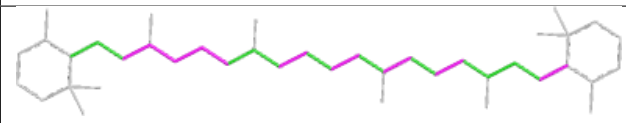
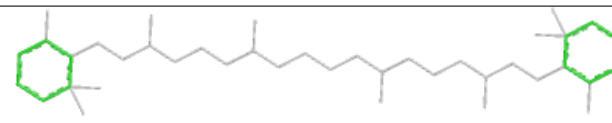
## Ligand CLA G 1601

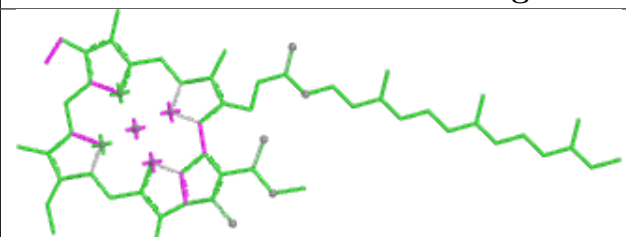
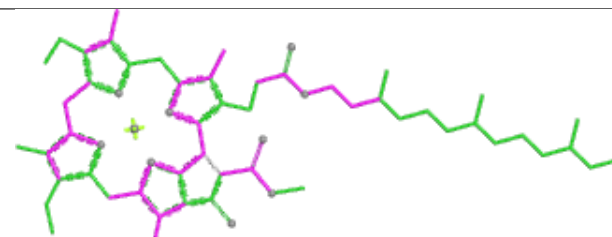
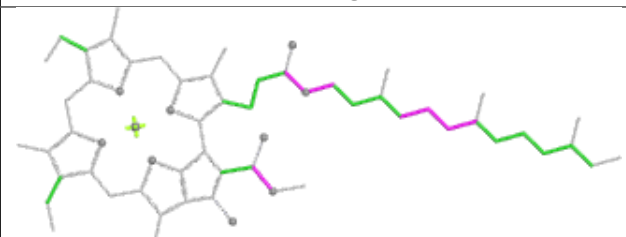
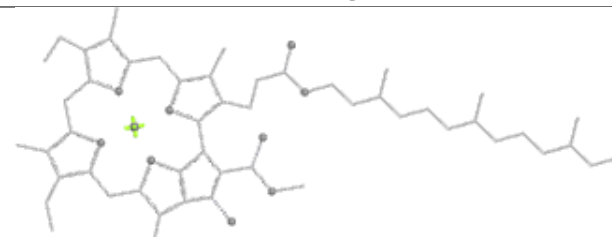


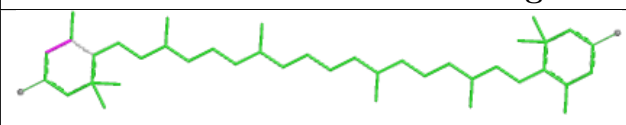
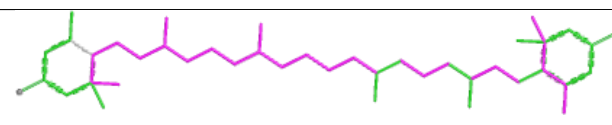
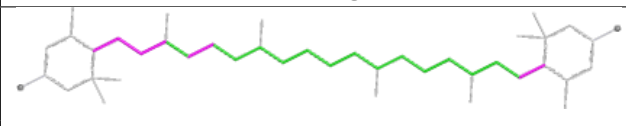
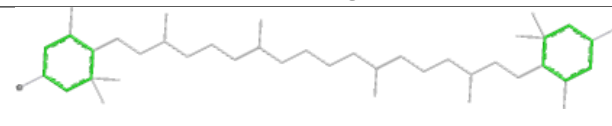
## Ligand CLA A 1123



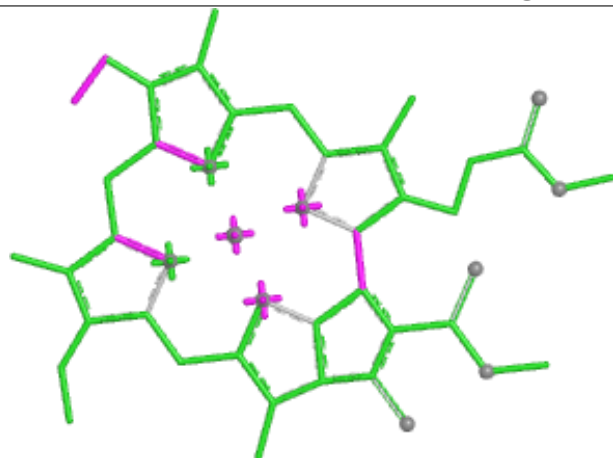
| Ligand BCR 3 503                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand BCR 6 503                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

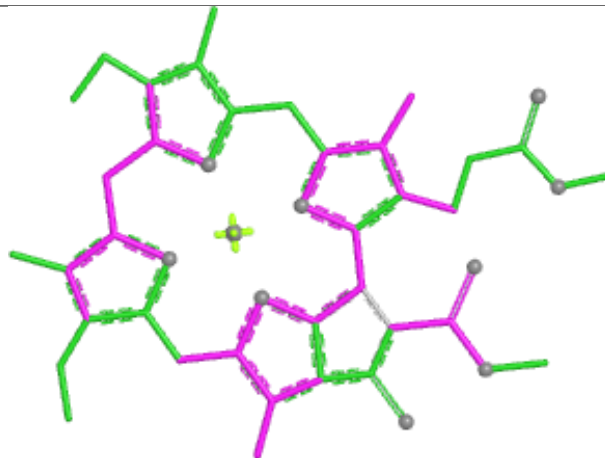
| Ligand CLA A 1114                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

| Ligand LUT 2 501                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

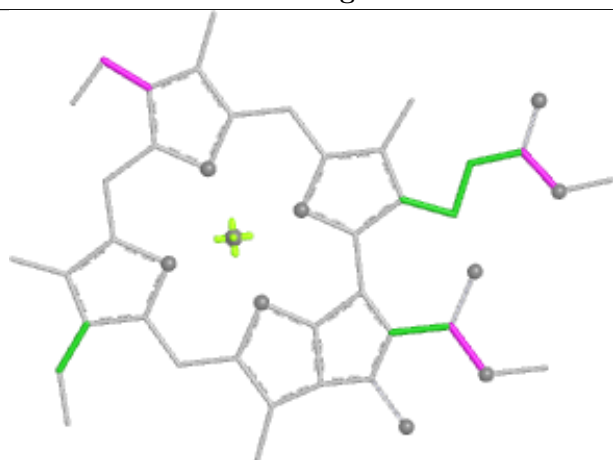
## Ligand CLA 2 615



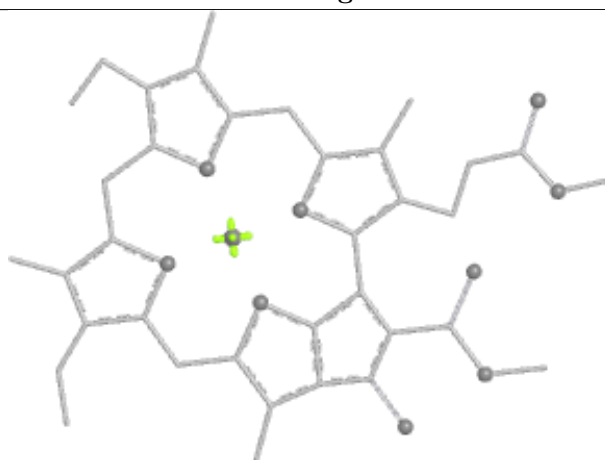
Bond lengths



Bond angles

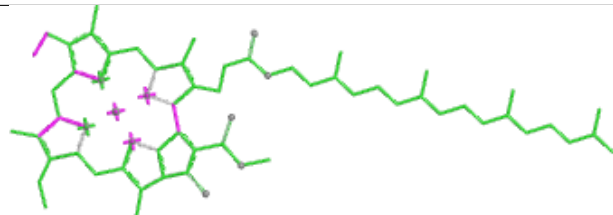


Torsions

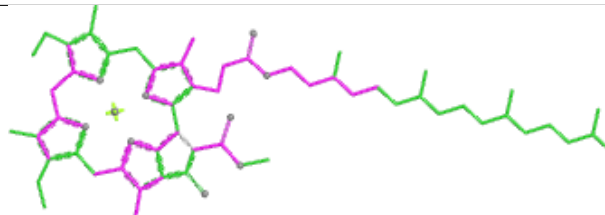


Rings

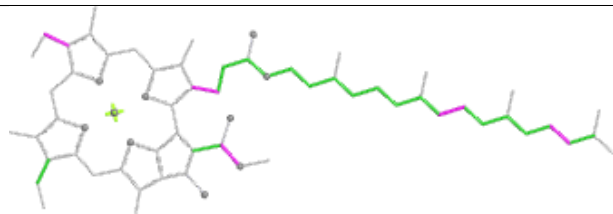
## Ligand CLA 8 603



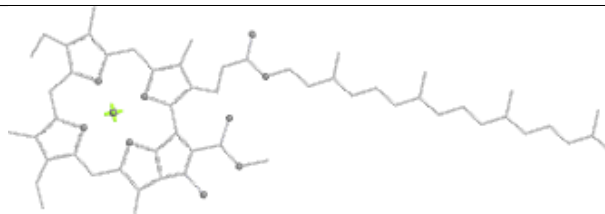
Bond lengths



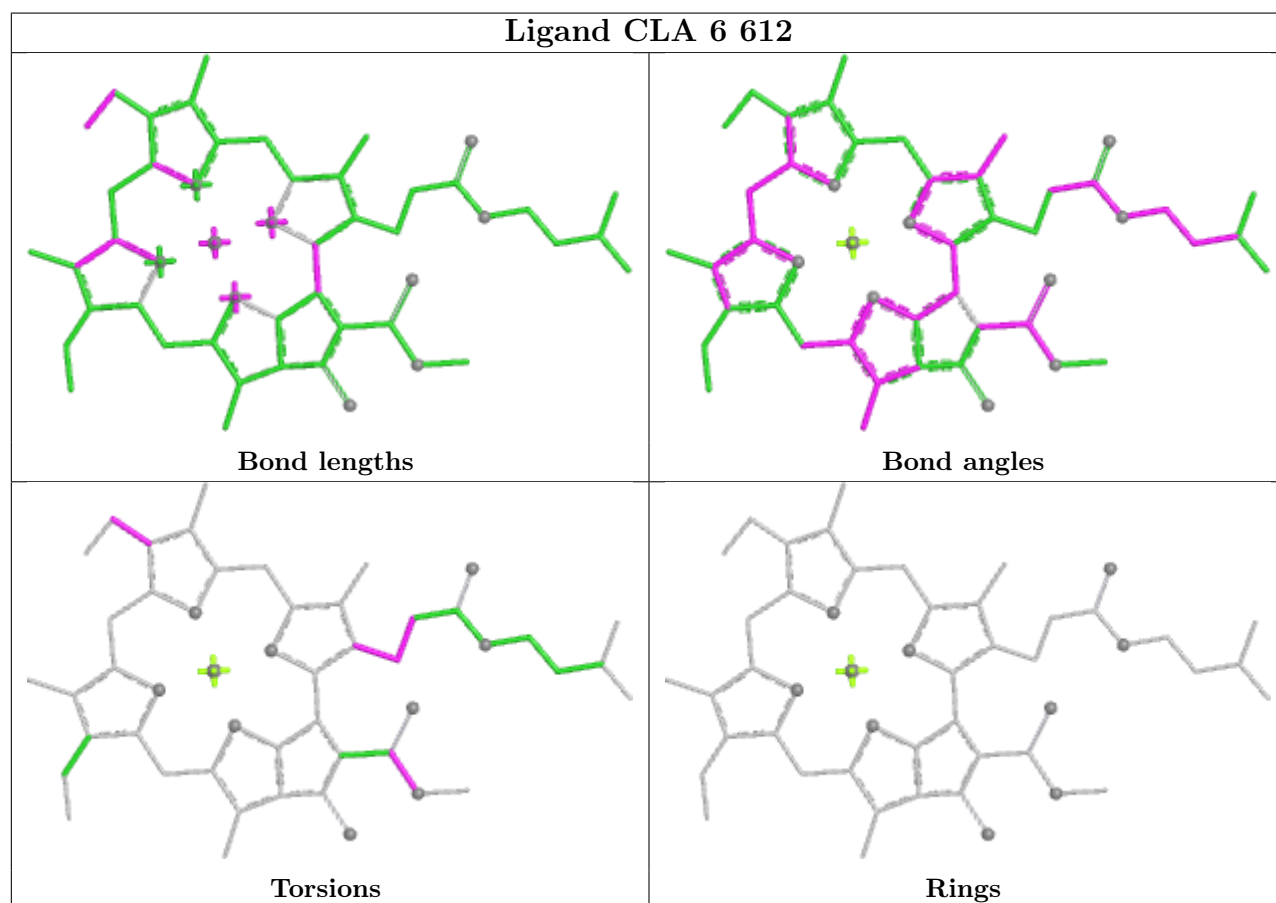
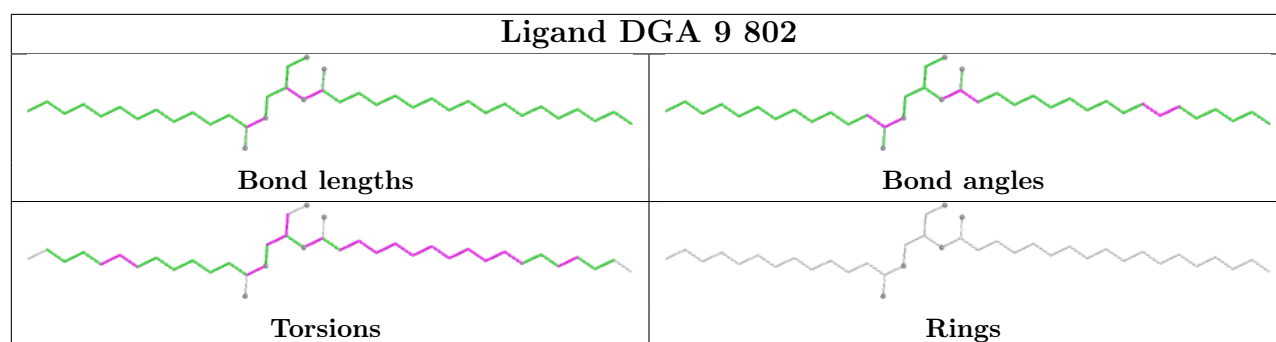
Bond angles



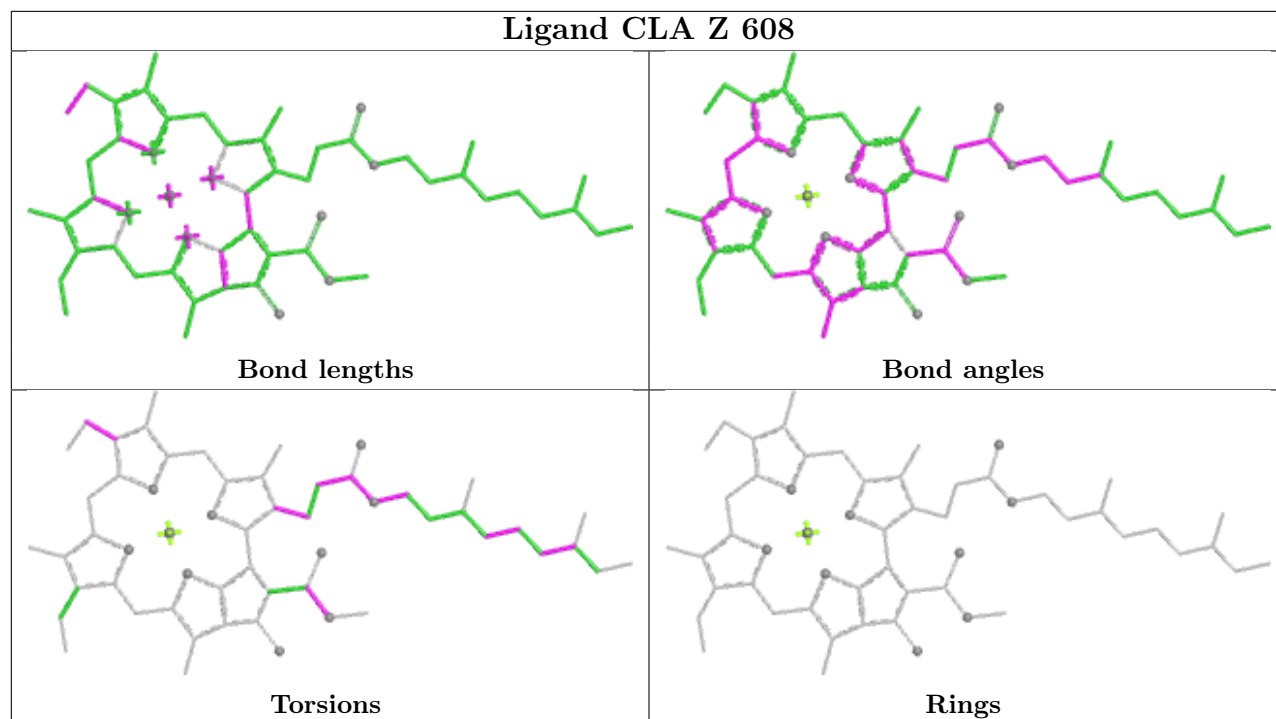
Torsions



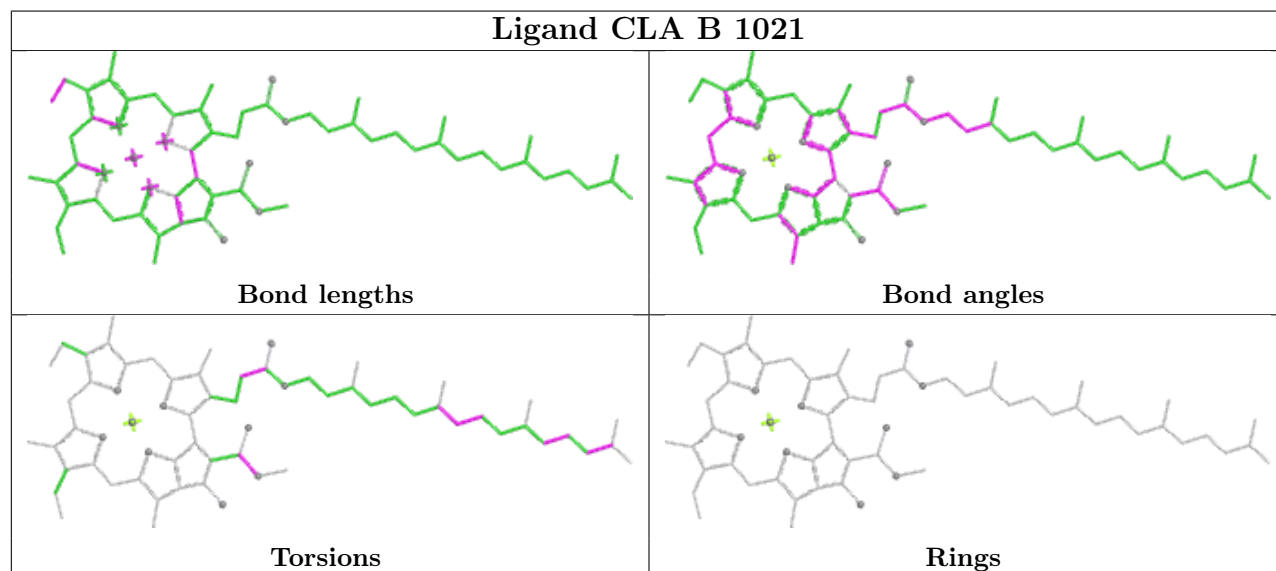
Rings

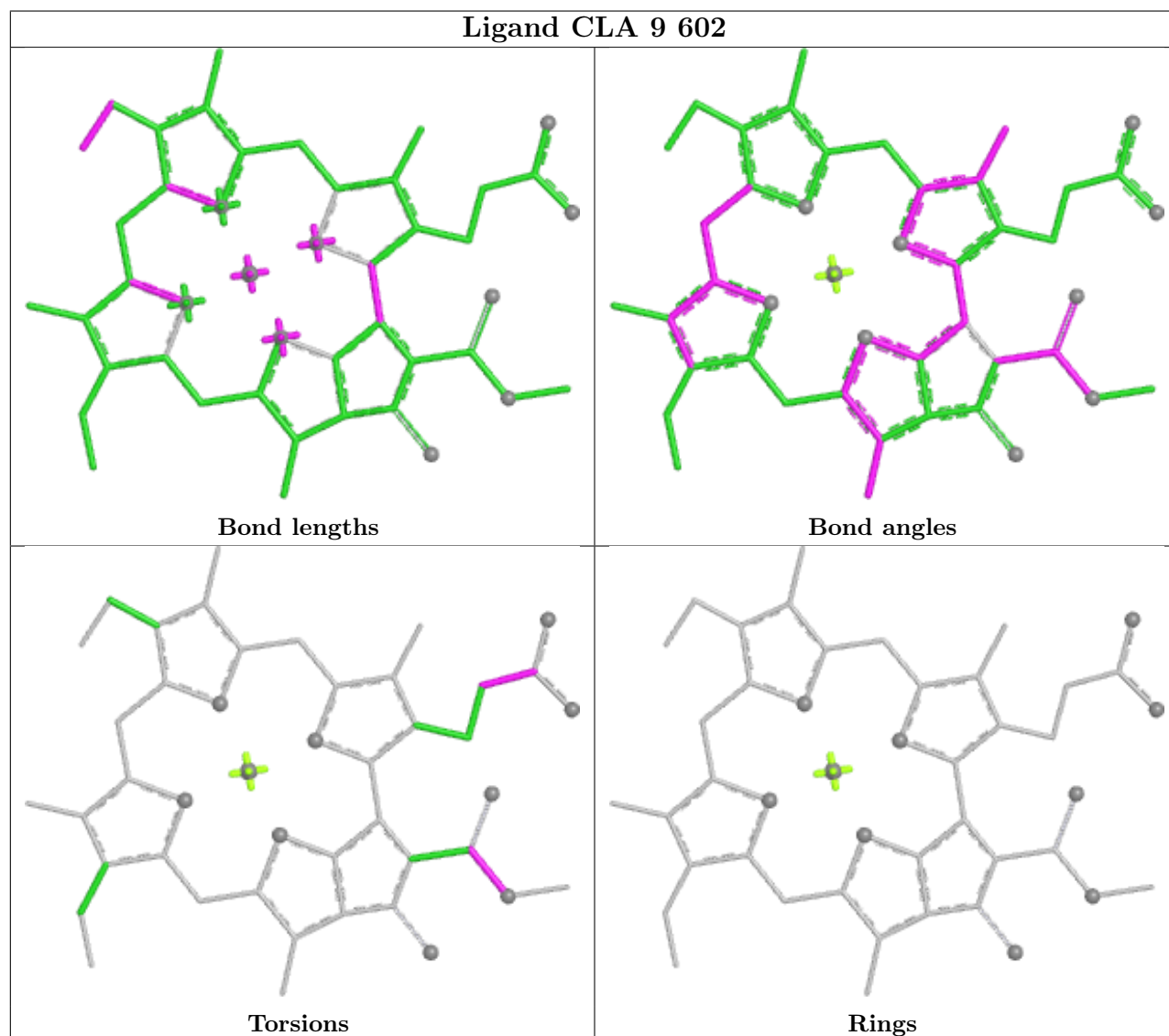
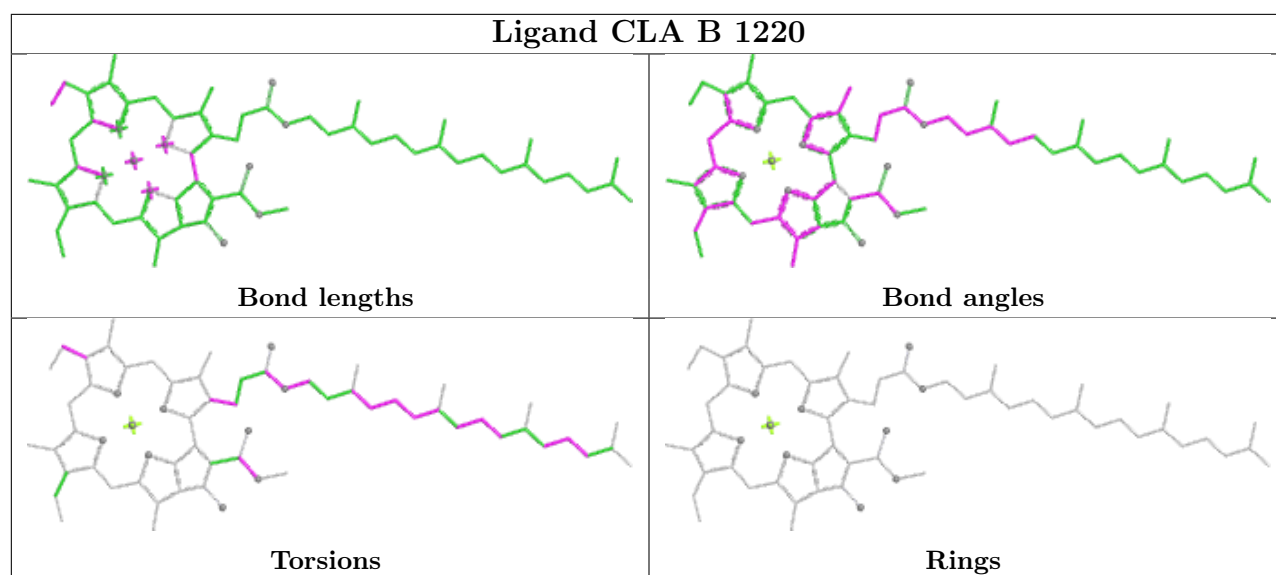


## Ligand CLA Z 608

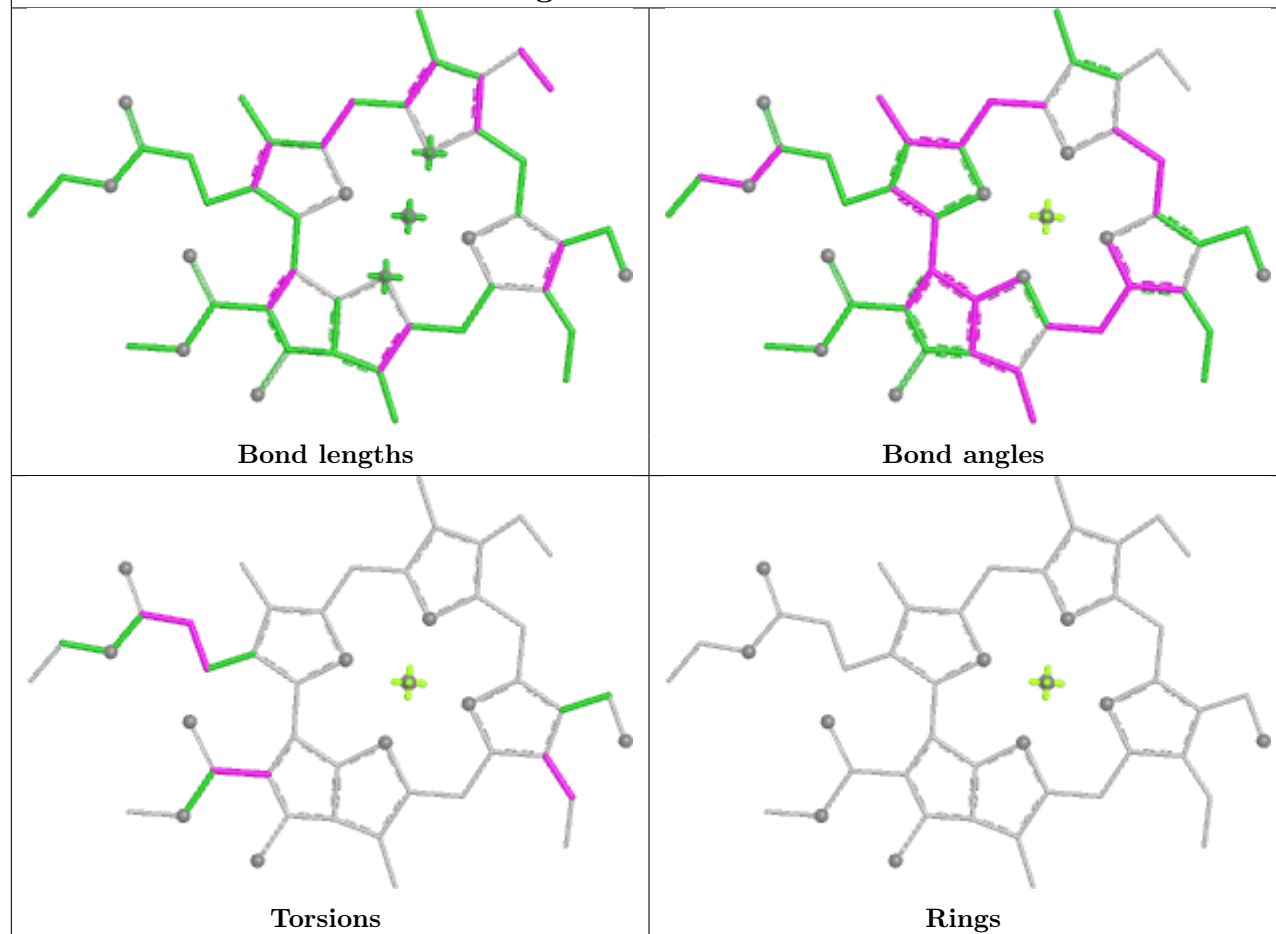


## Ligand CLA B 1021

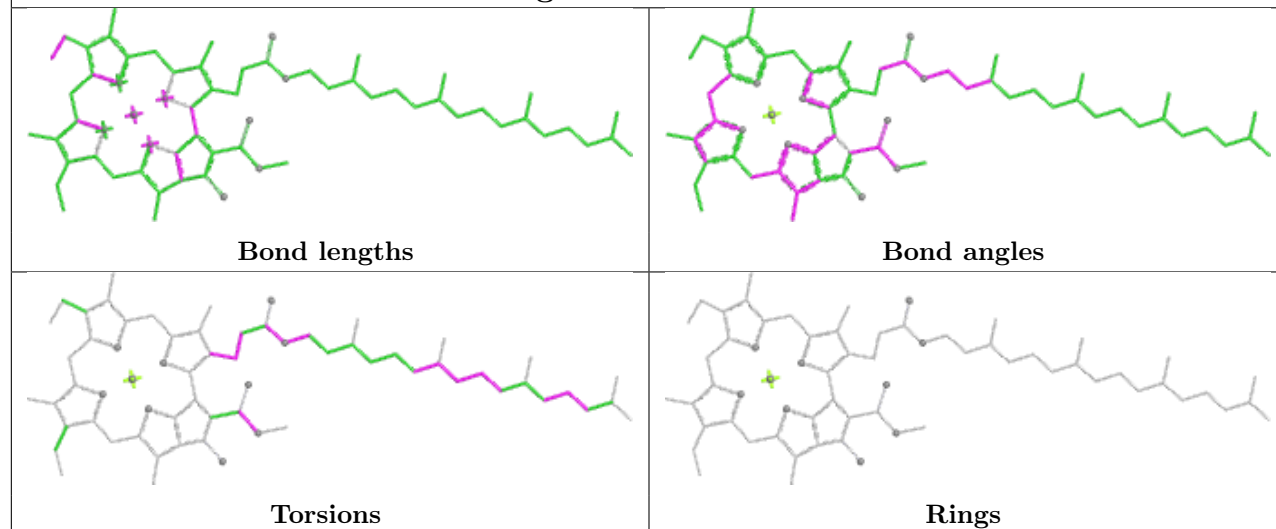


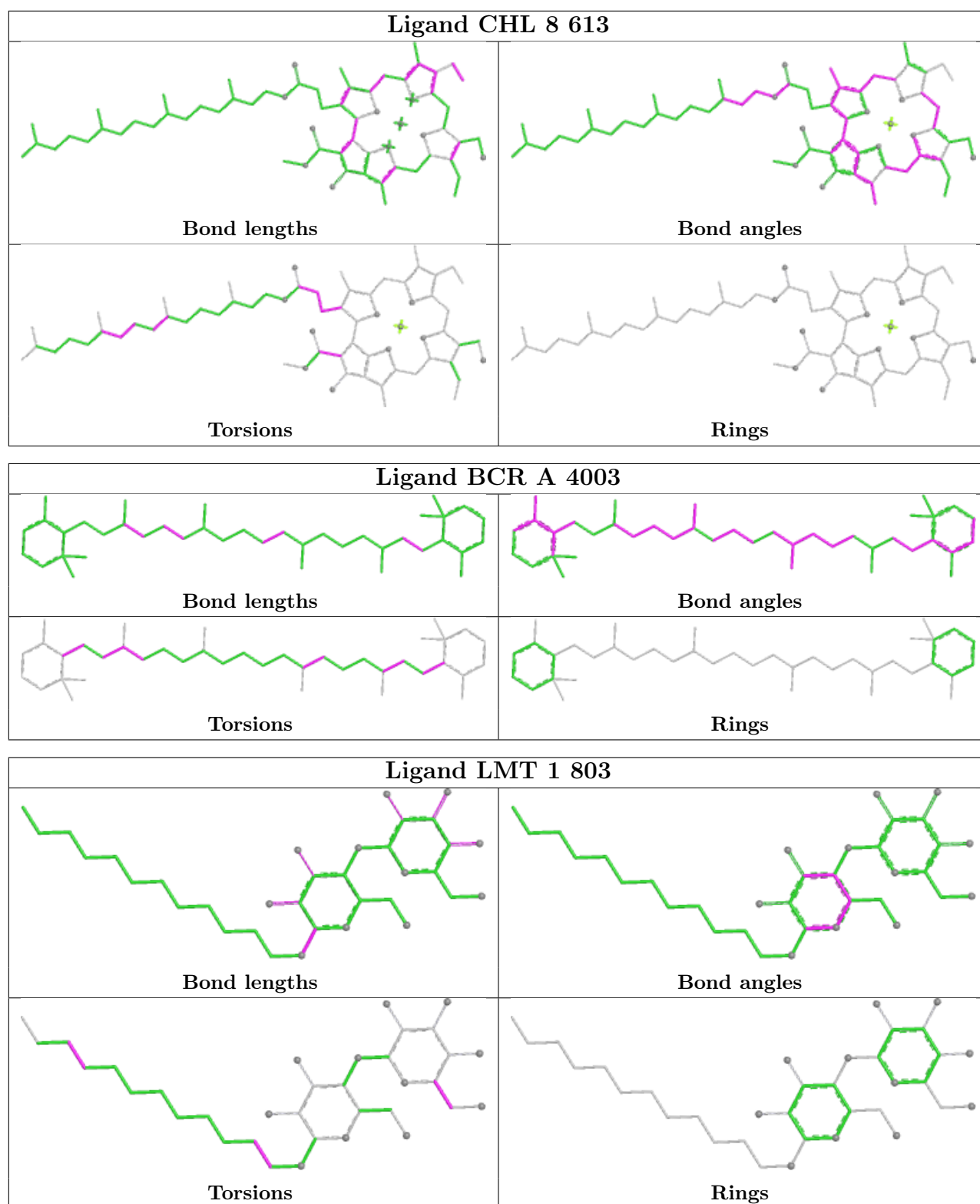


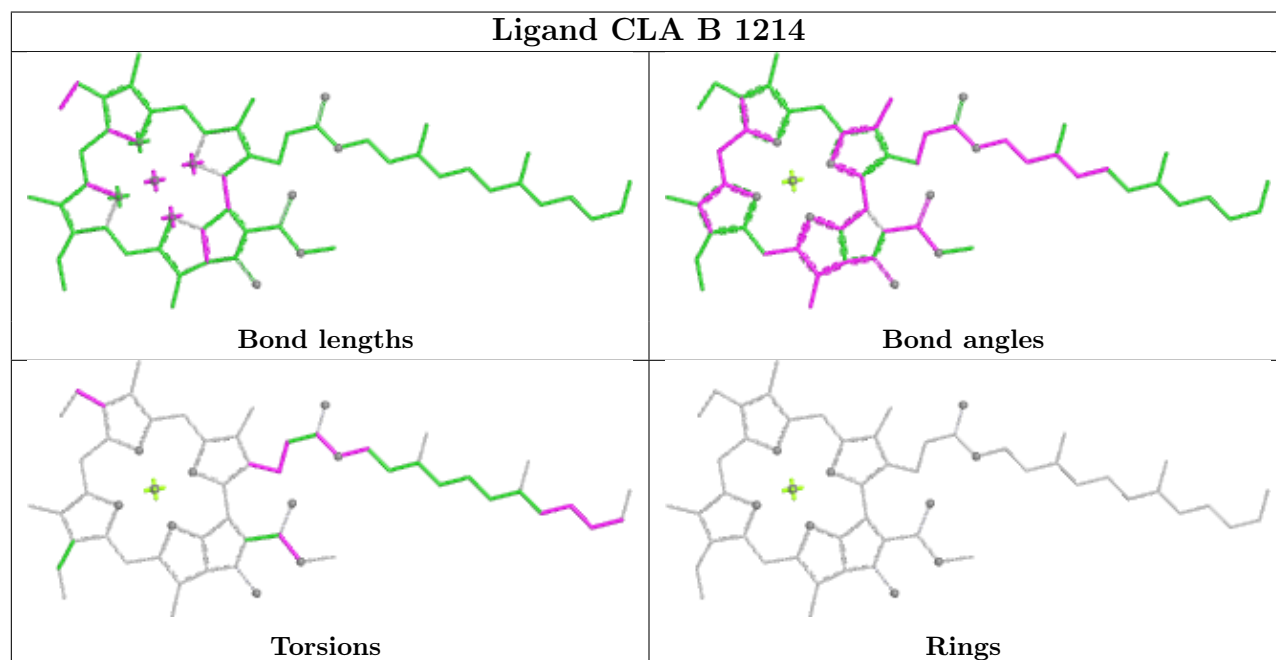
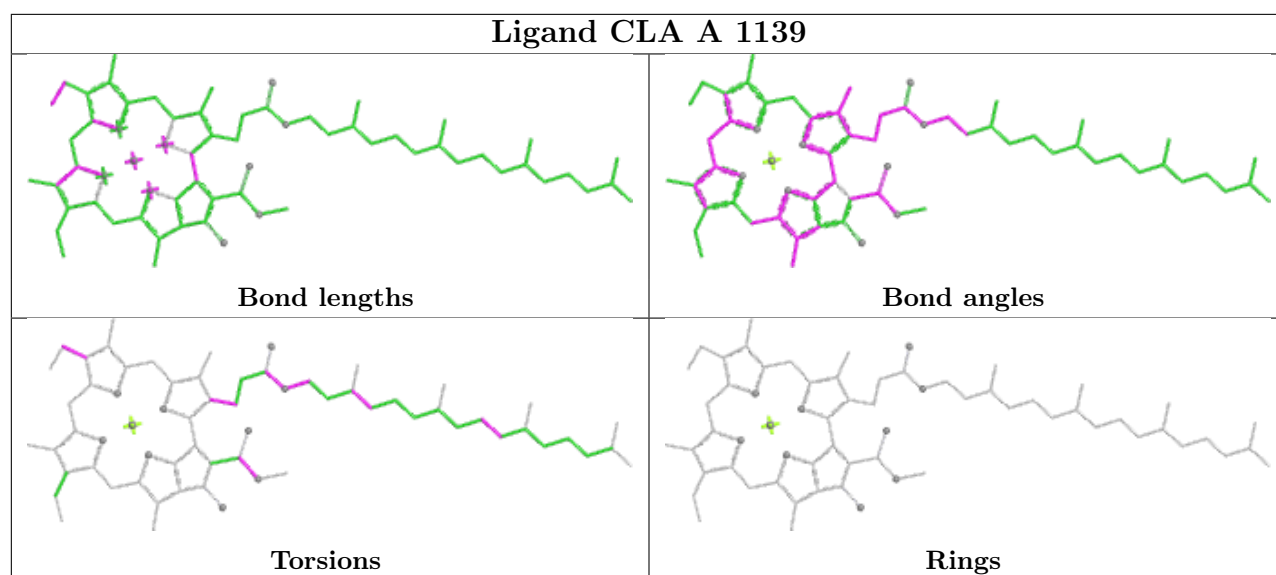
## Ligand CHL 1 610

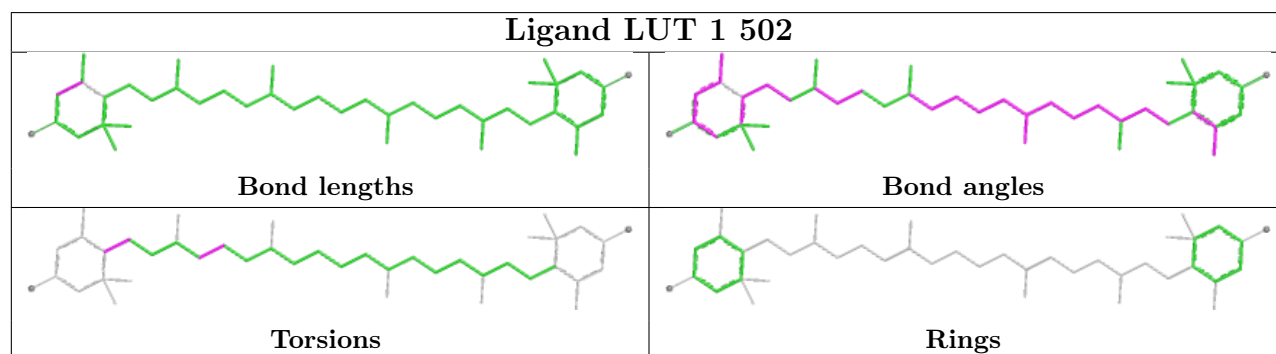
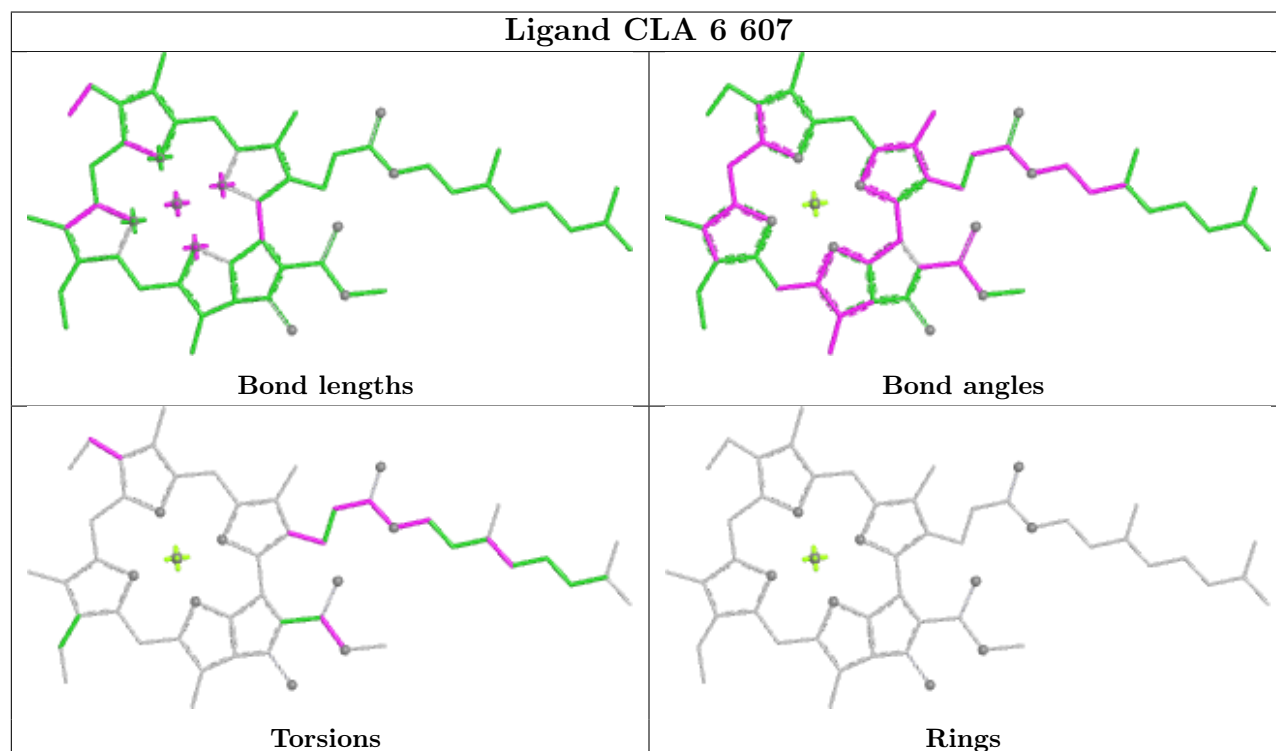
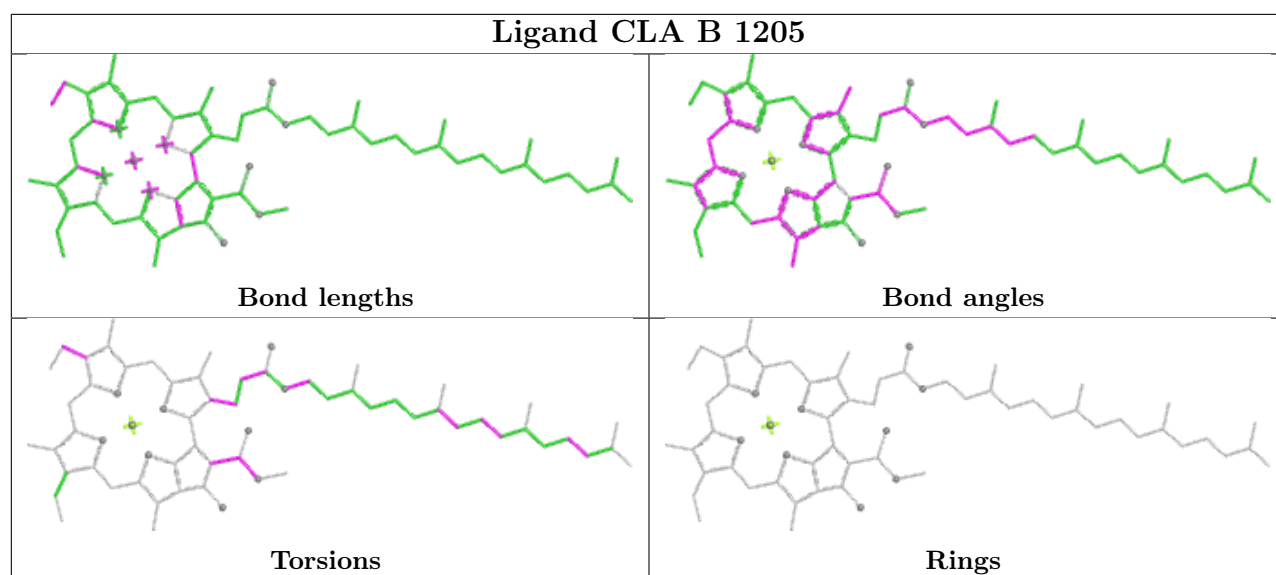


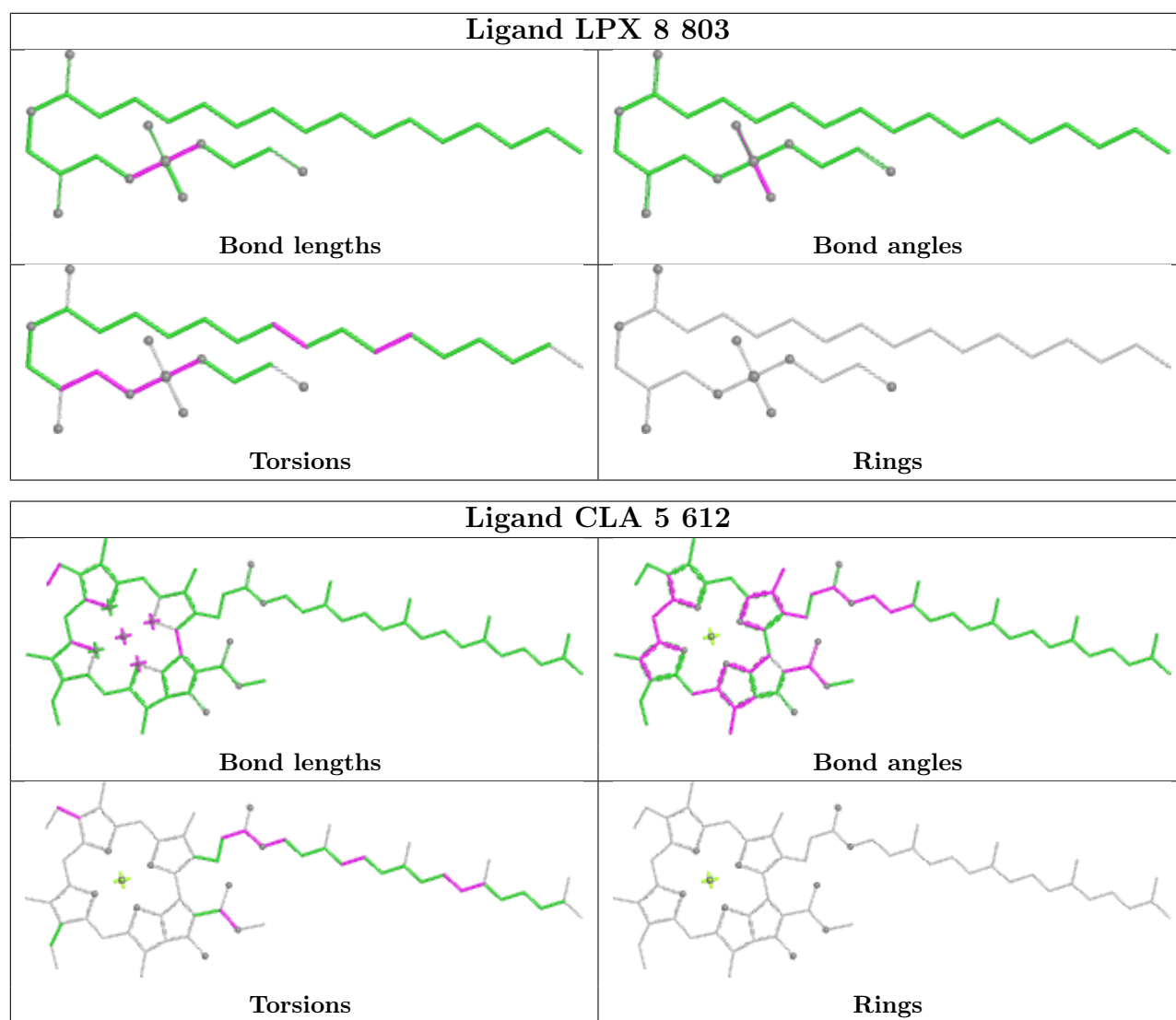
## Ligand CLA 3 606



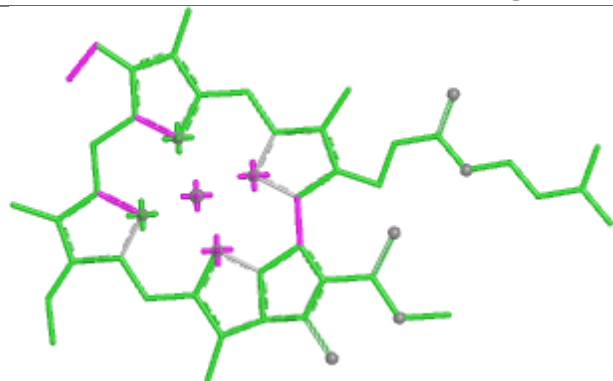




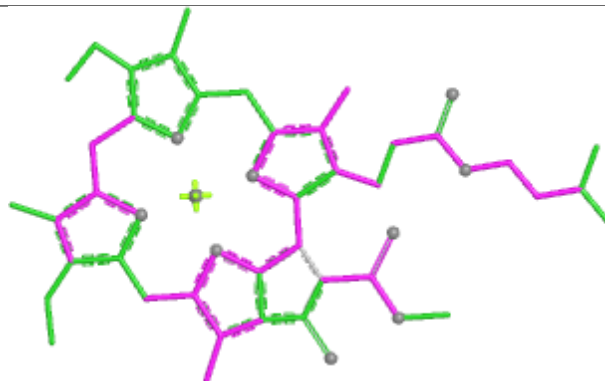




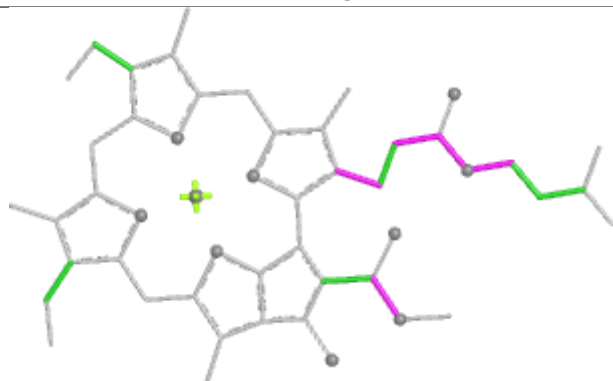
## Ligand CLA L 1503



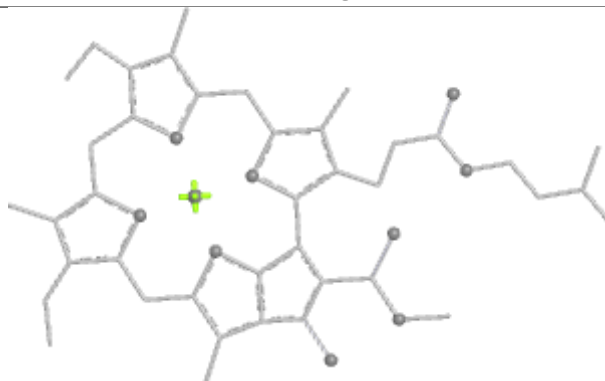
Bond lengths



Bond angles

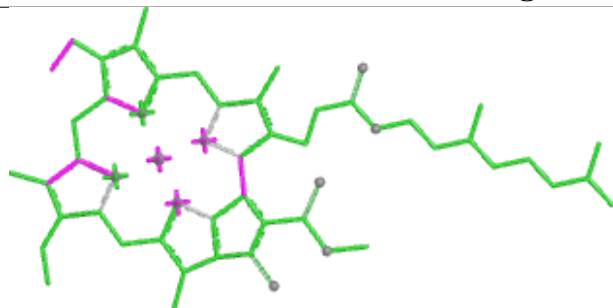


Torsions

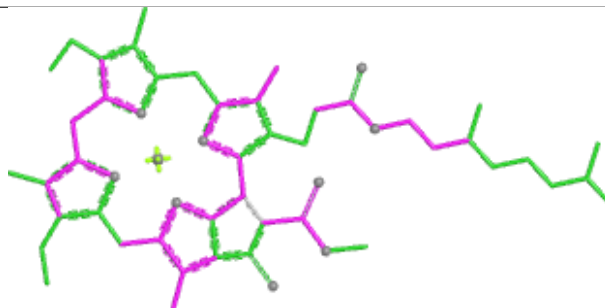


Rings

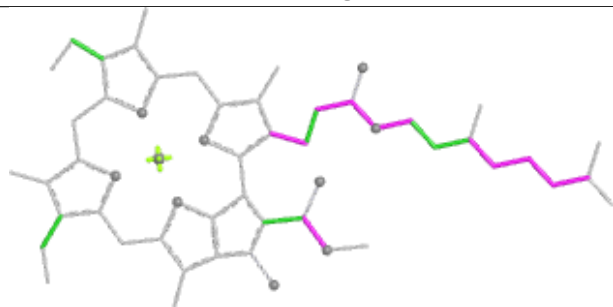
## Ligand CLA 6 605



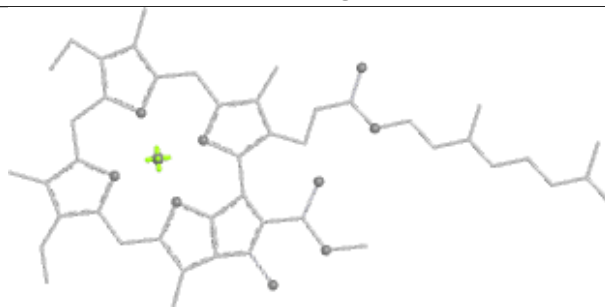
Bond lengths



Bond angles

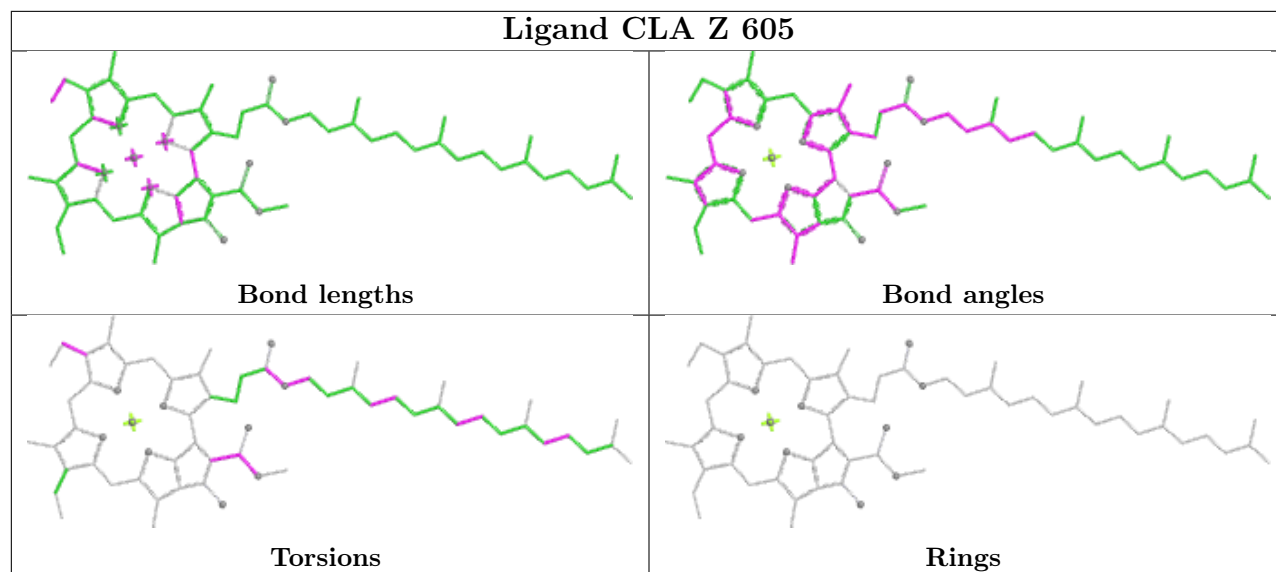


Torsions

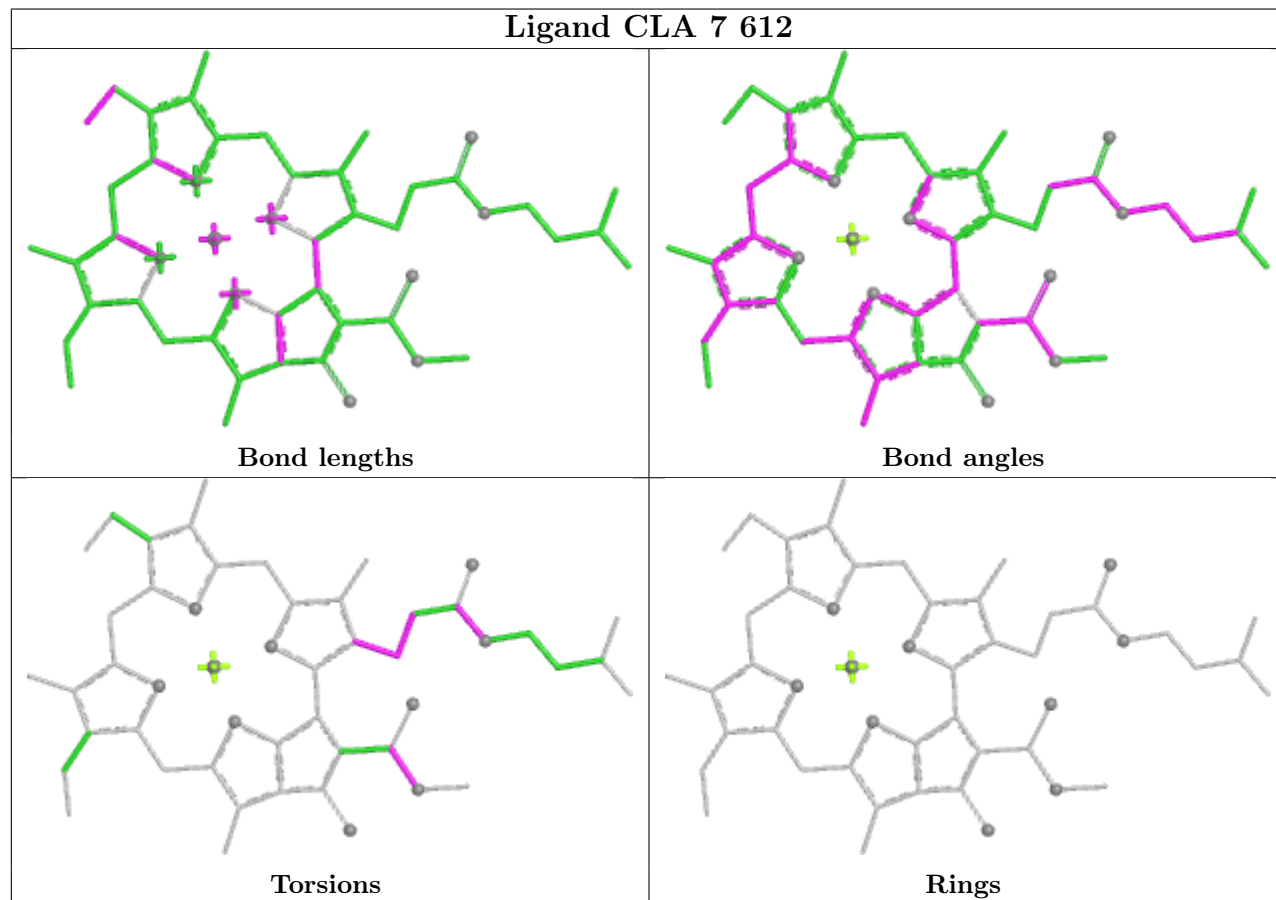


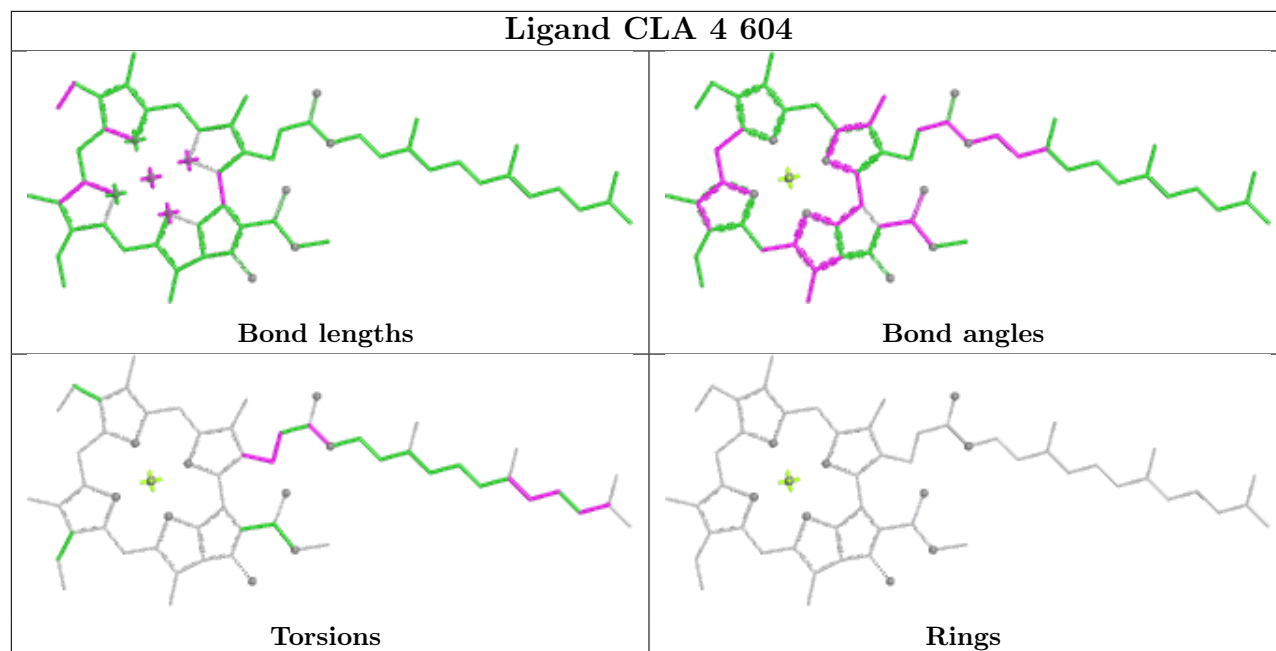
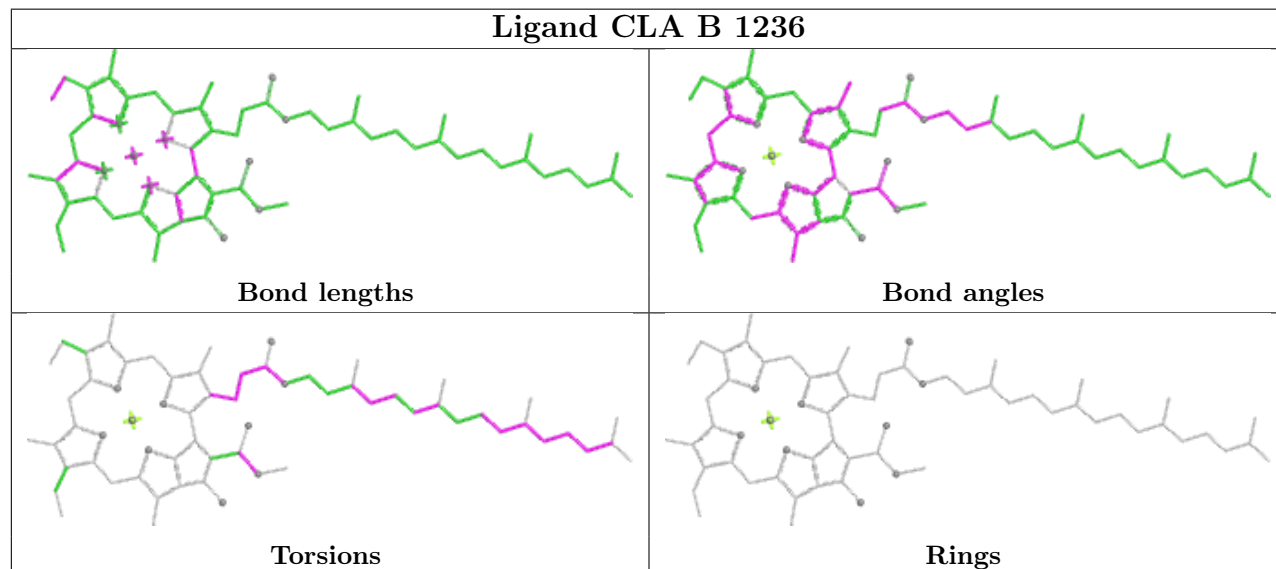
Rings

## Ligand CLA Z 605

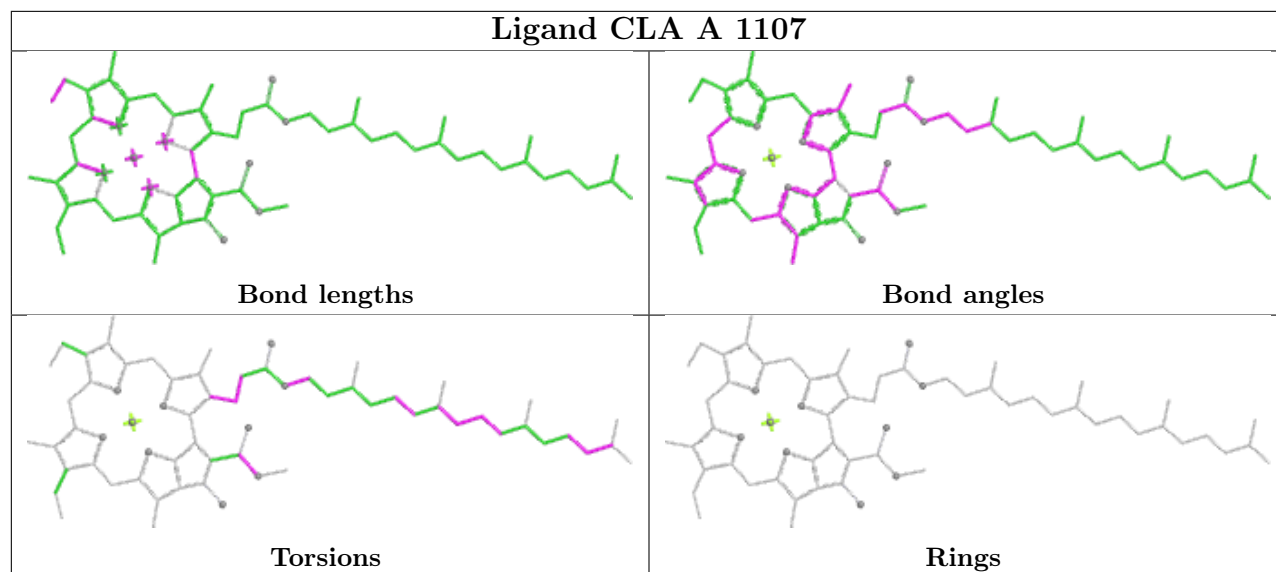


## Ligand CLA 7 612

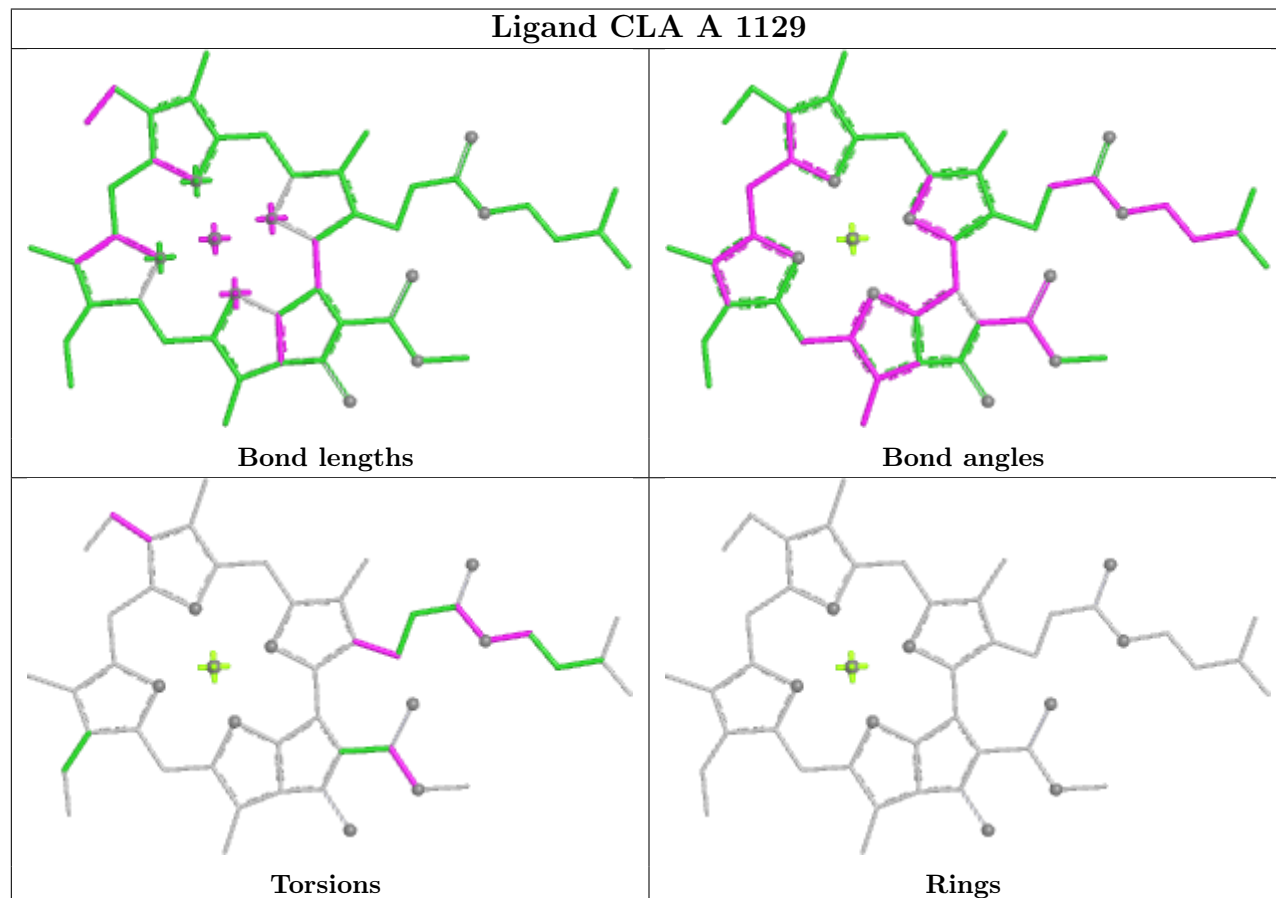


**Ligand CLA 4 604****Ligand CLA B 1236**

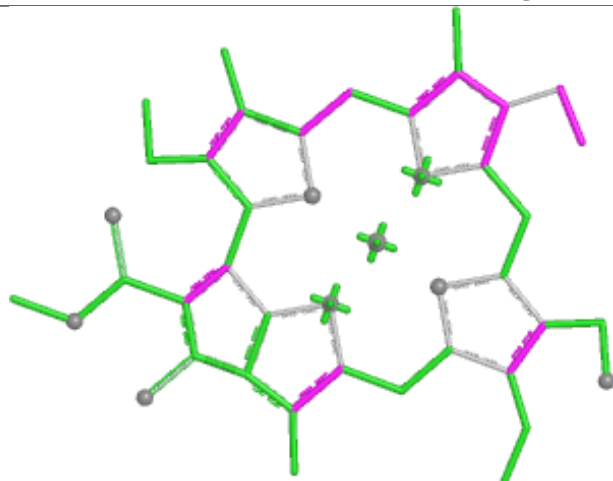
## Ligand CLA A 1107



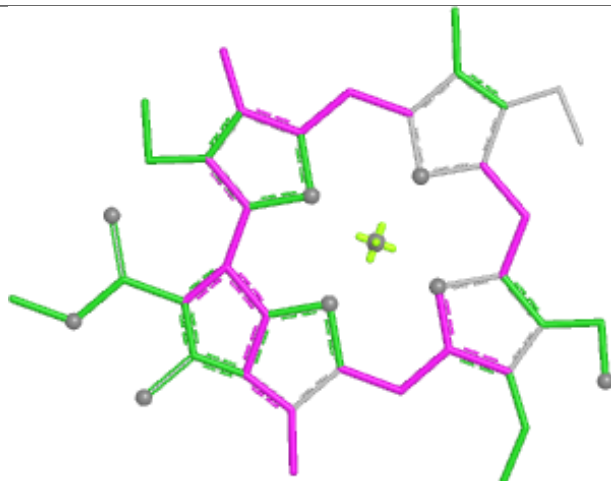
## Ligand CLA A 1129



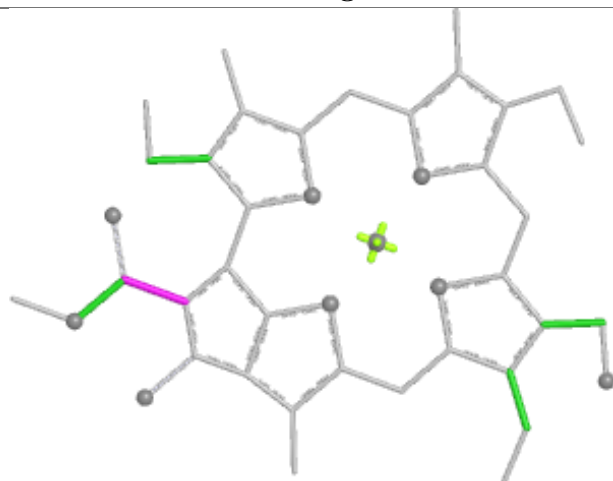
## Ligand CHL 5 617



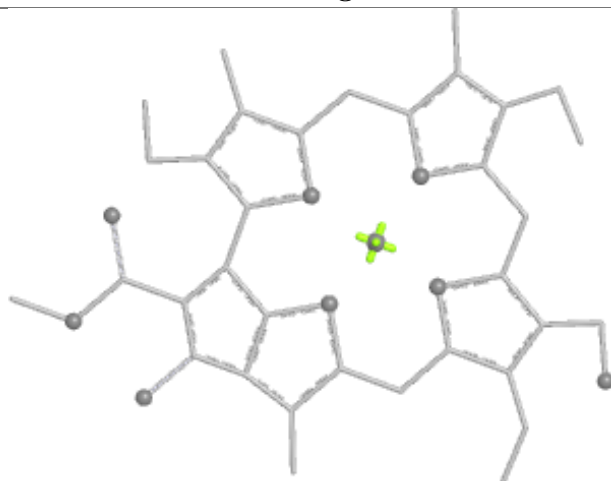
Bond lengths



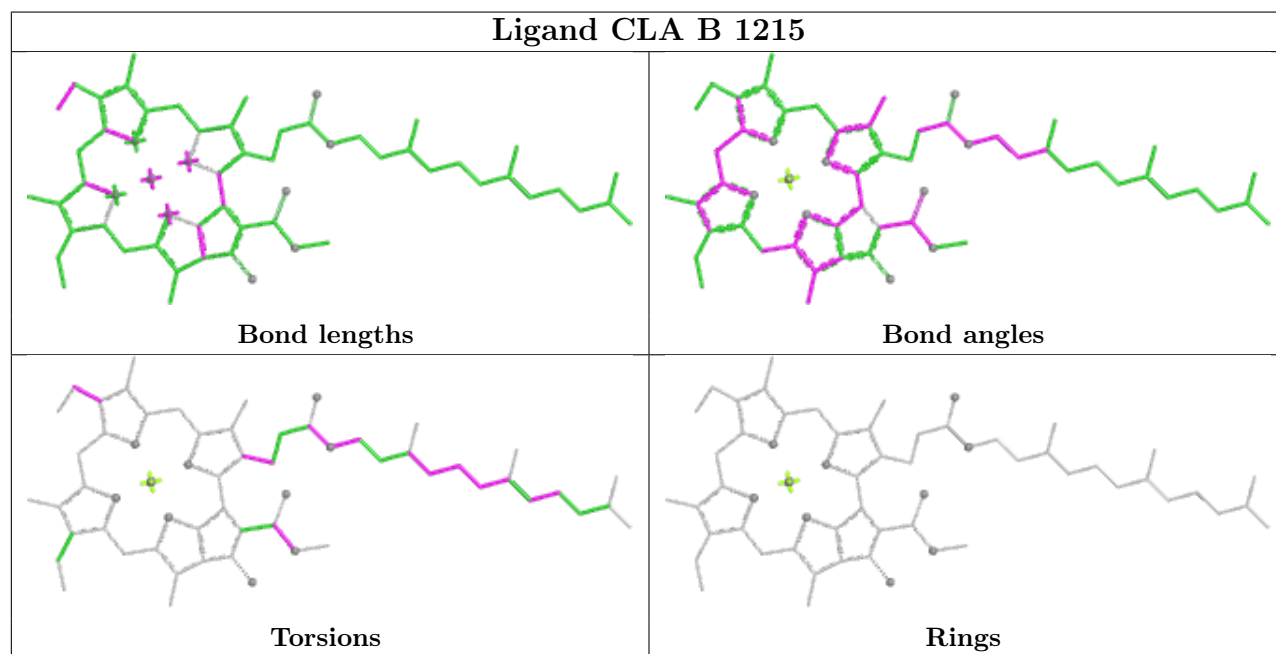
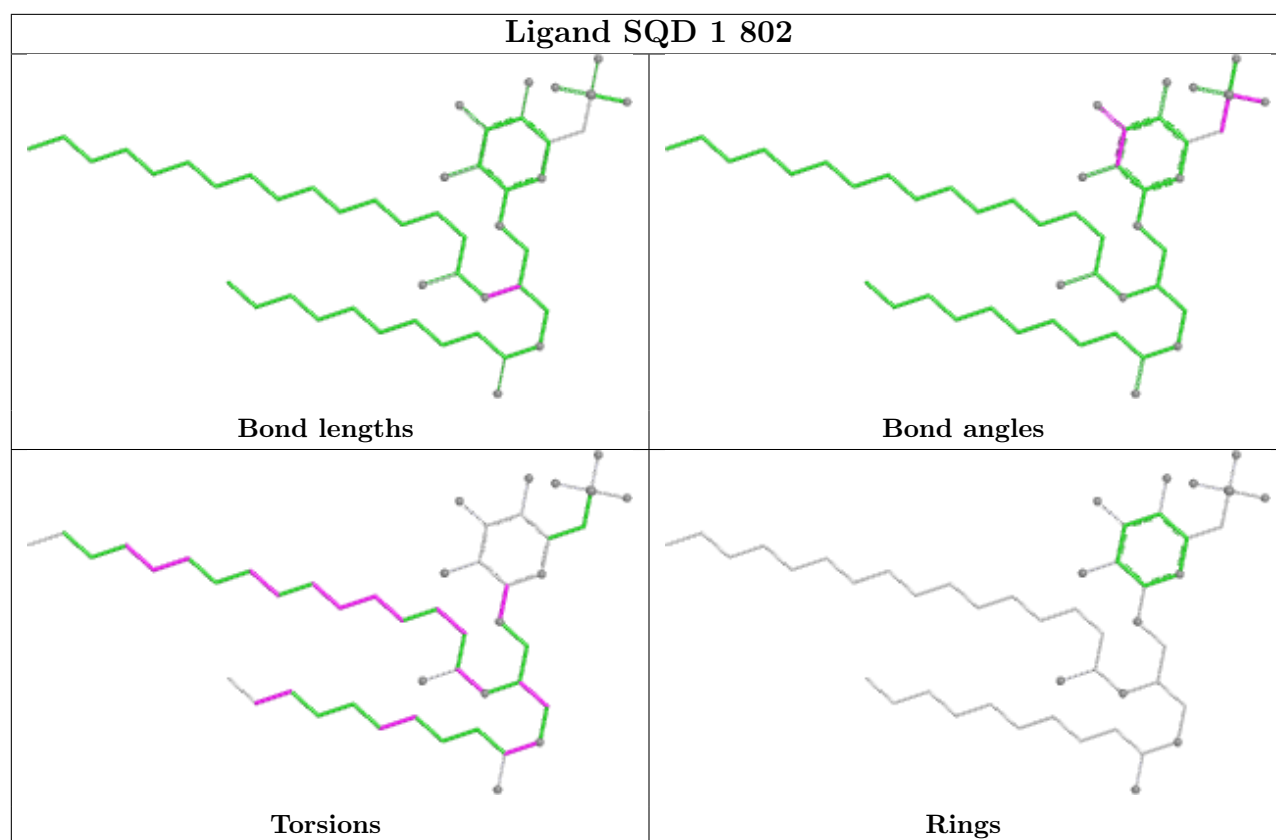
Bond angles

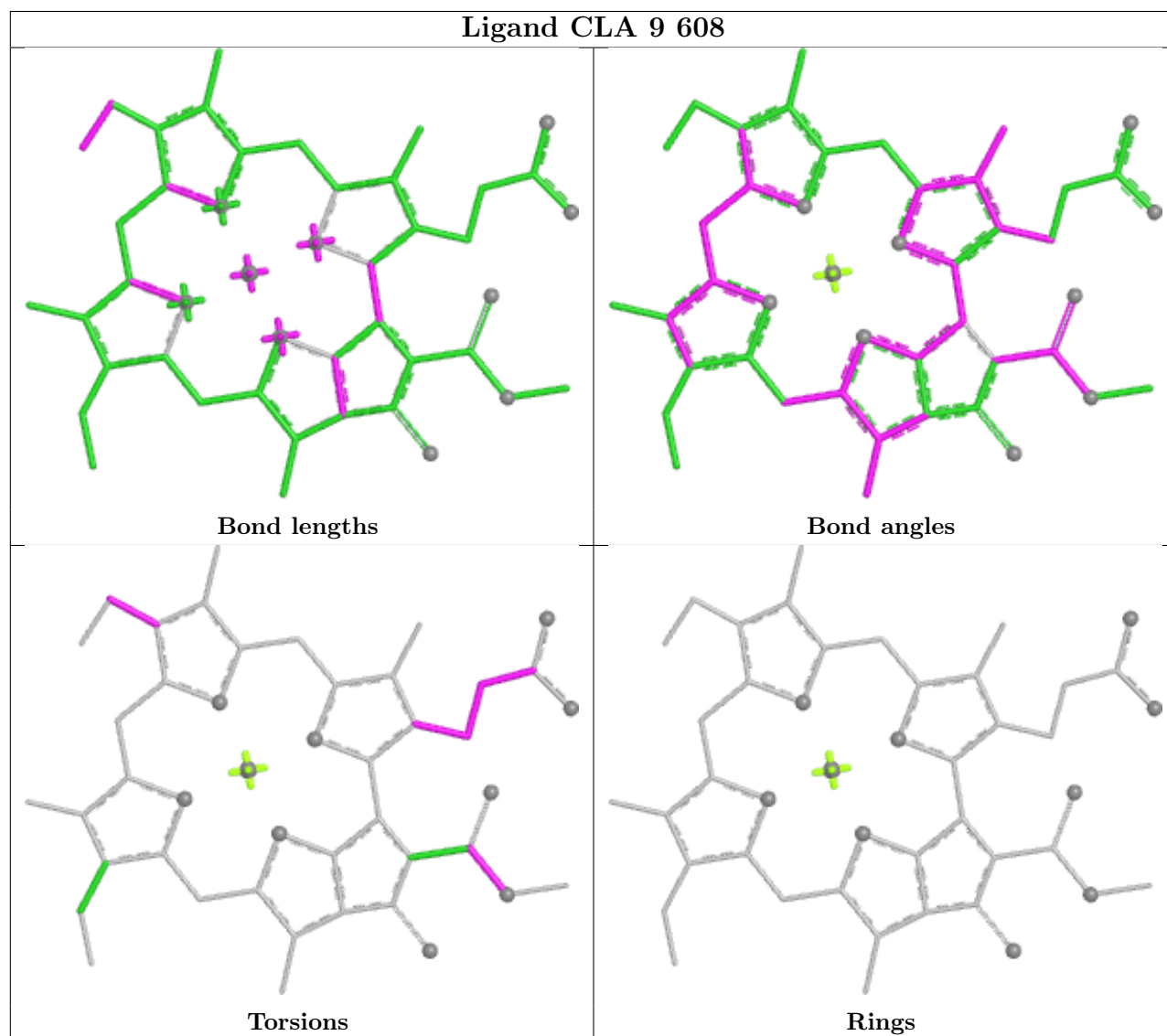
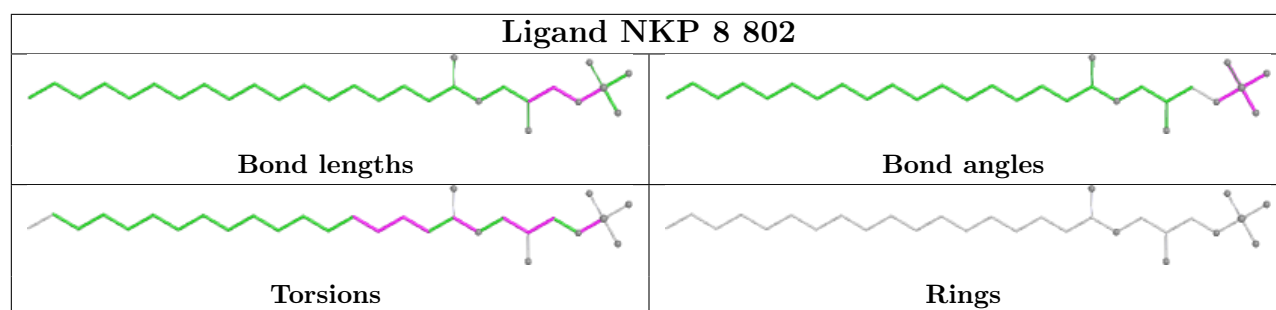


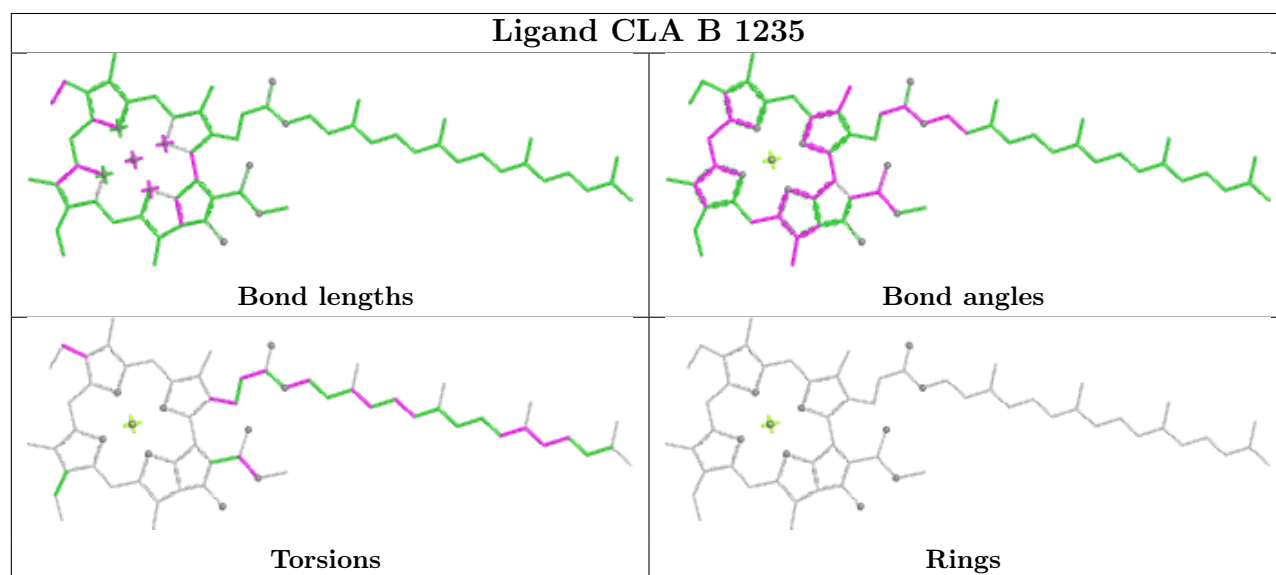
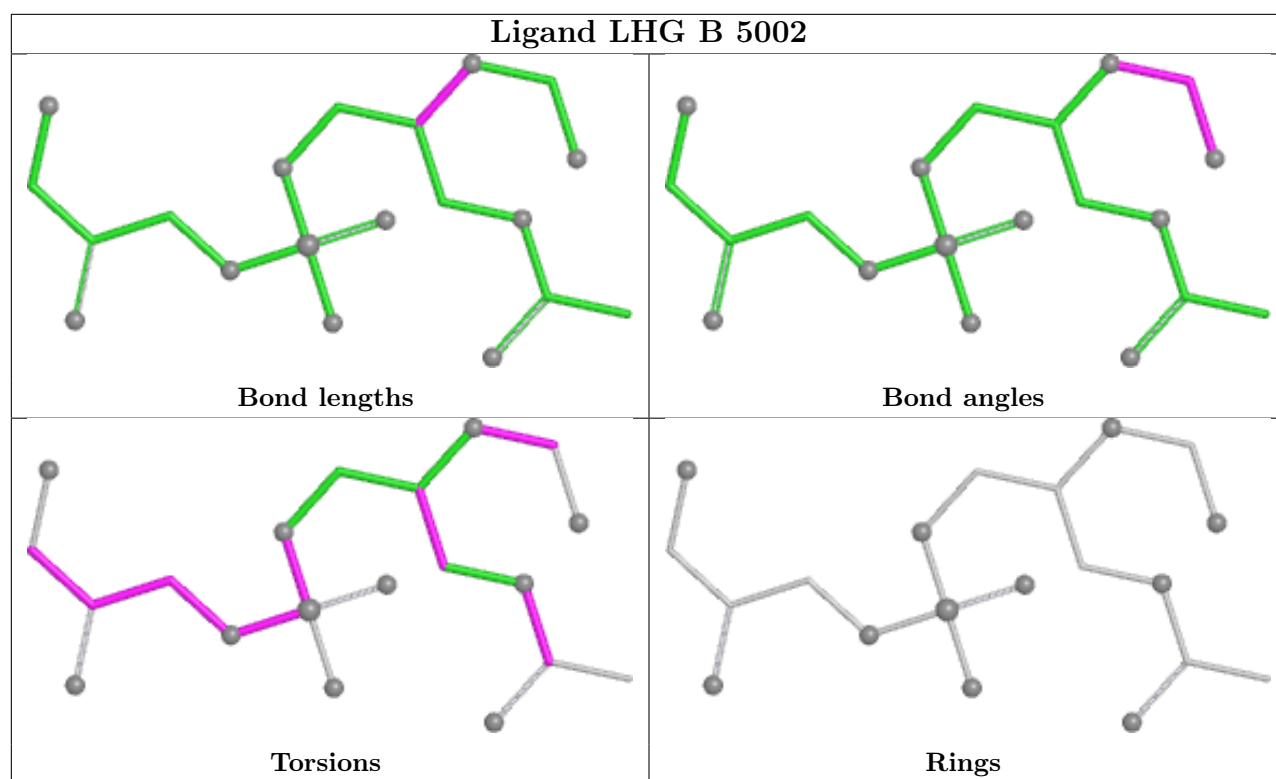
Torsions

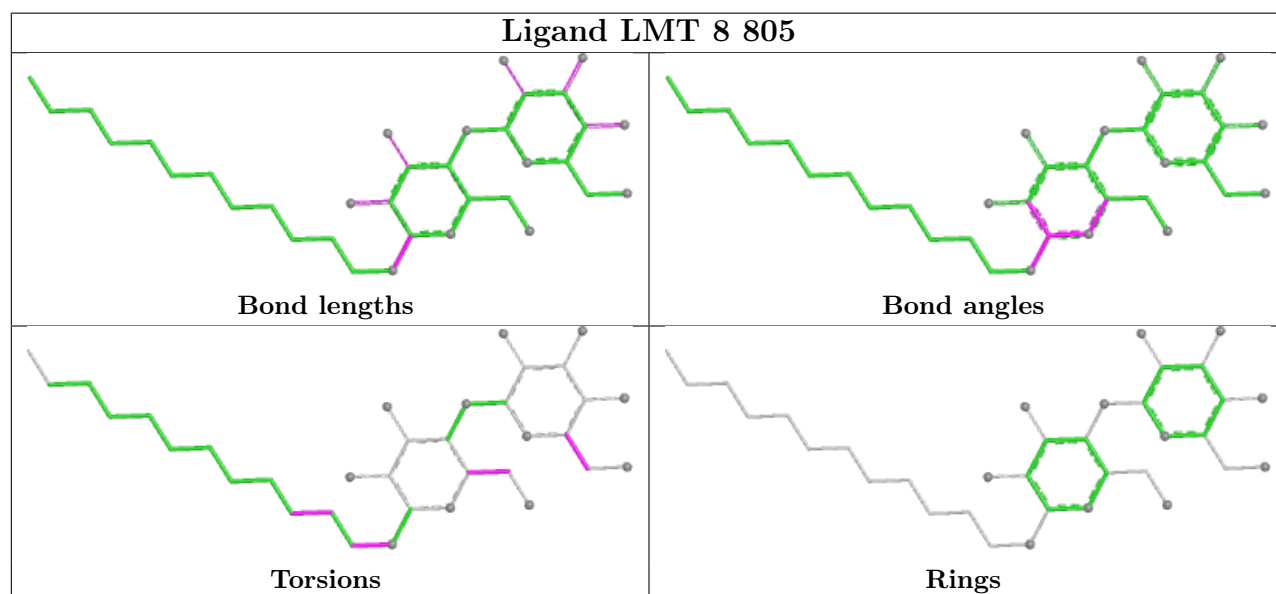
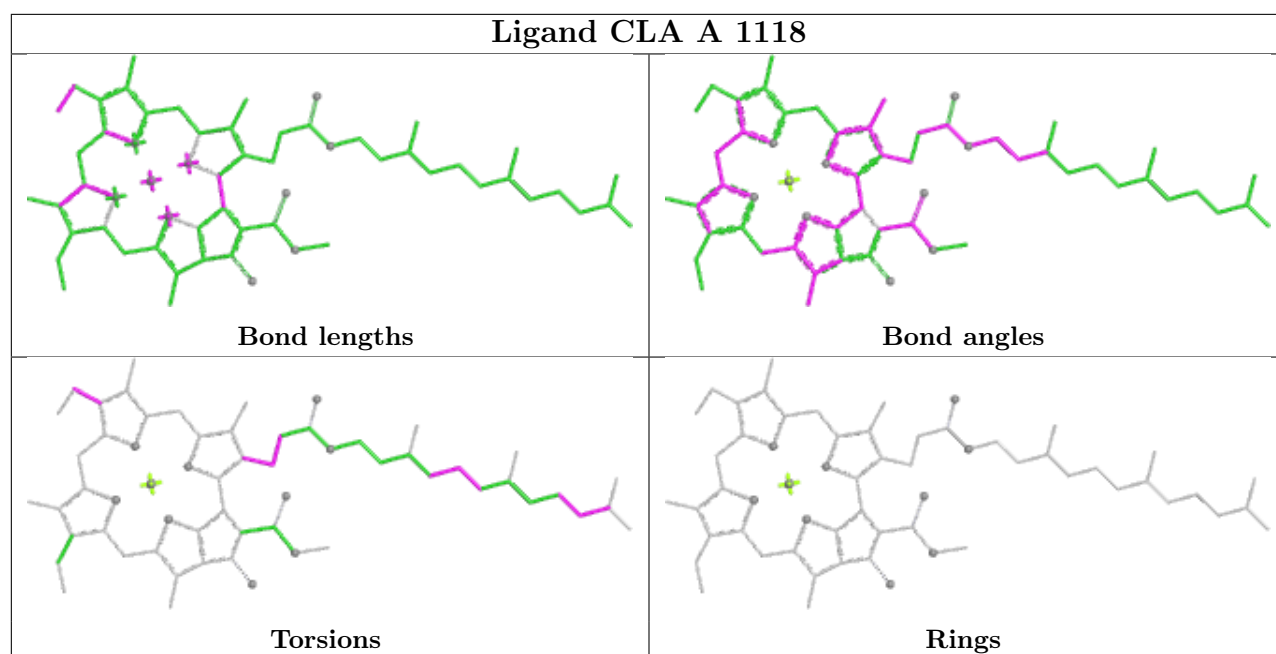


Rings

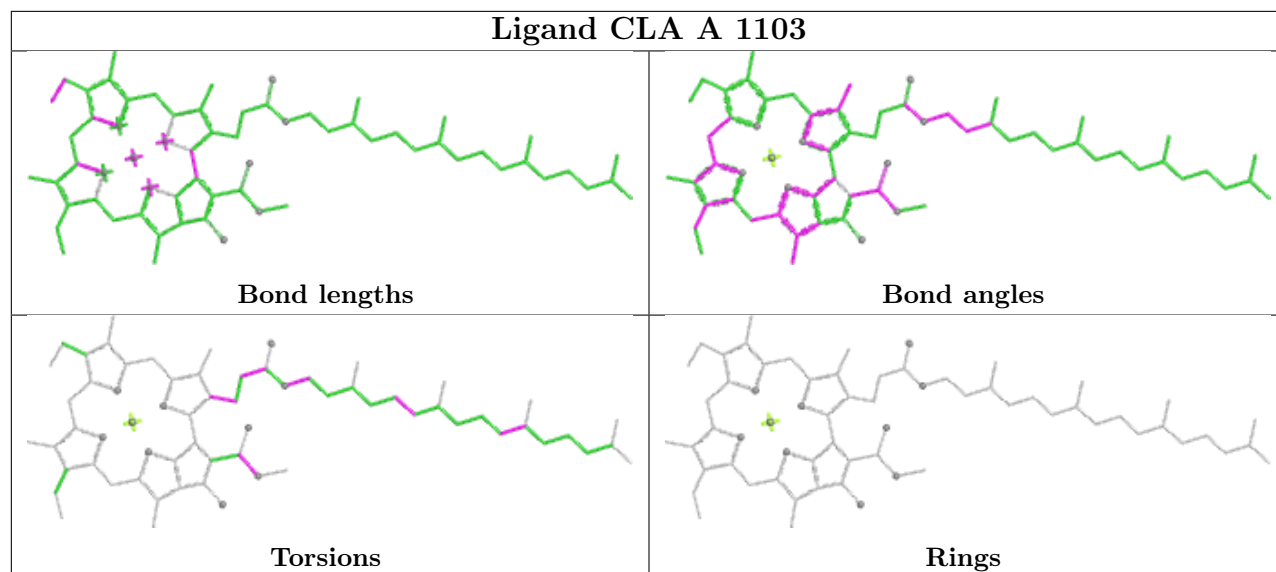




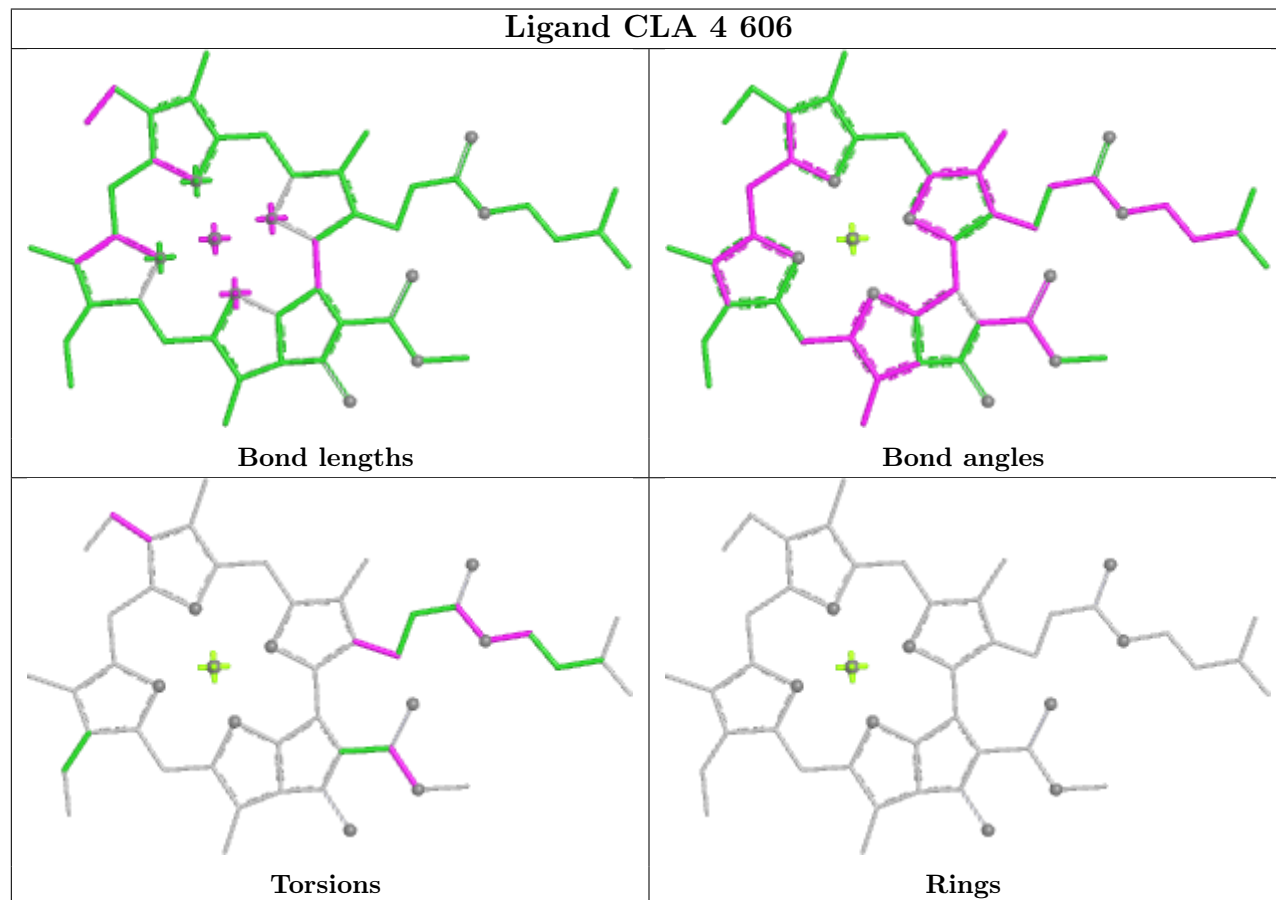


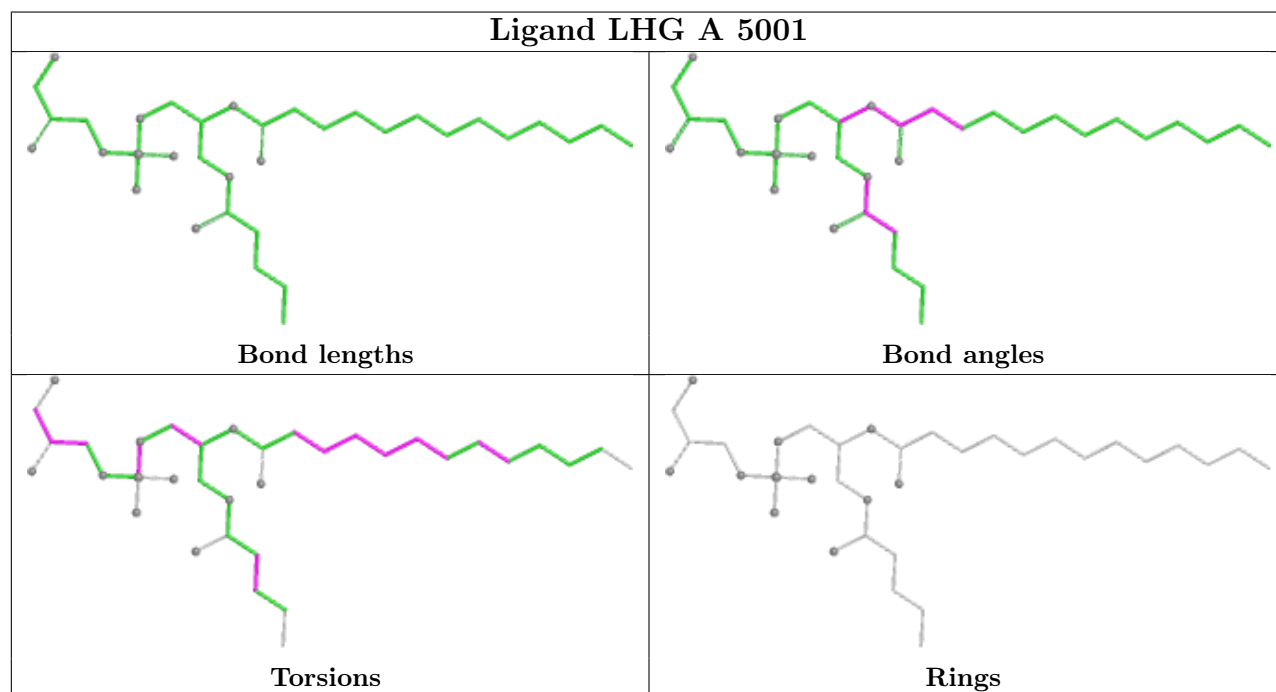
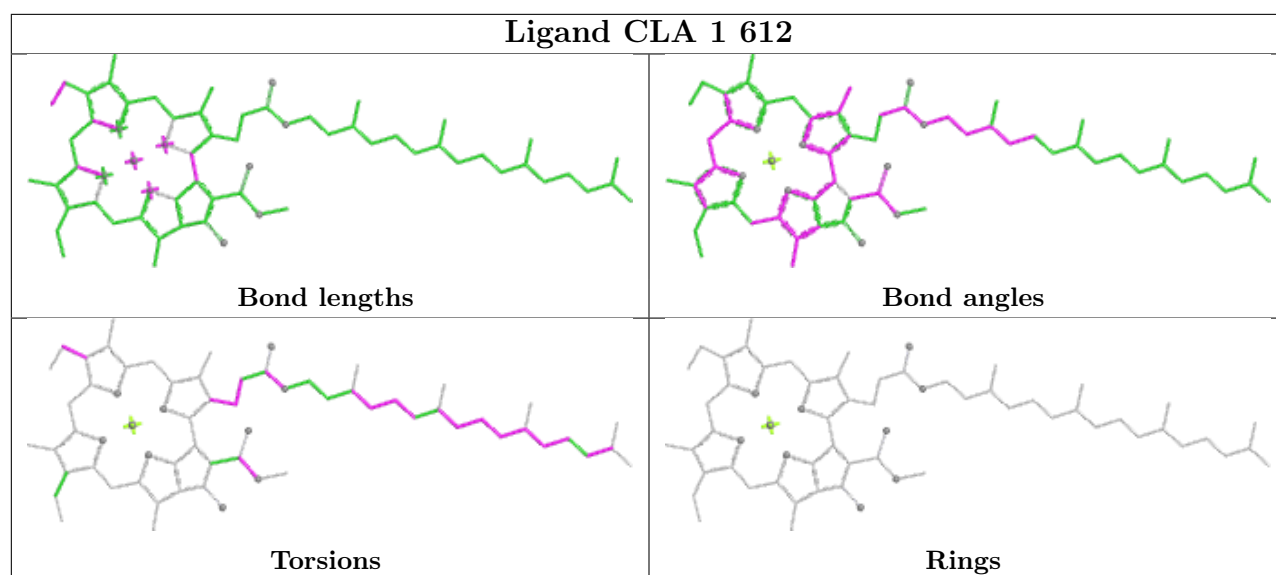


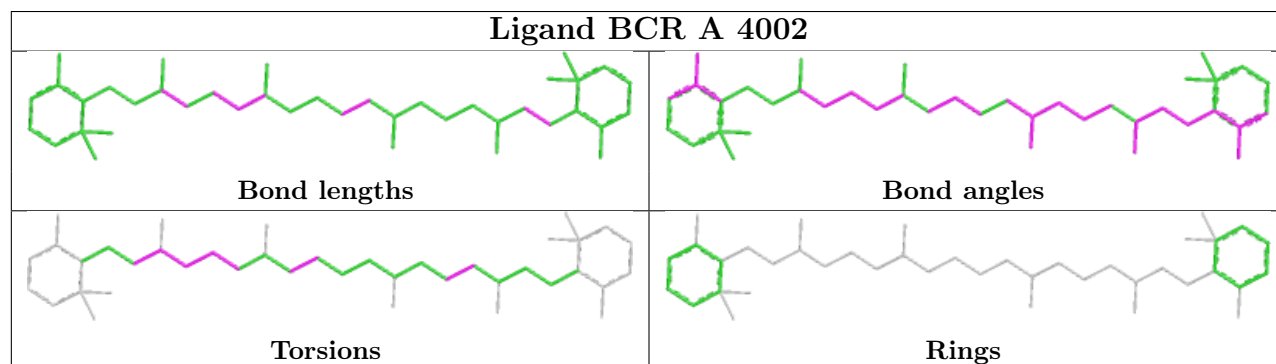
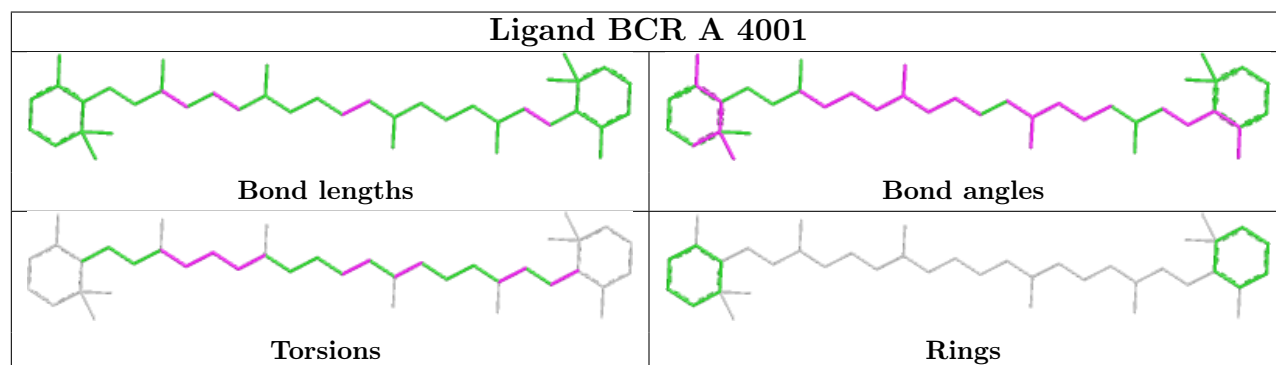
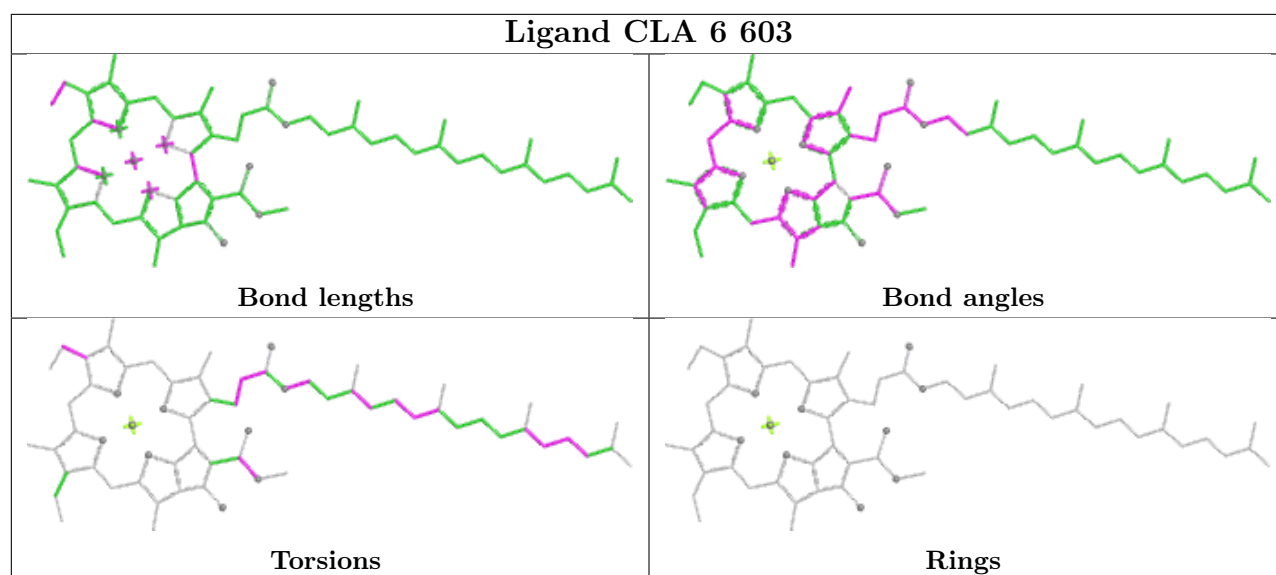
## Ligand CLA A 1103

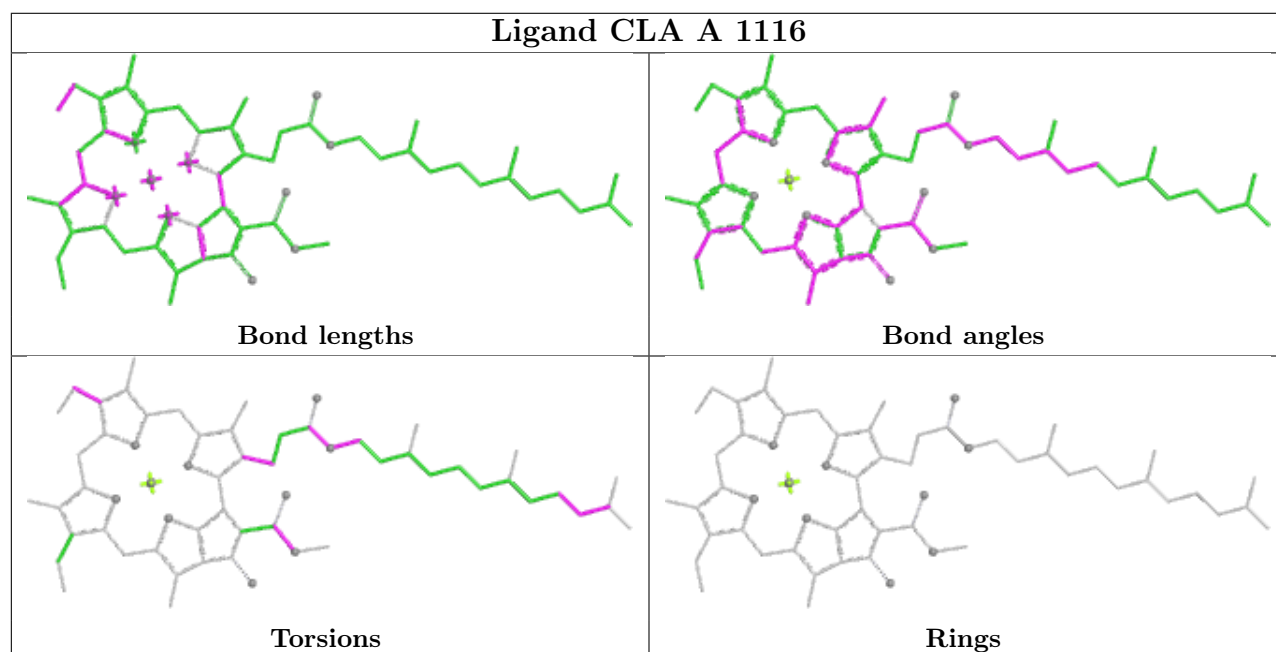
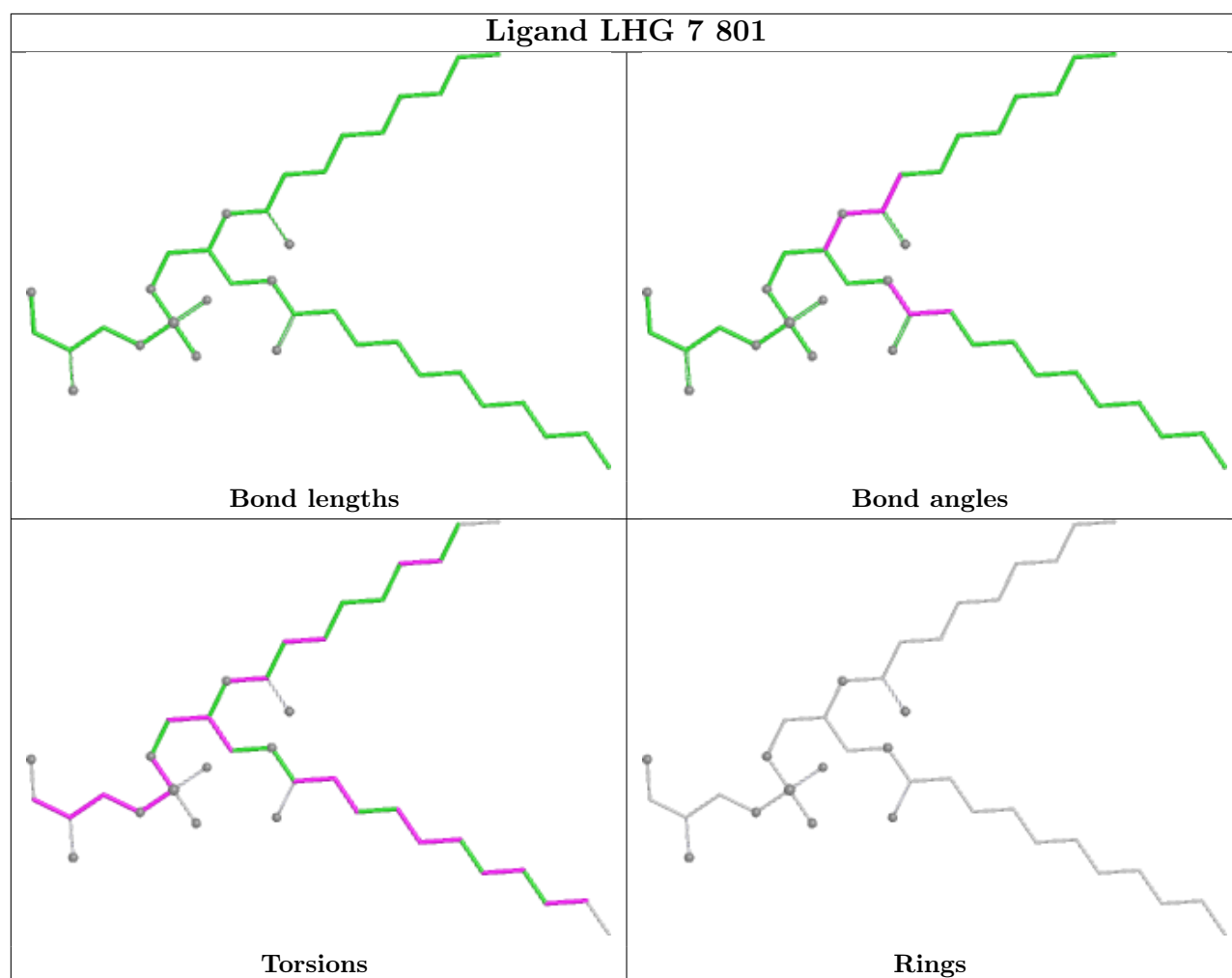


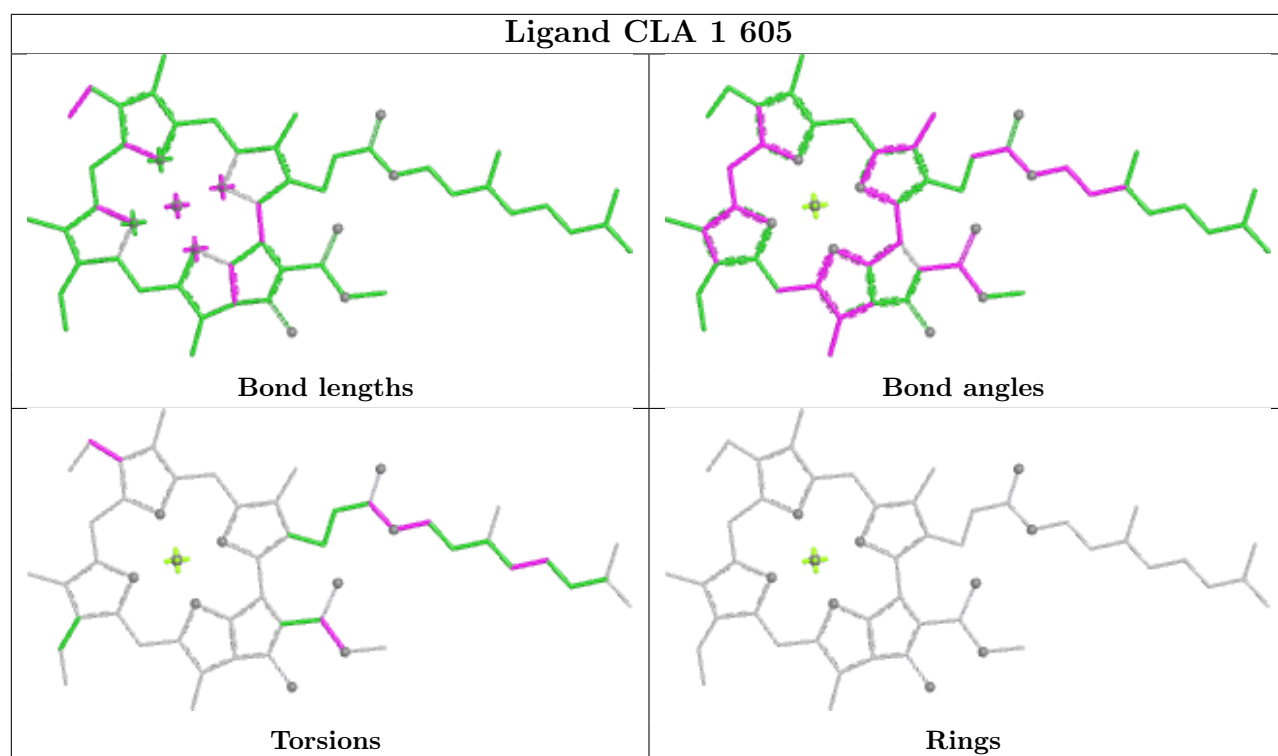
## Ligand CLA 4 606

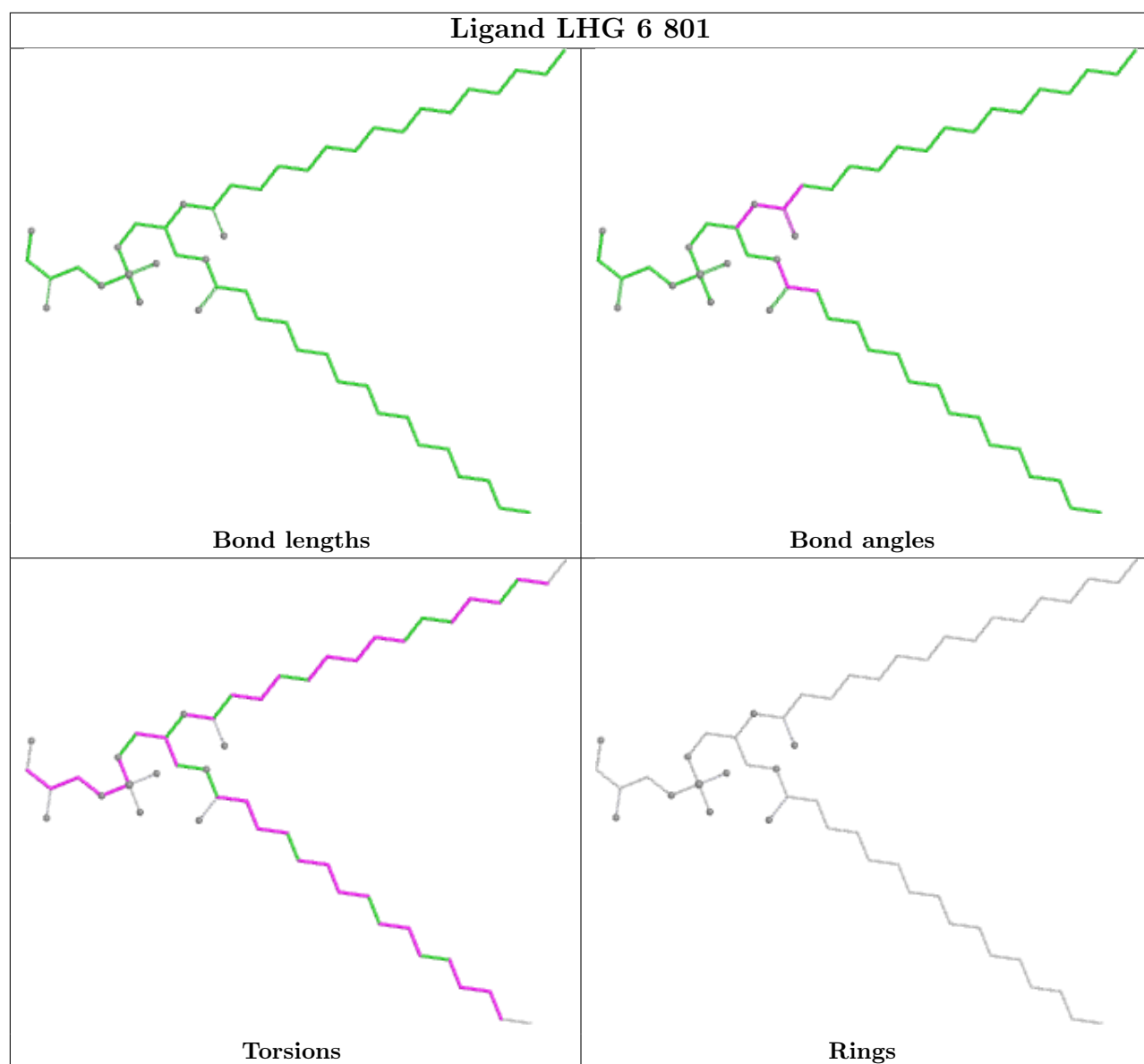


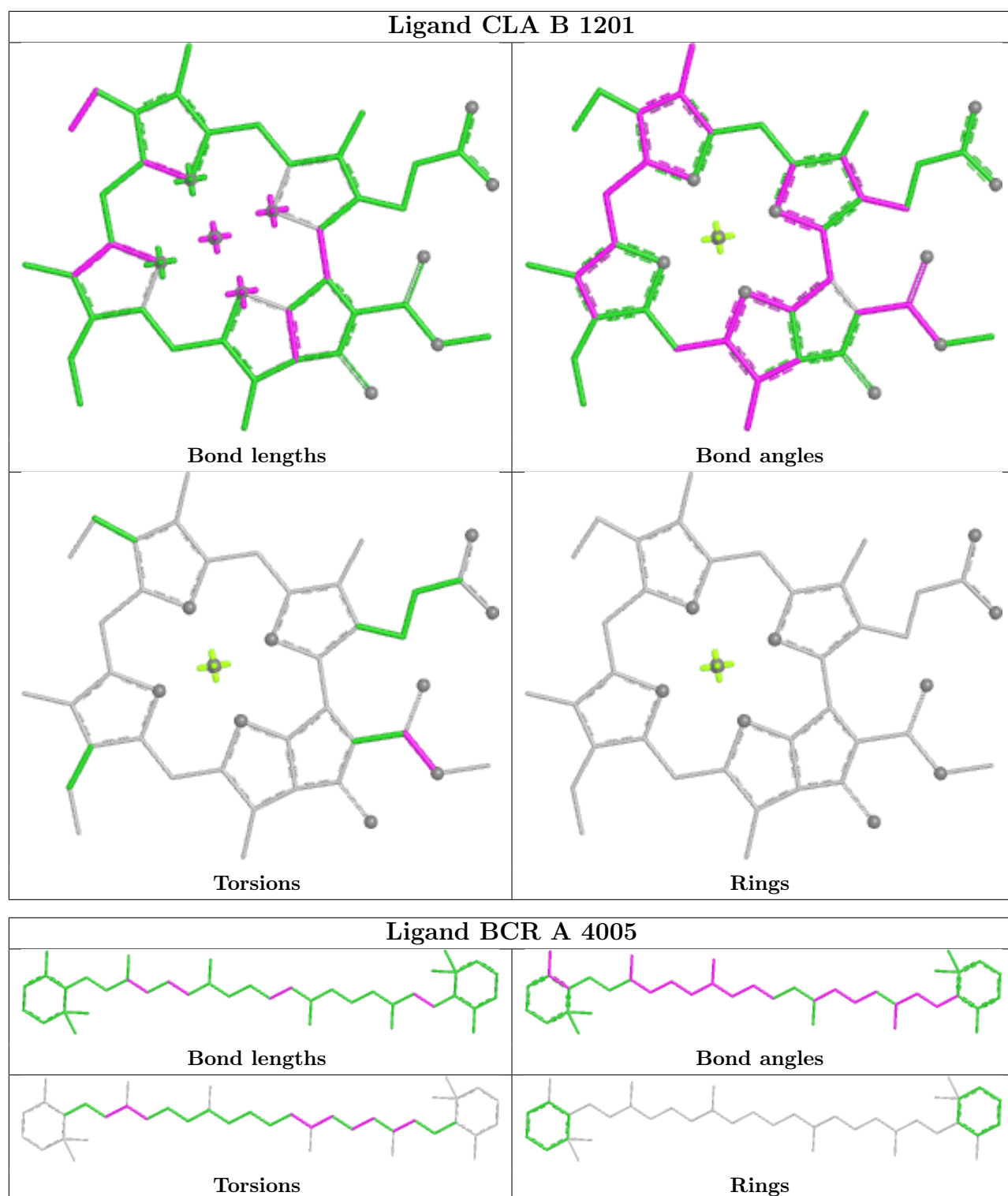


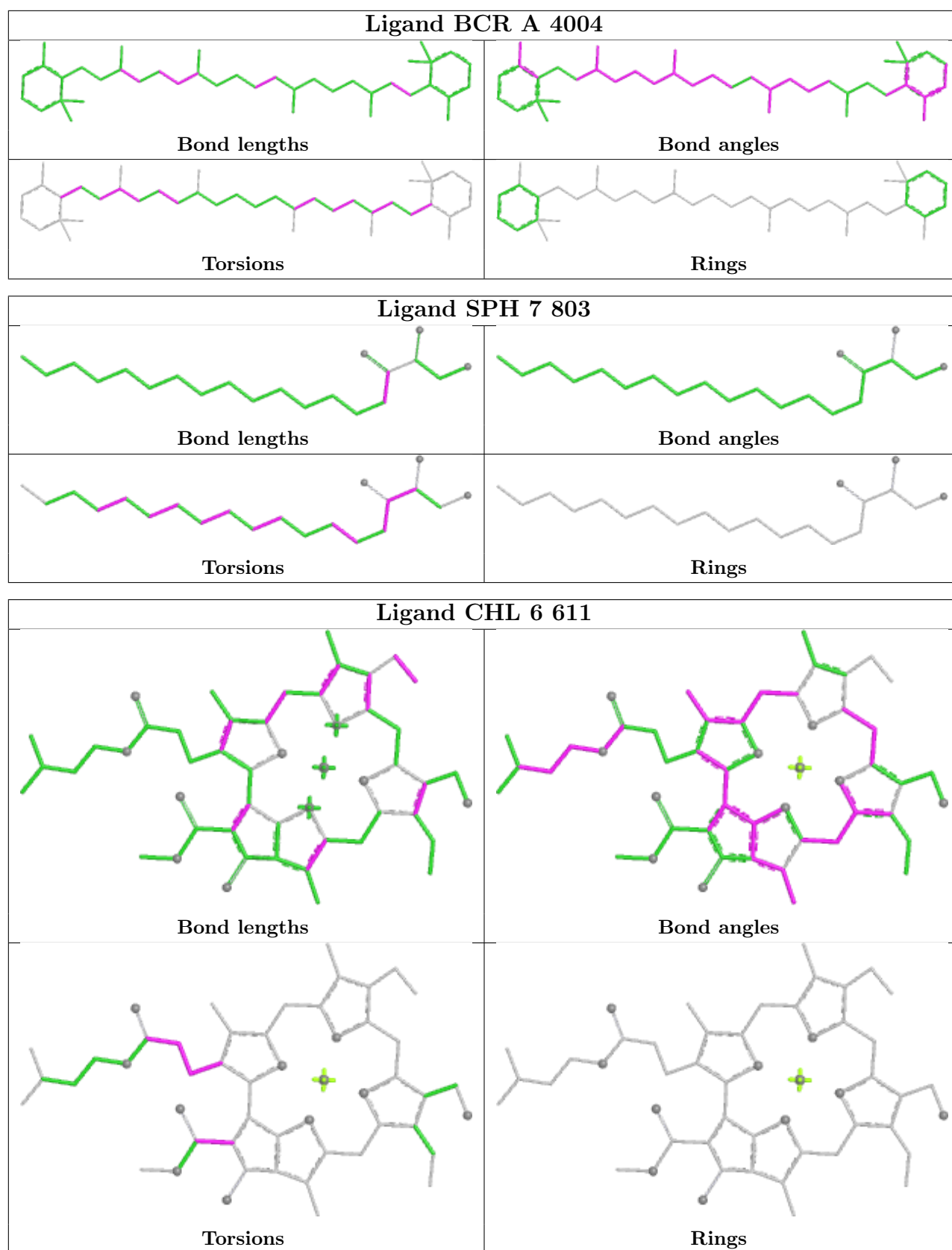


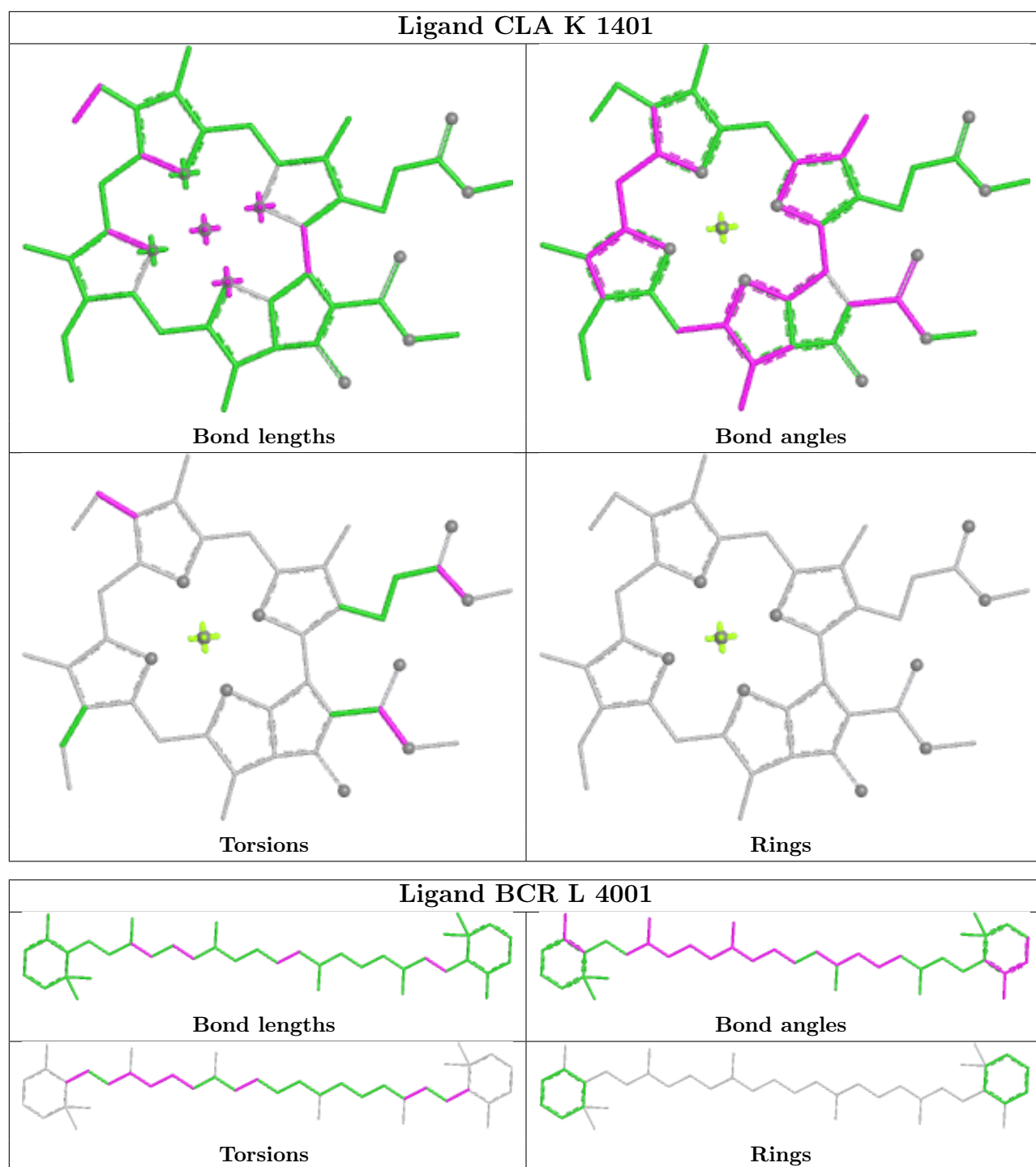


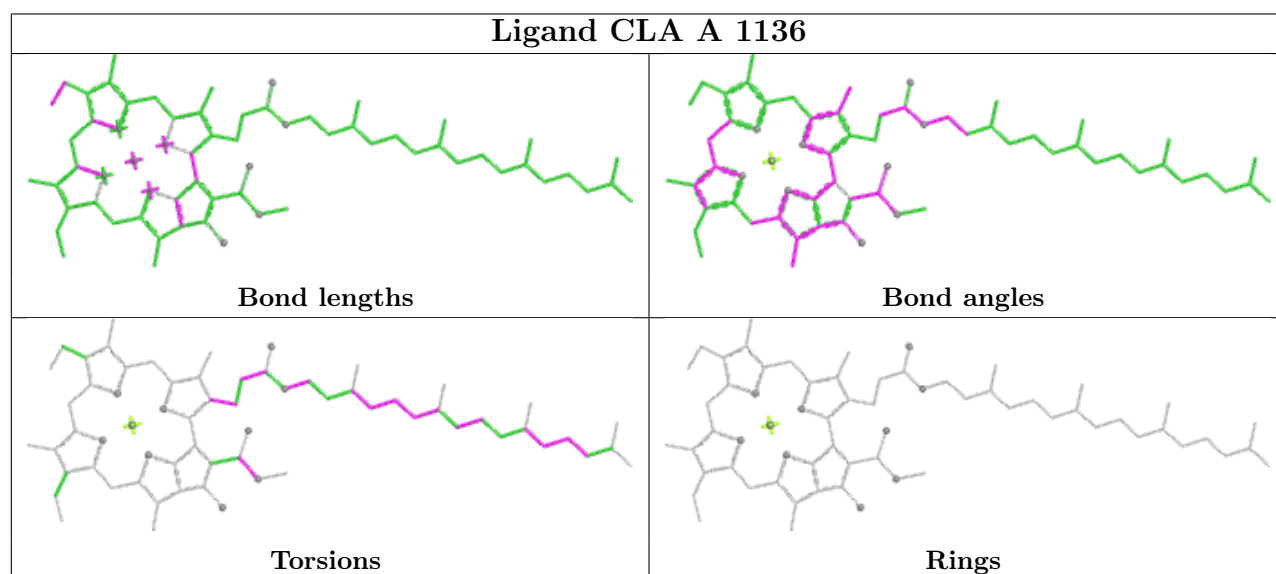
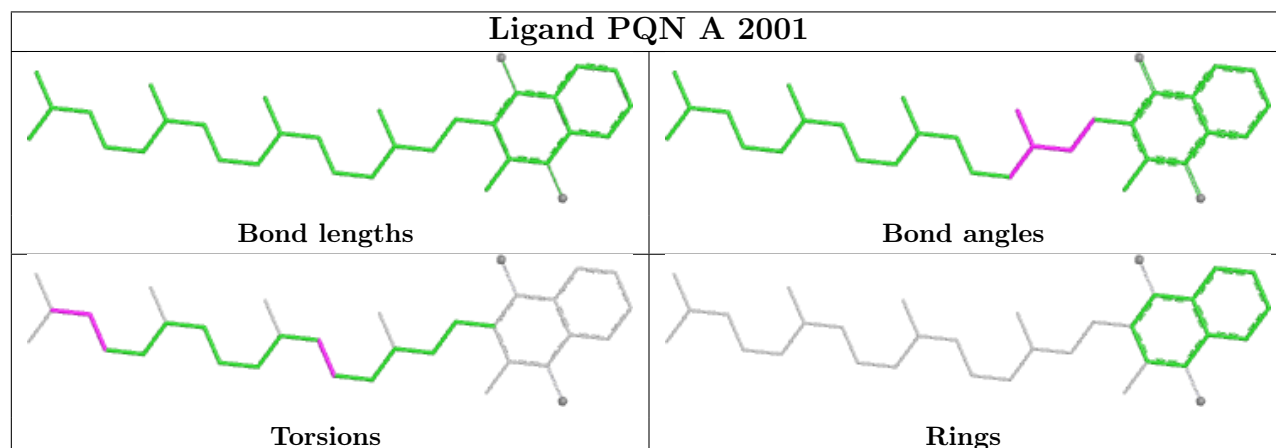
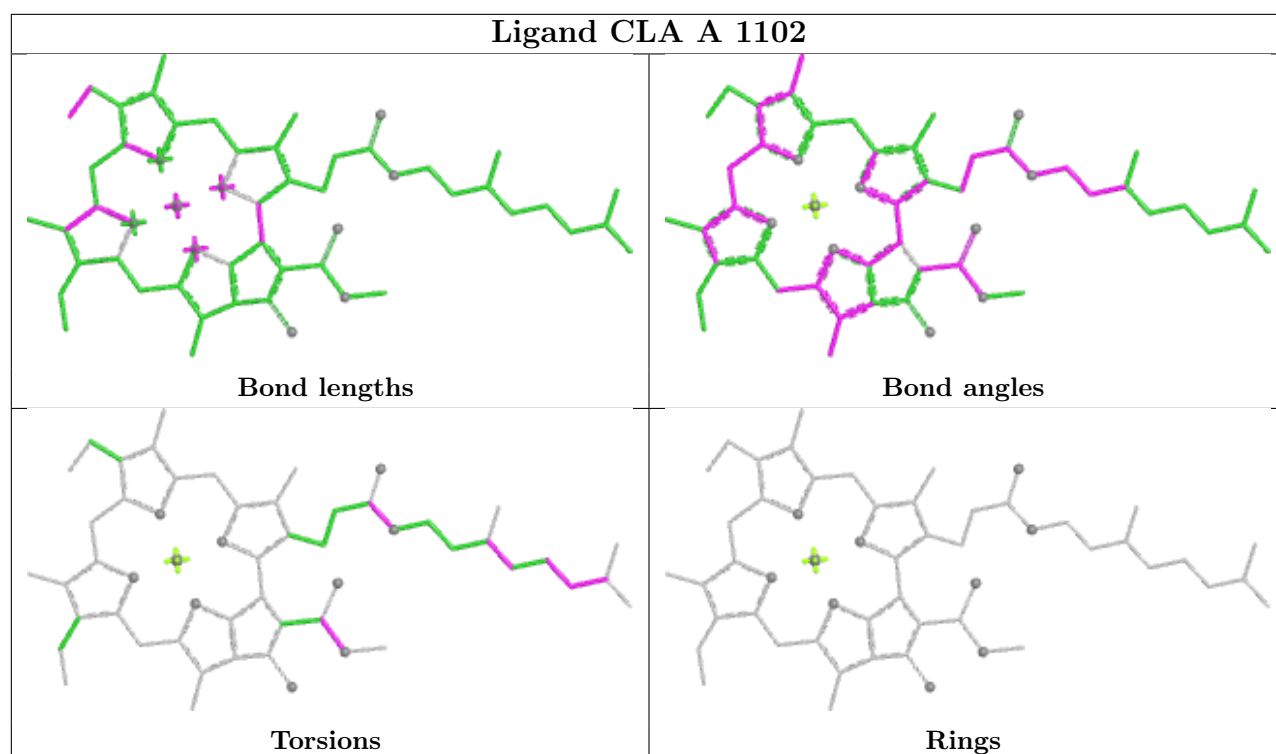


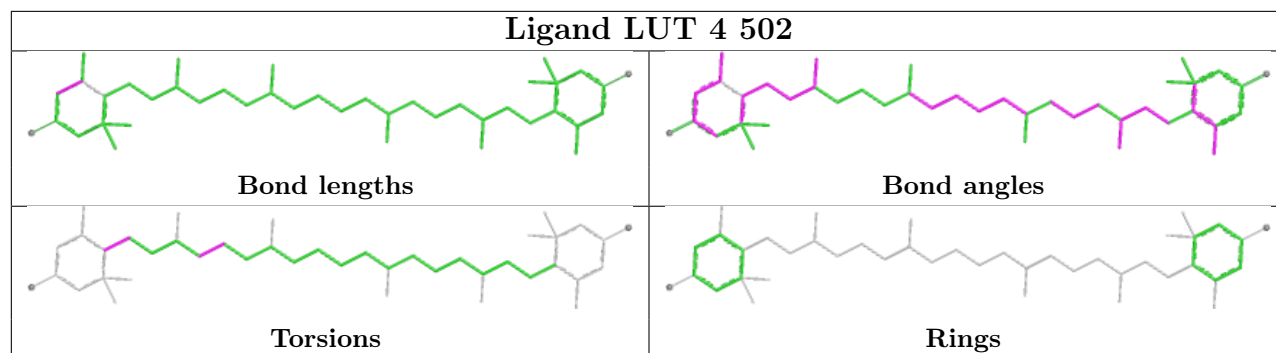
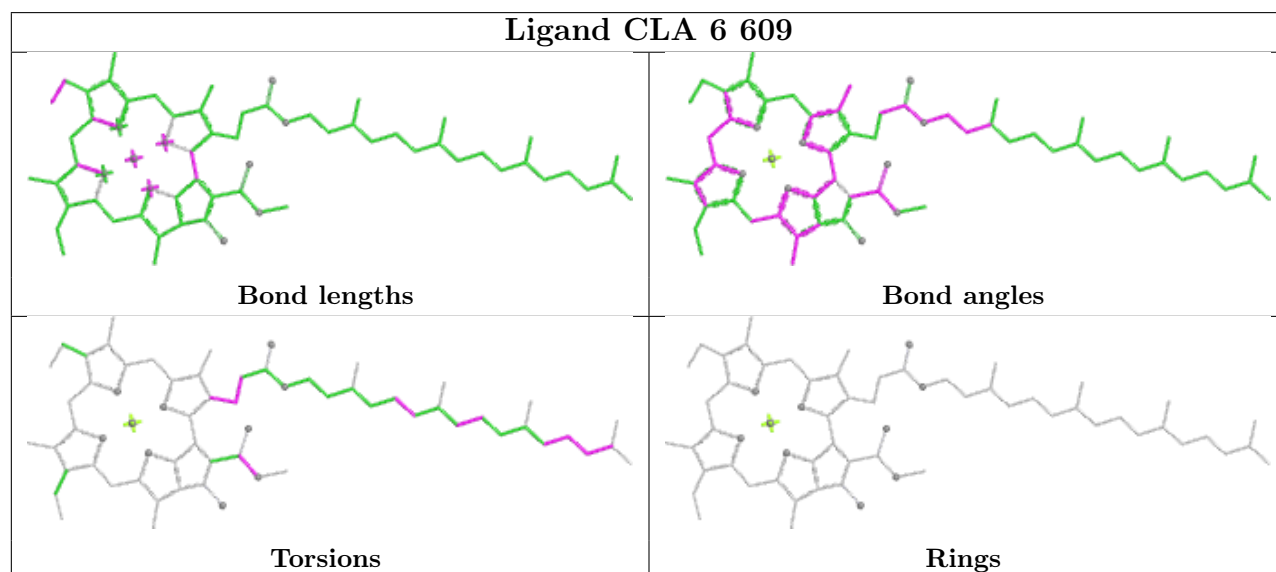
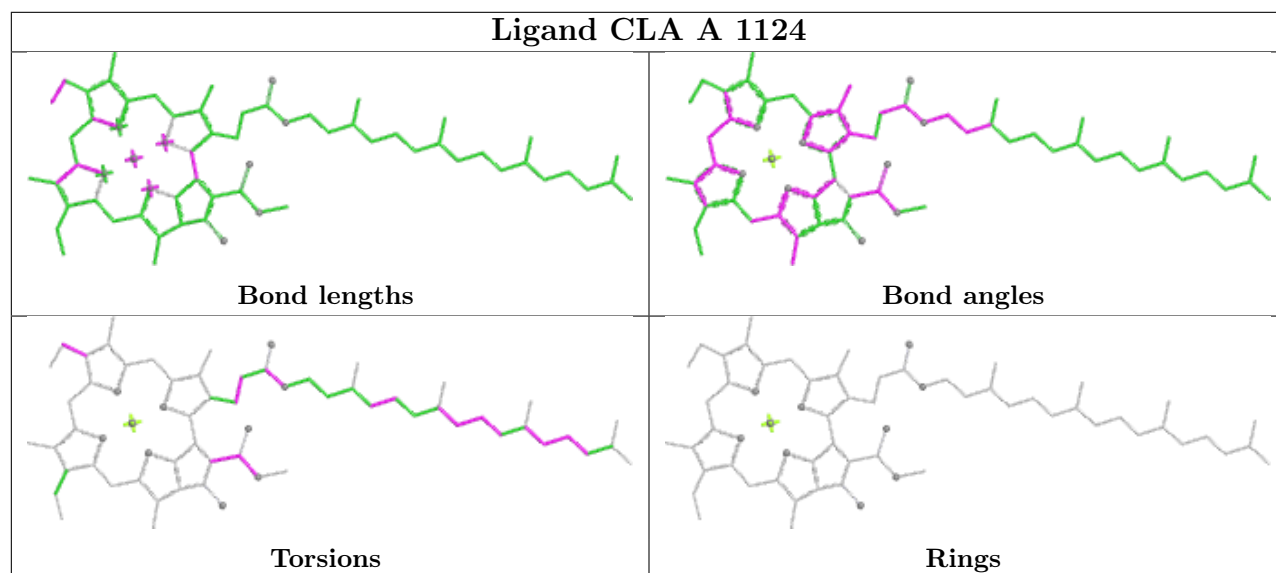




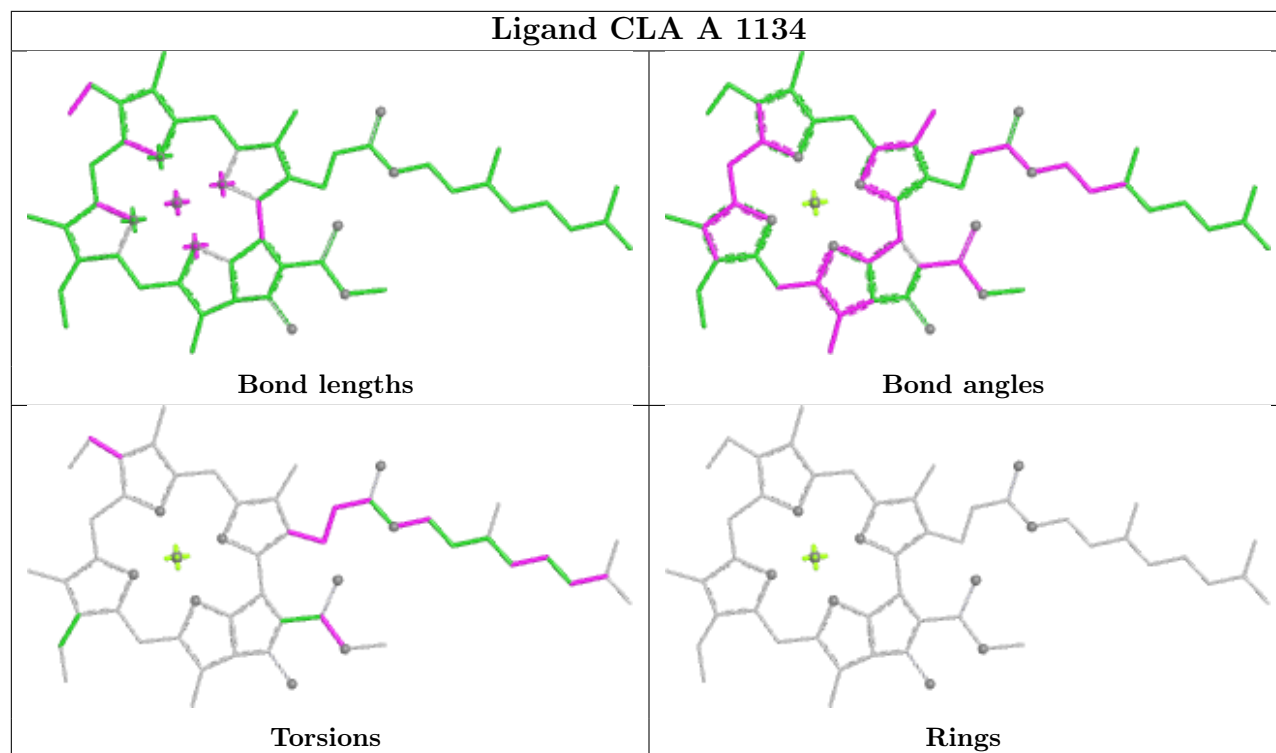




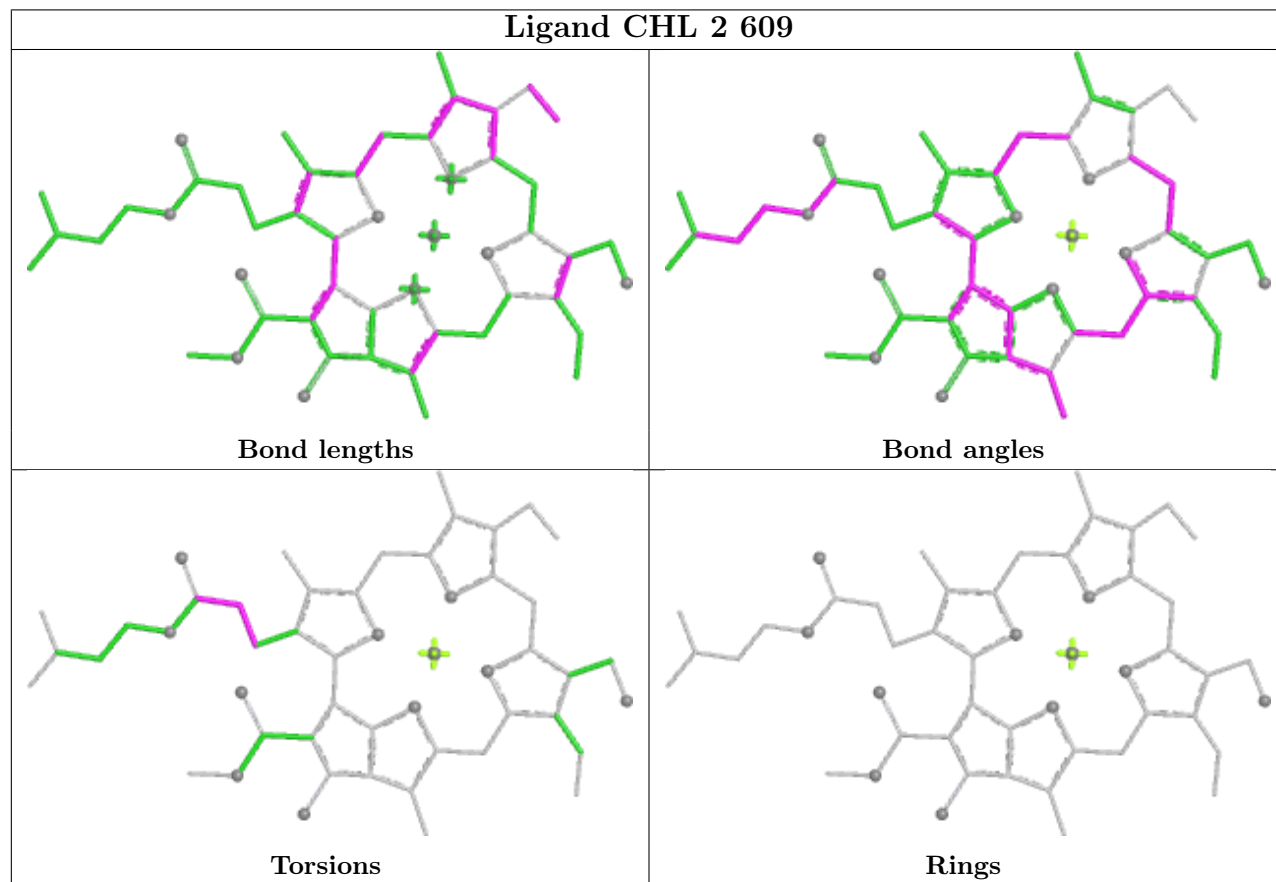


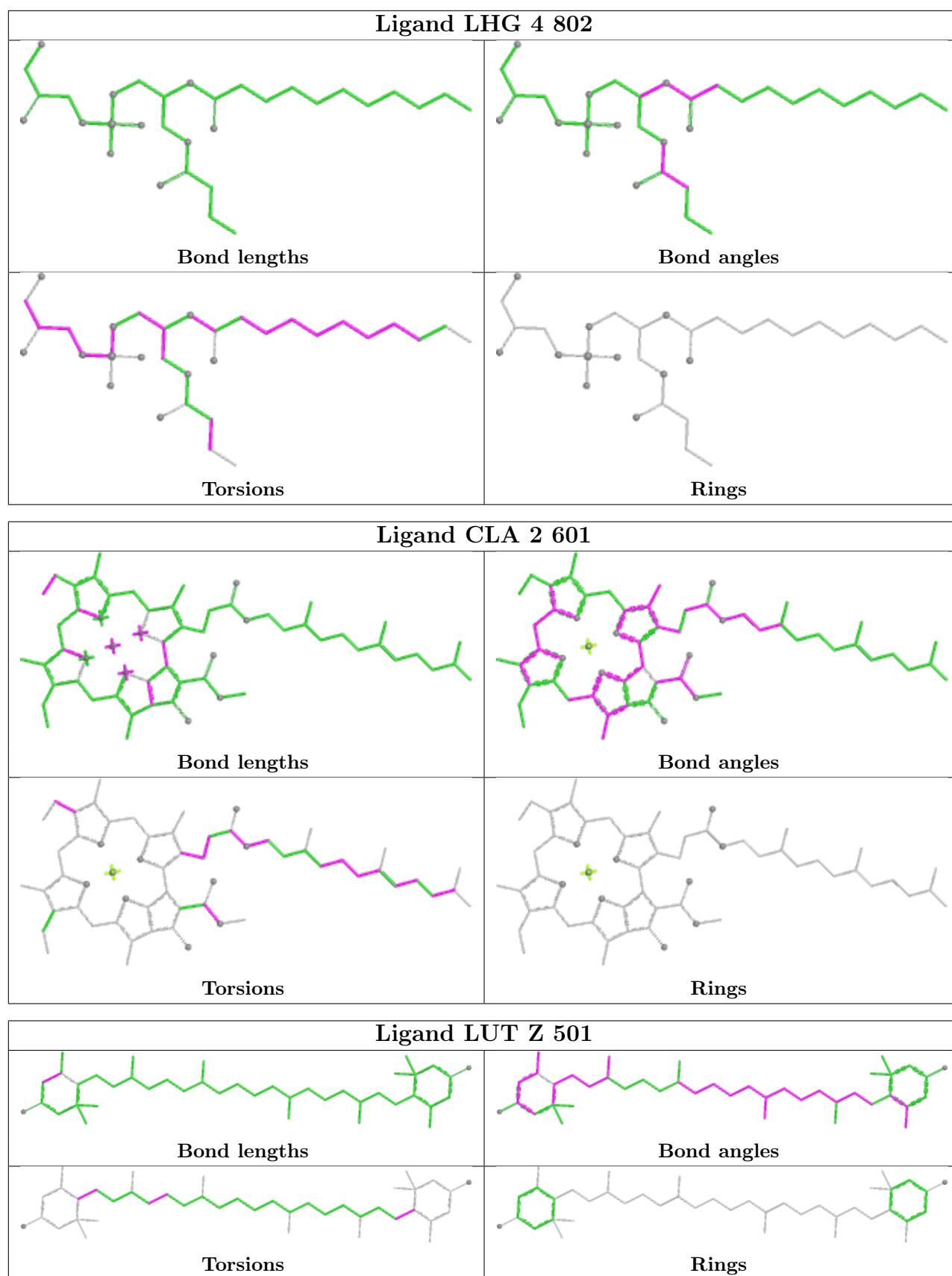
**Ligand LUT 4 502****Ligand CLA 6 609****Ligand CLA A 1124**

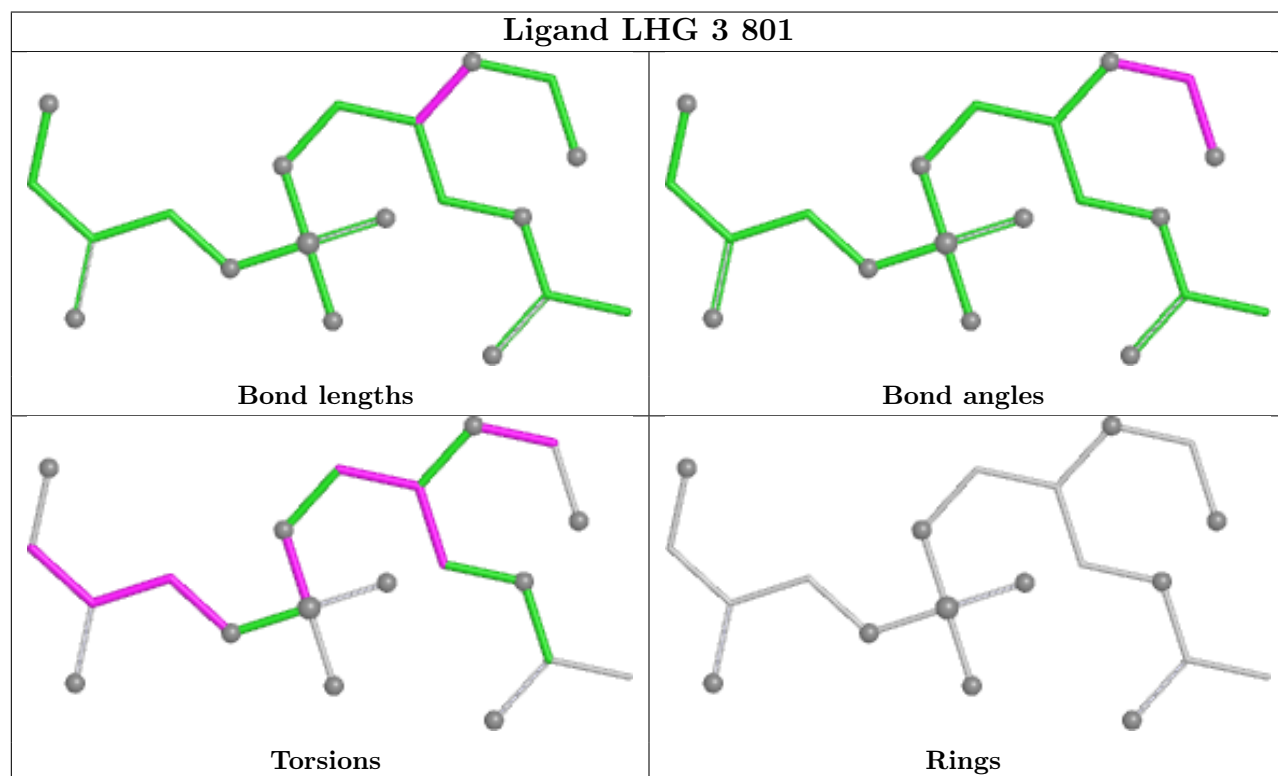
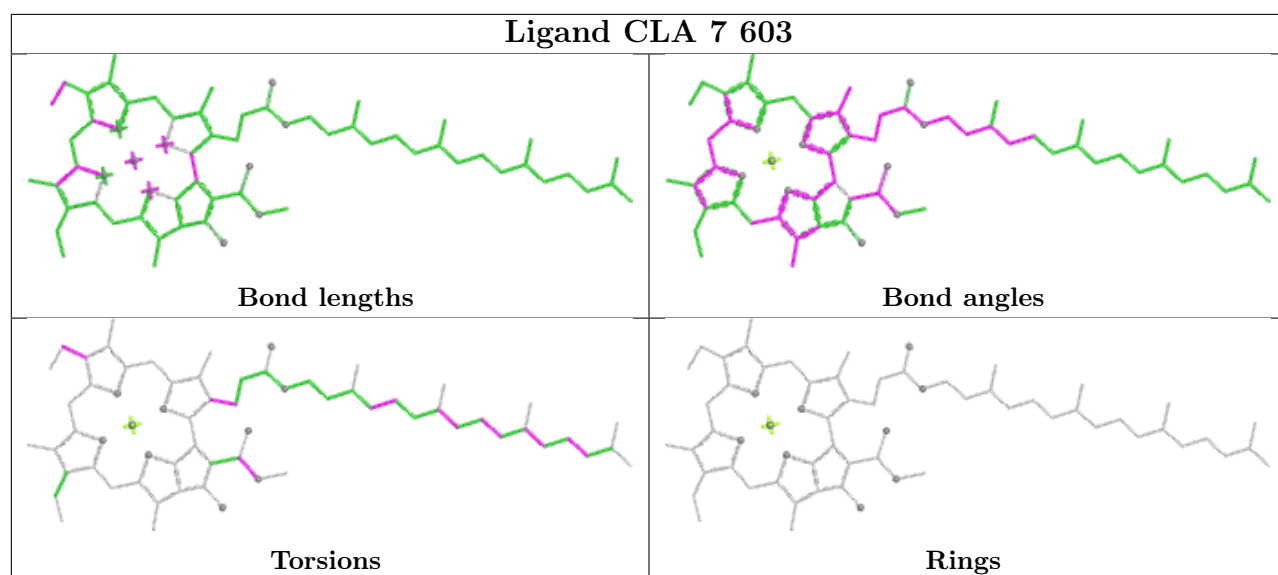
## Ligand CLA A 1134

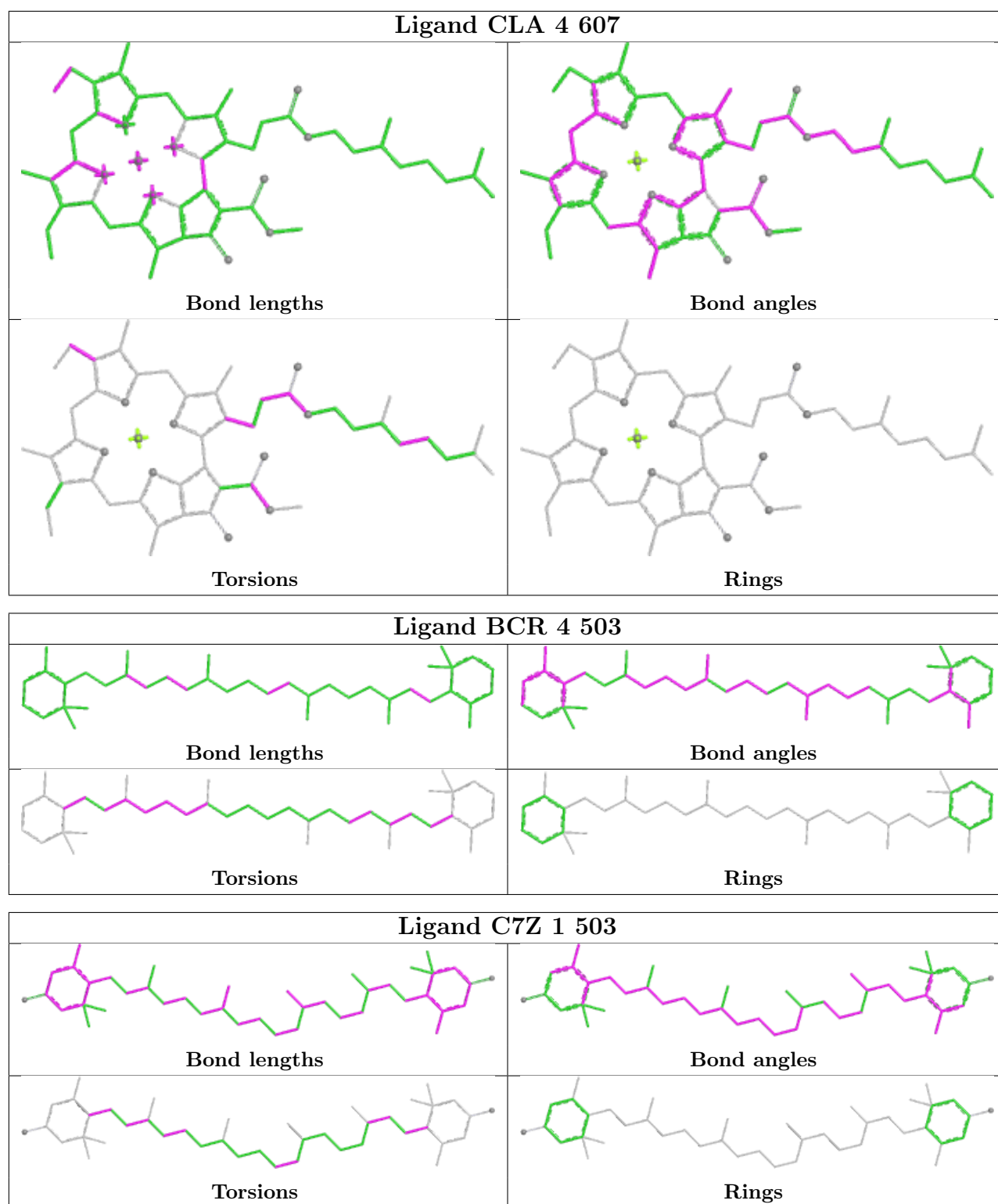


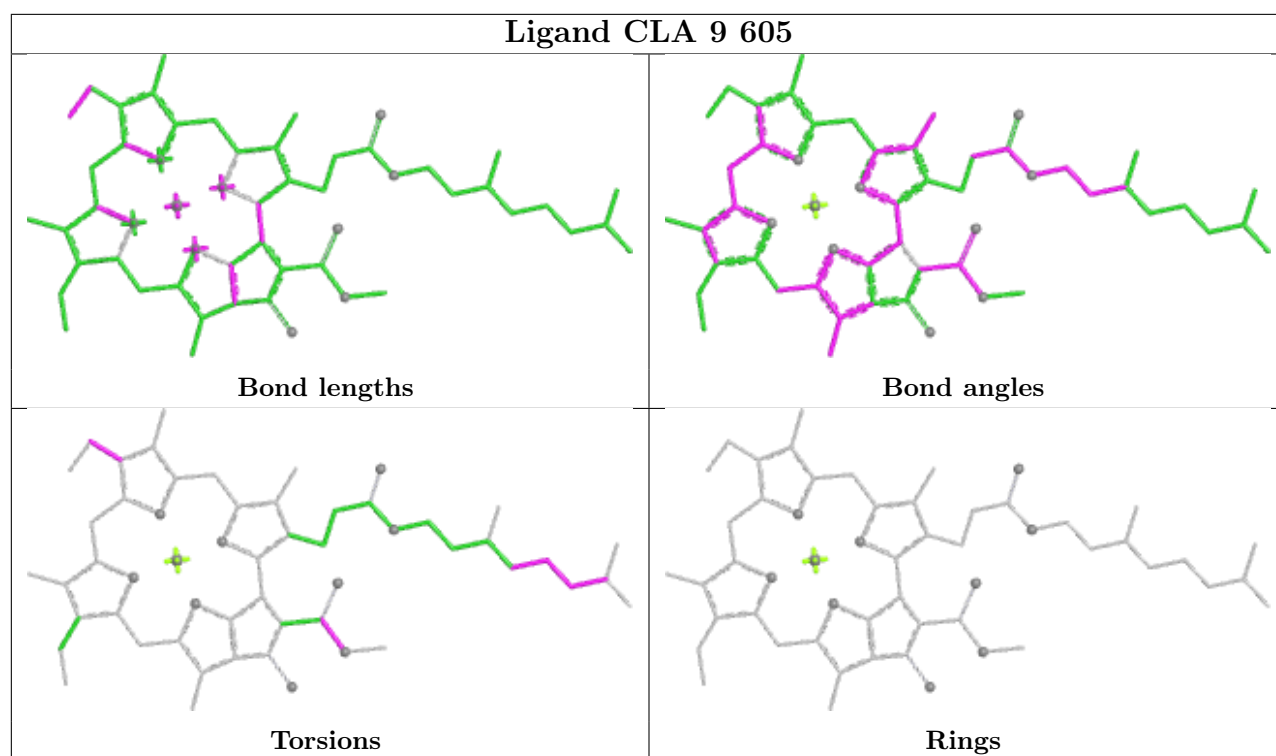
## Ligand CHL 2 609

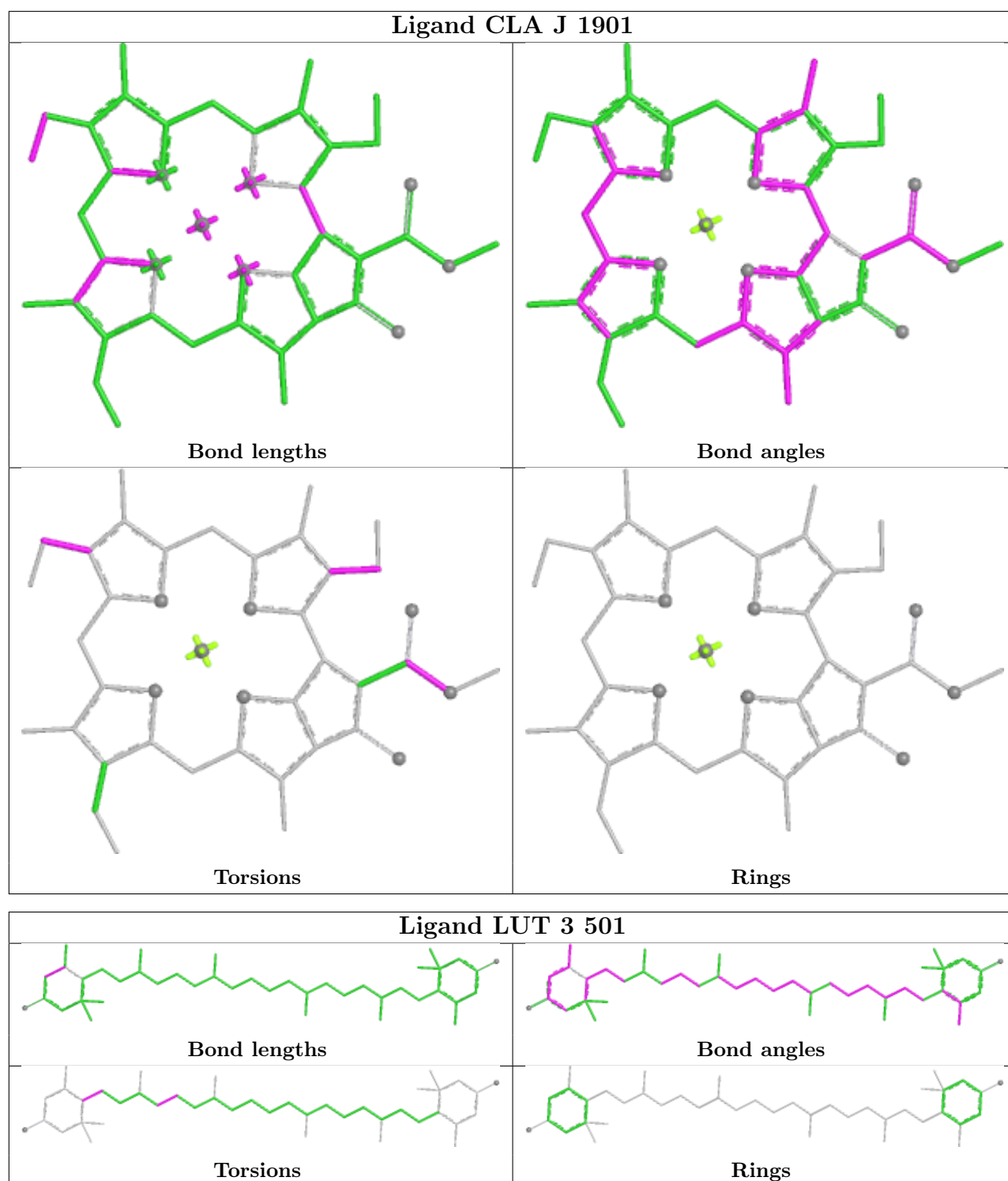


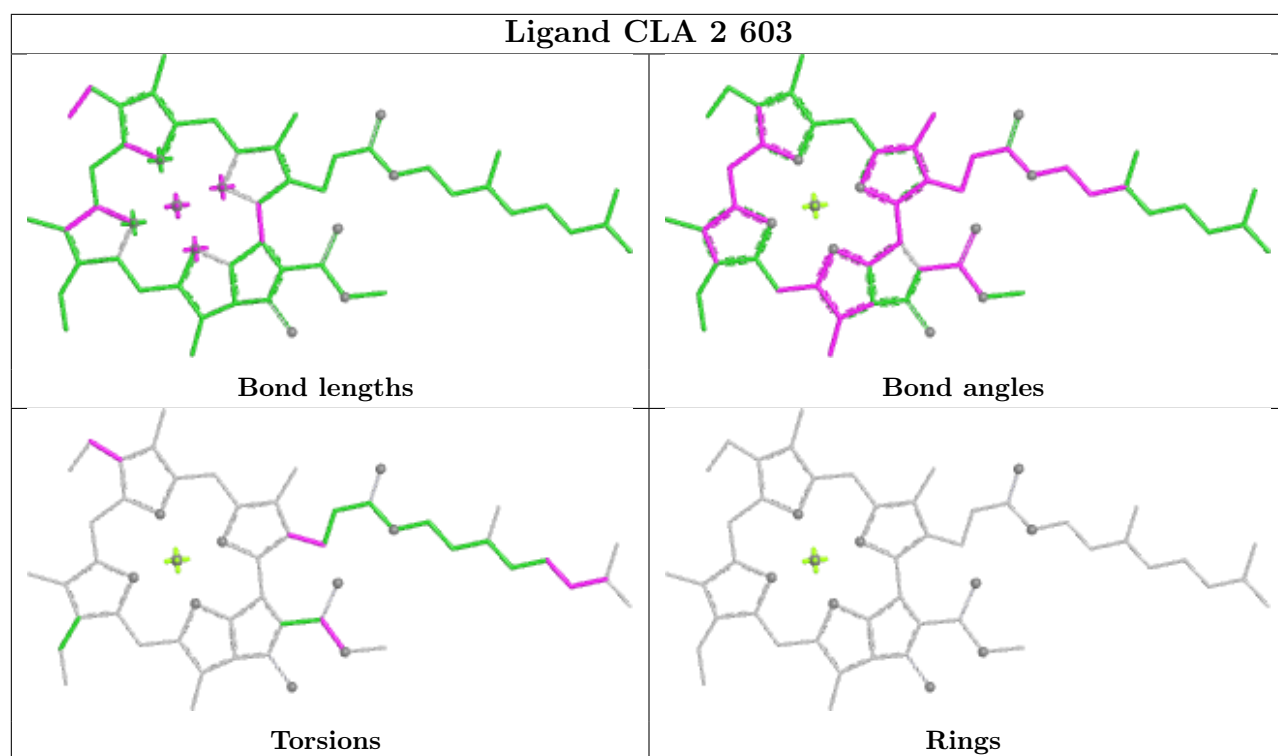


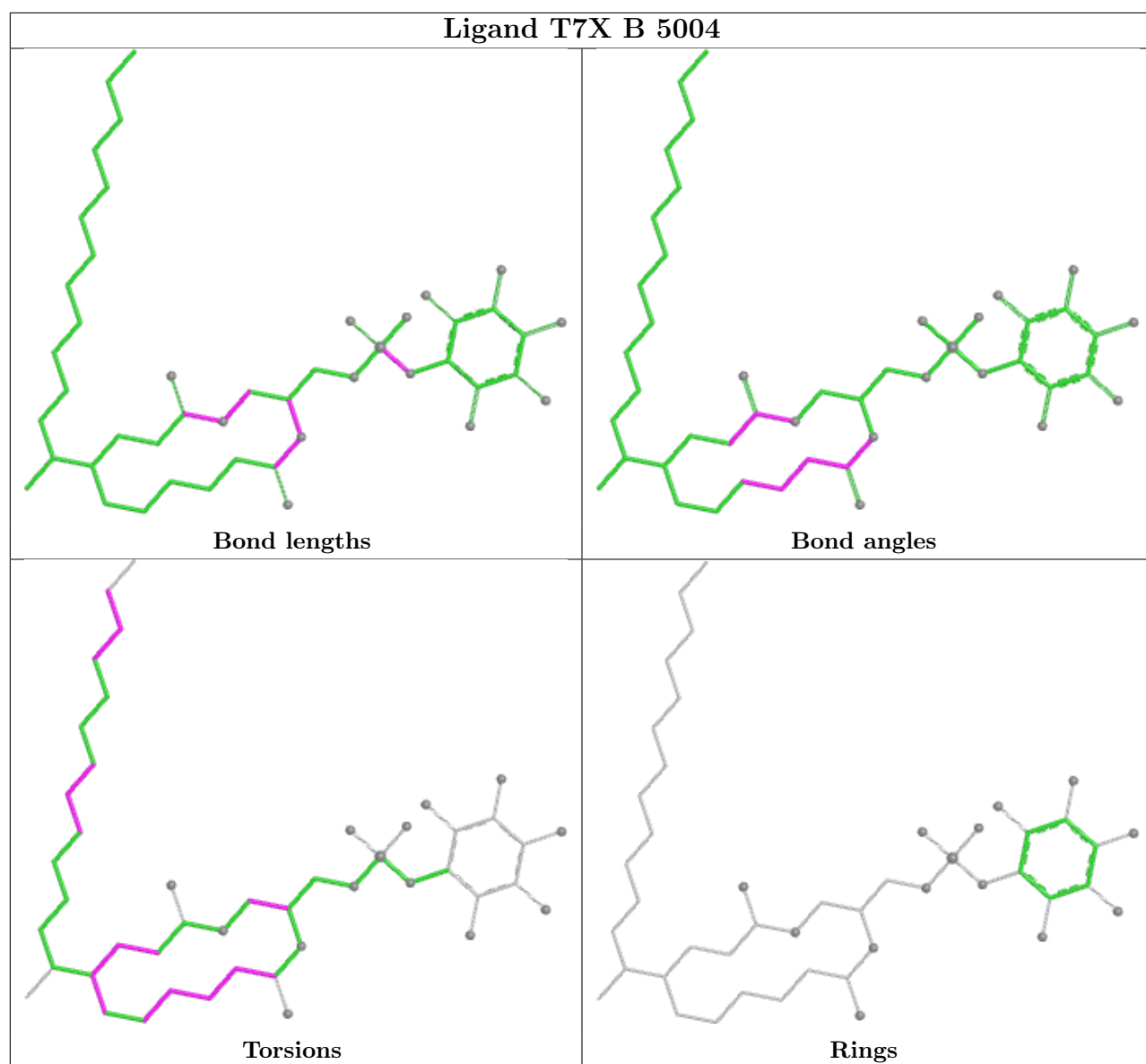




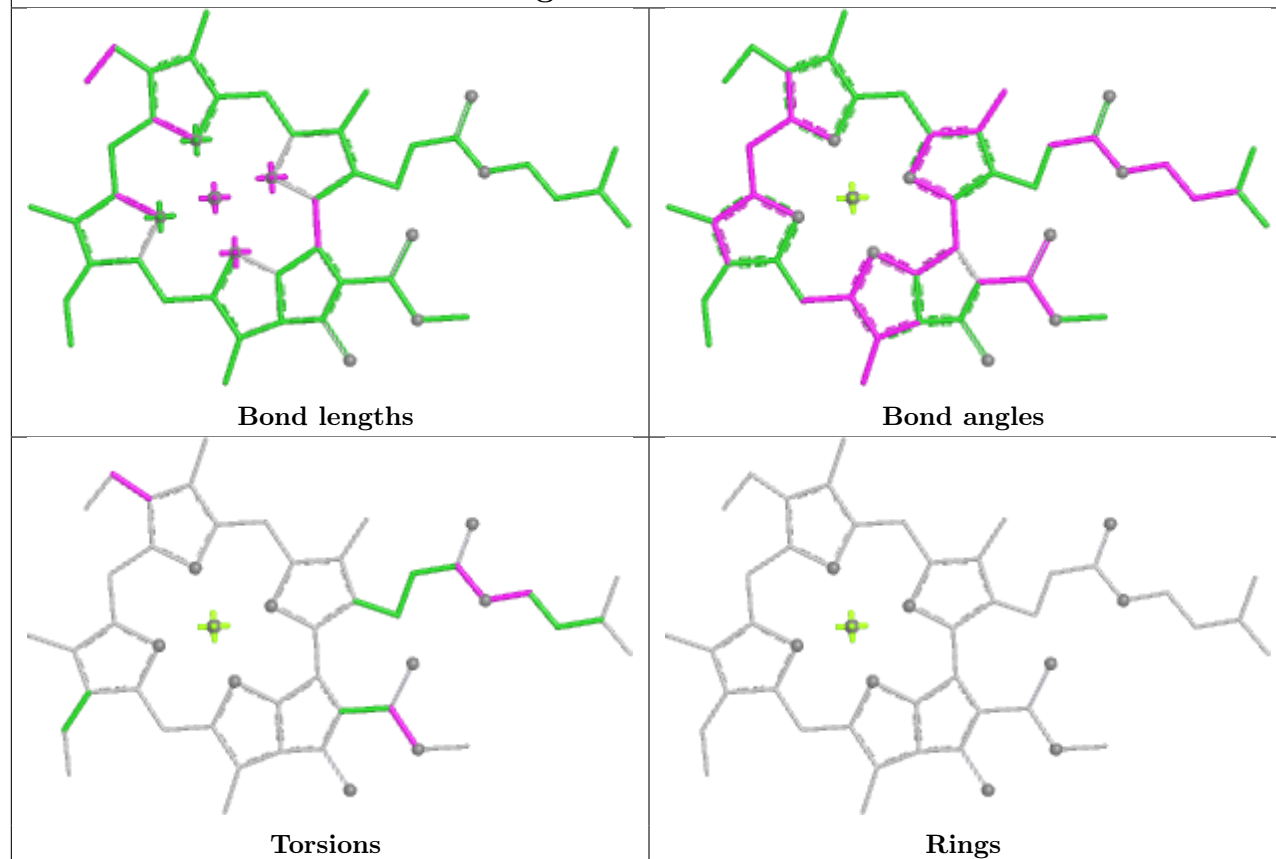




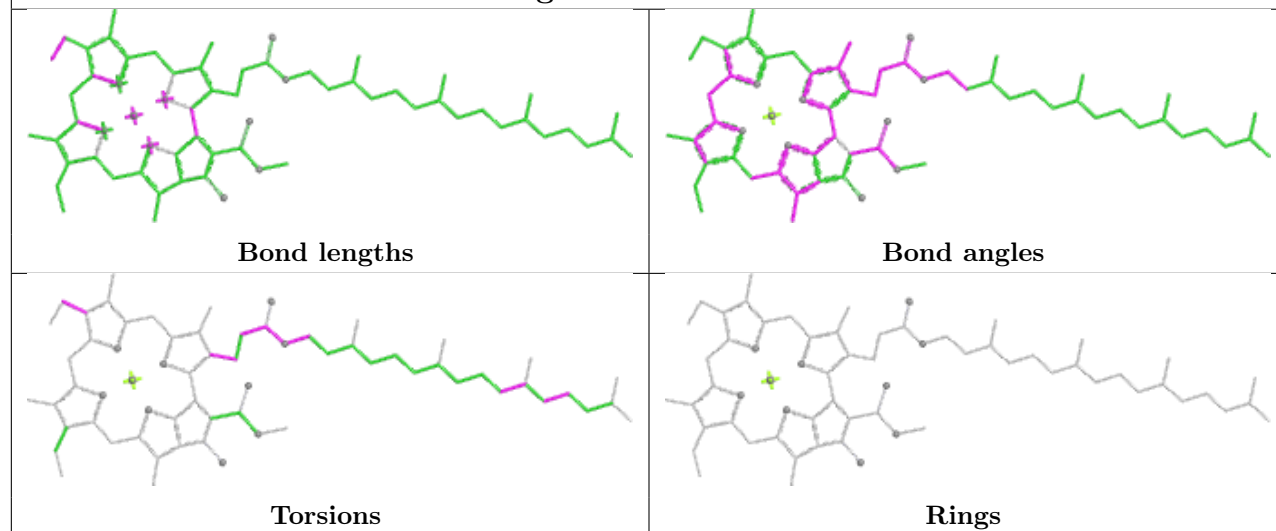


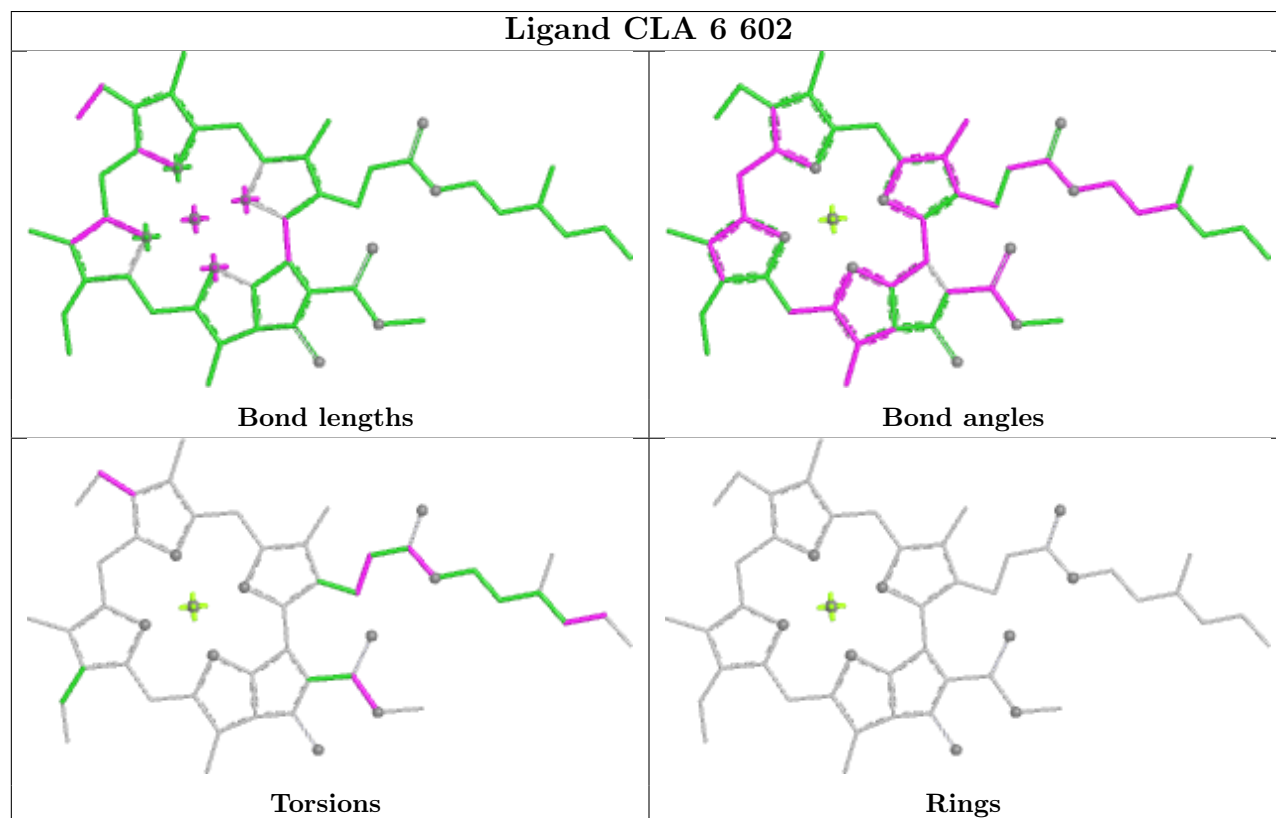
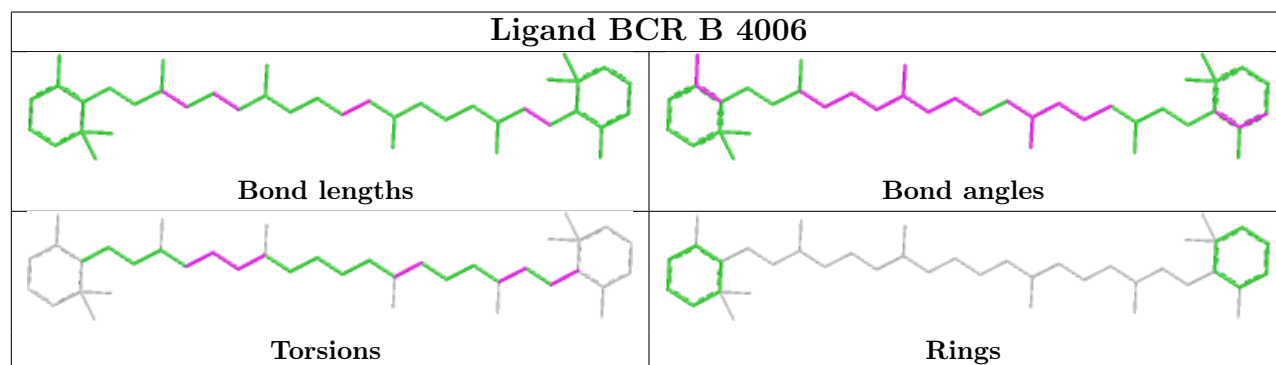
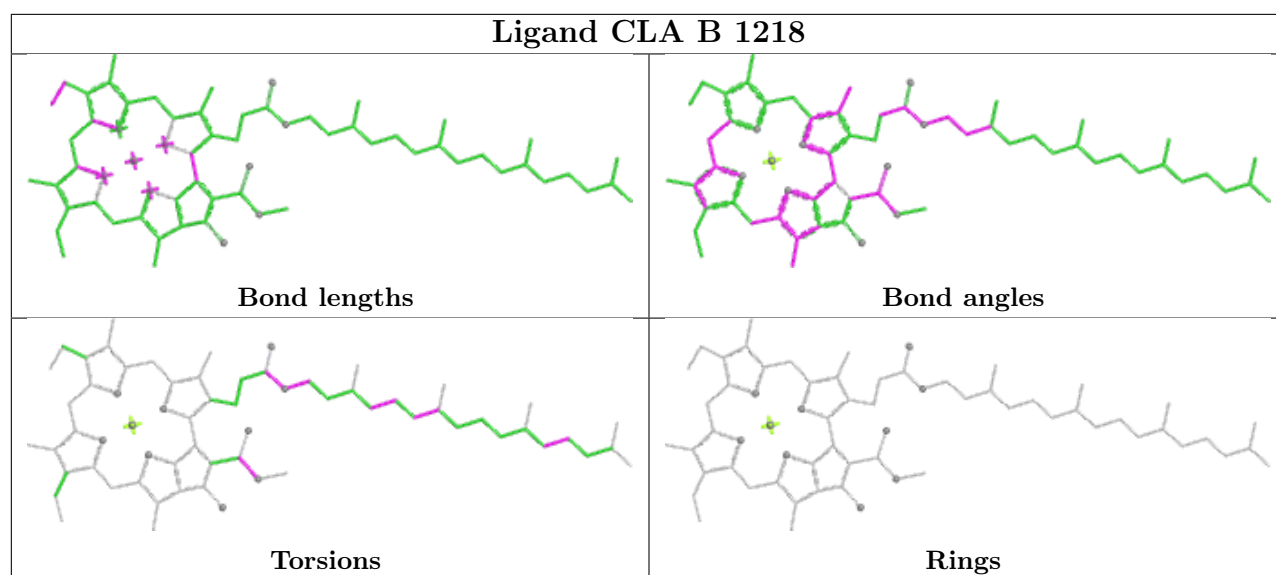


## Ligand CLA 7 602

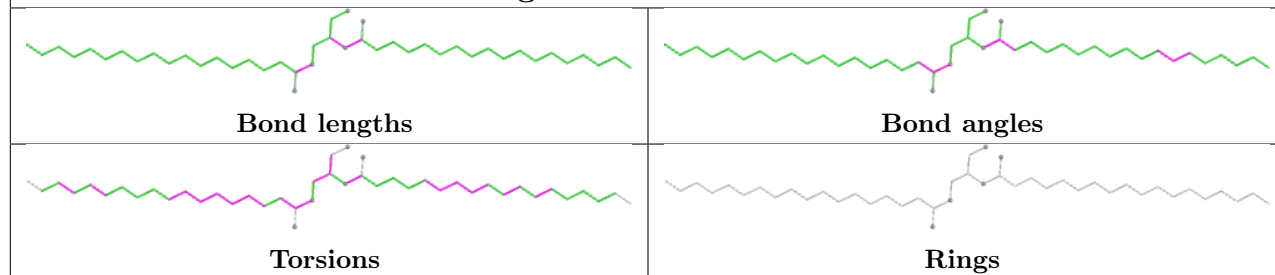


## Ligand CLA 6 604

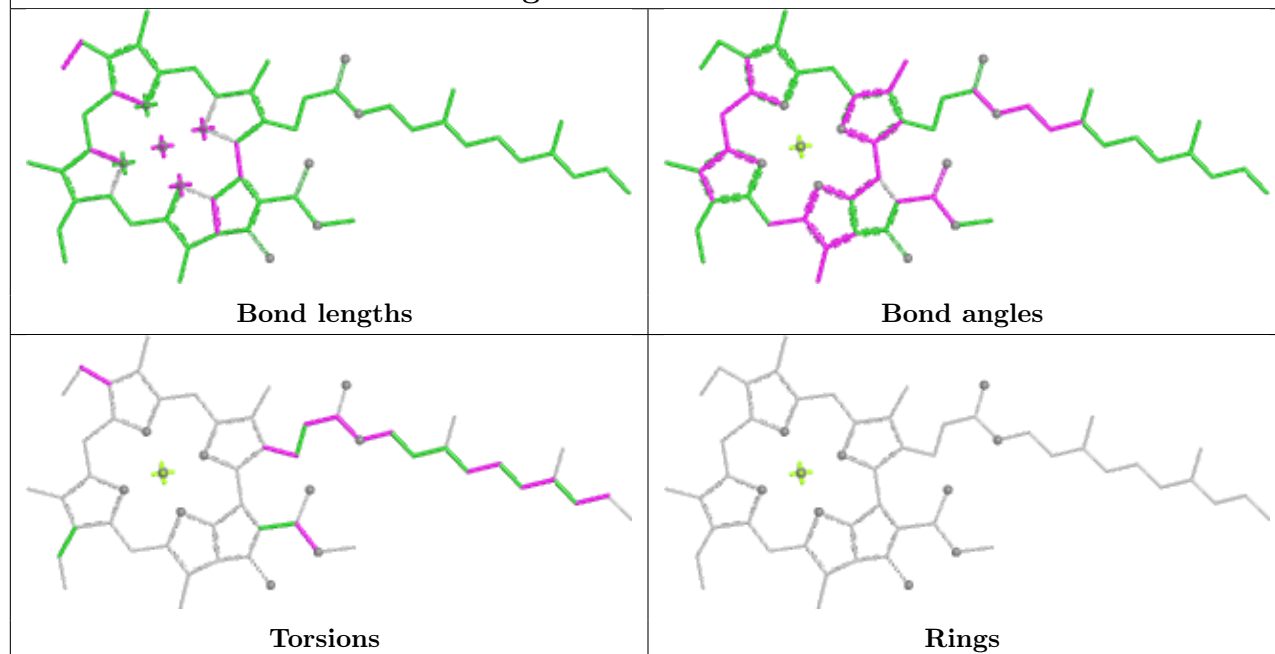




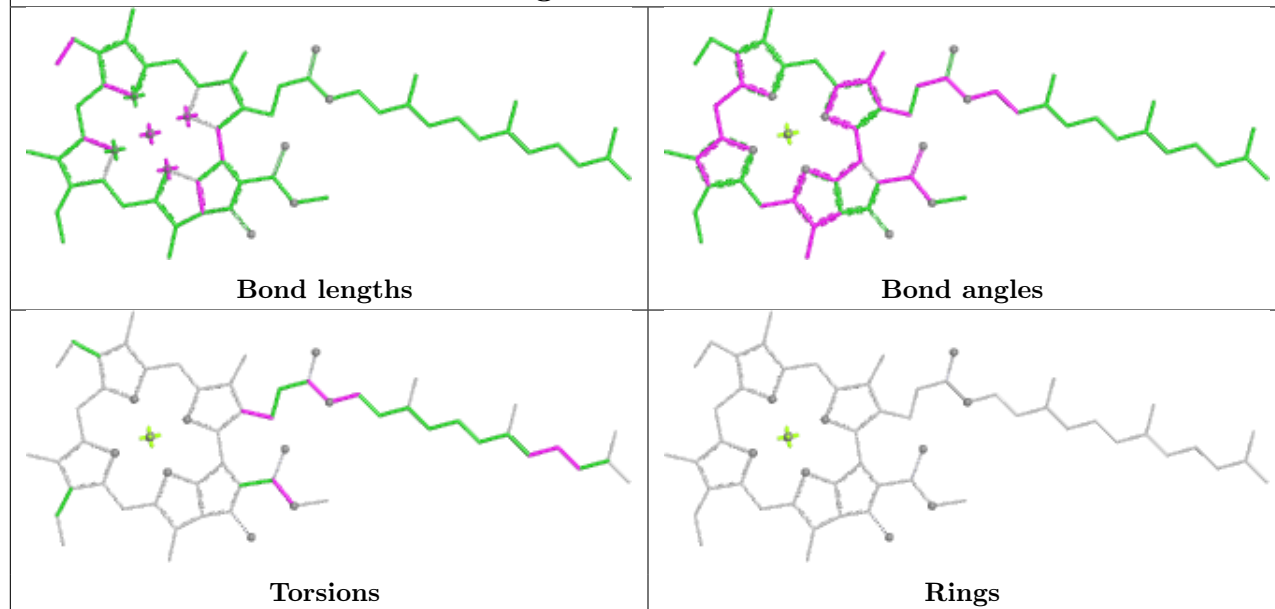
## Ligand DGA A 5005



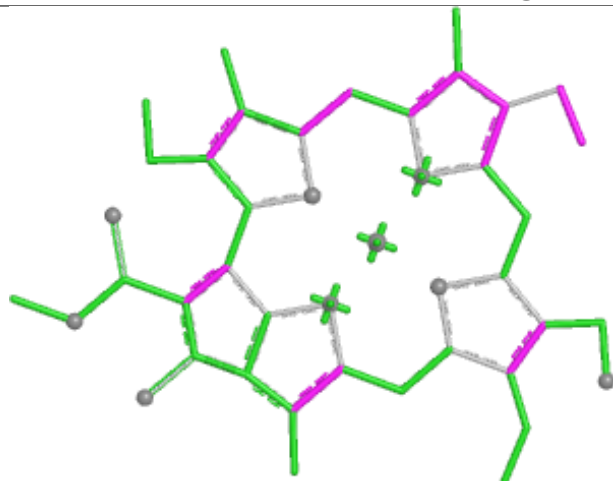
## Ligand CLA B 1212



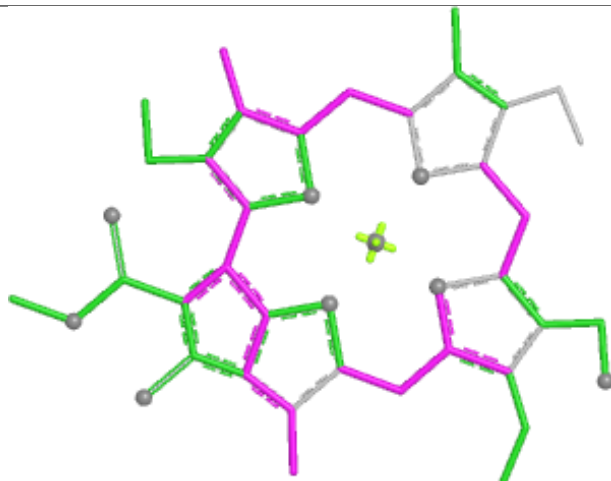
## Ligand CLA 7 601



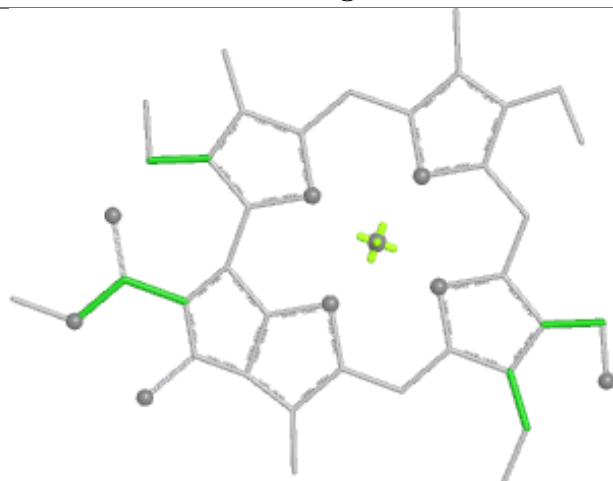
## Ligand CHL 4 617



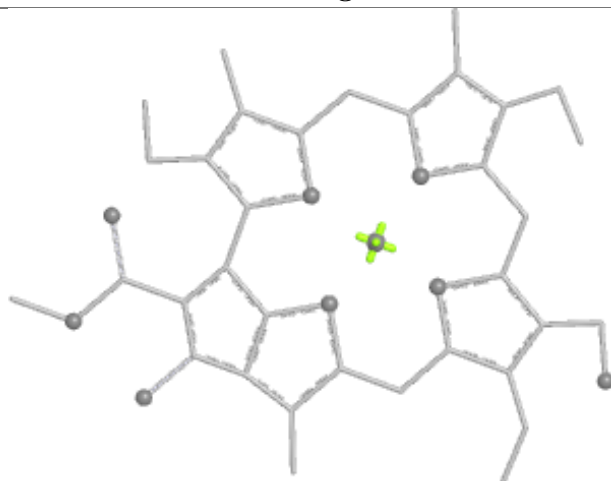
Bond lengths



Bond angles

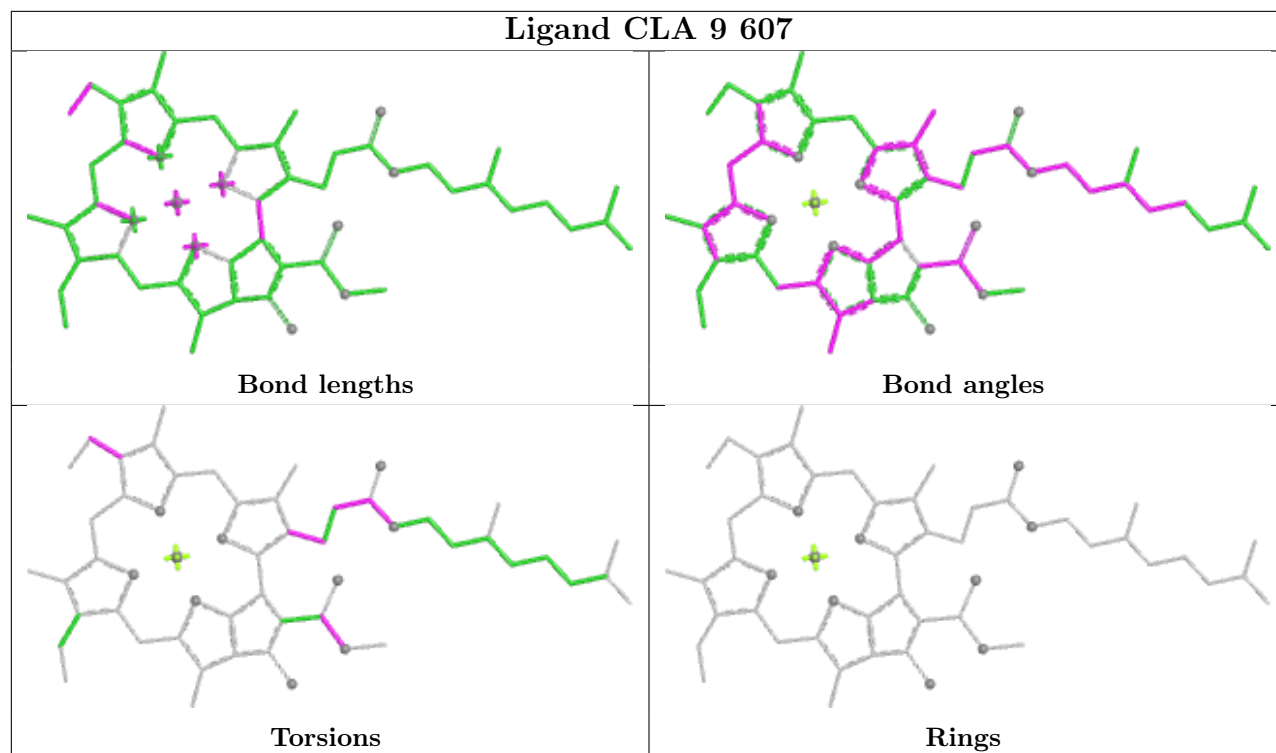


Torsions

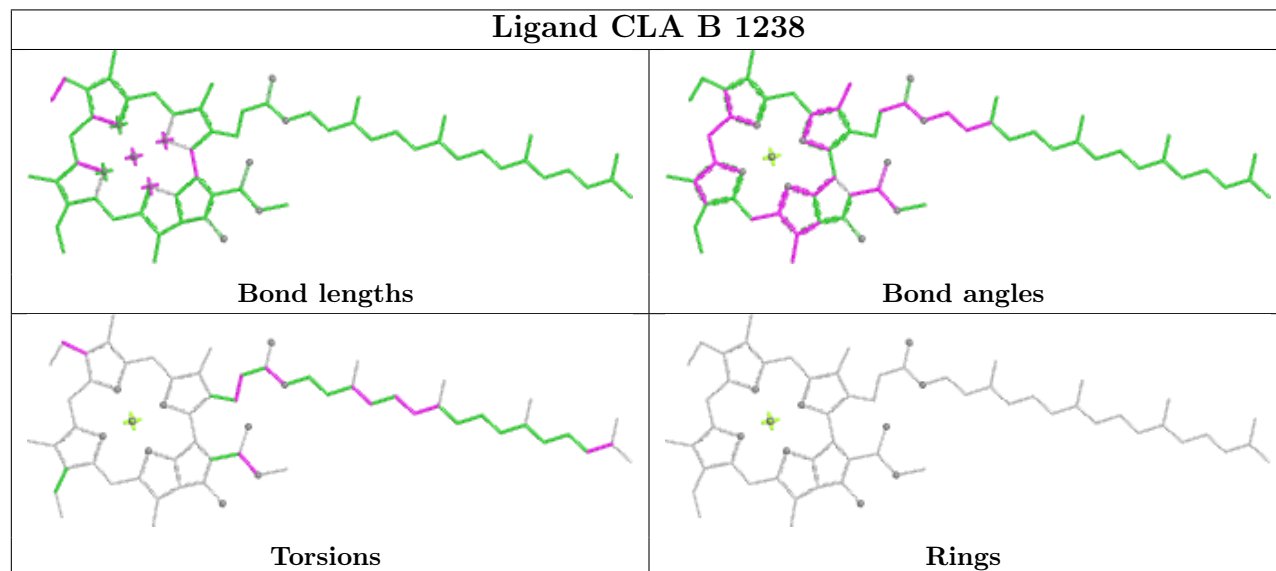


Rings

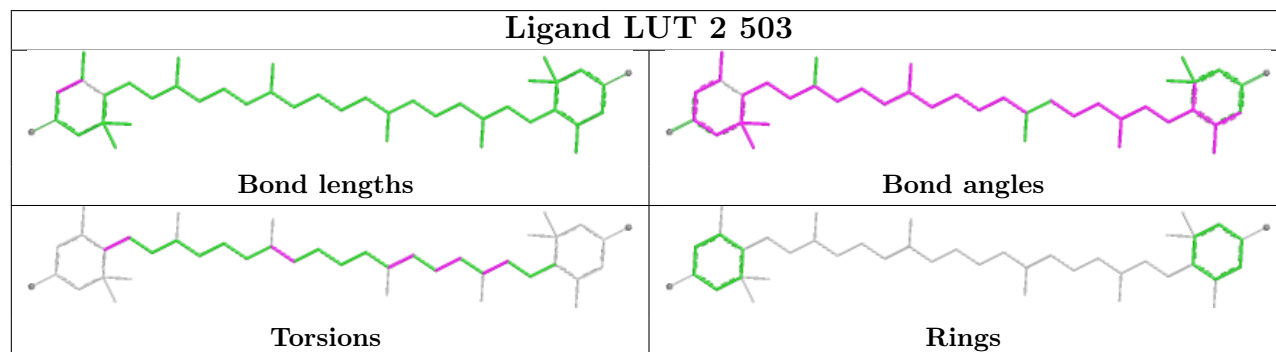
## Ligand CLA 9 607

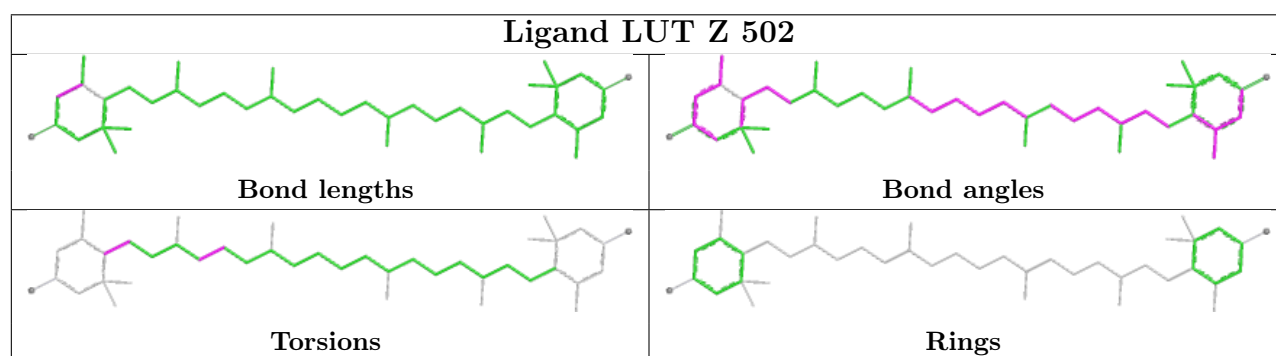
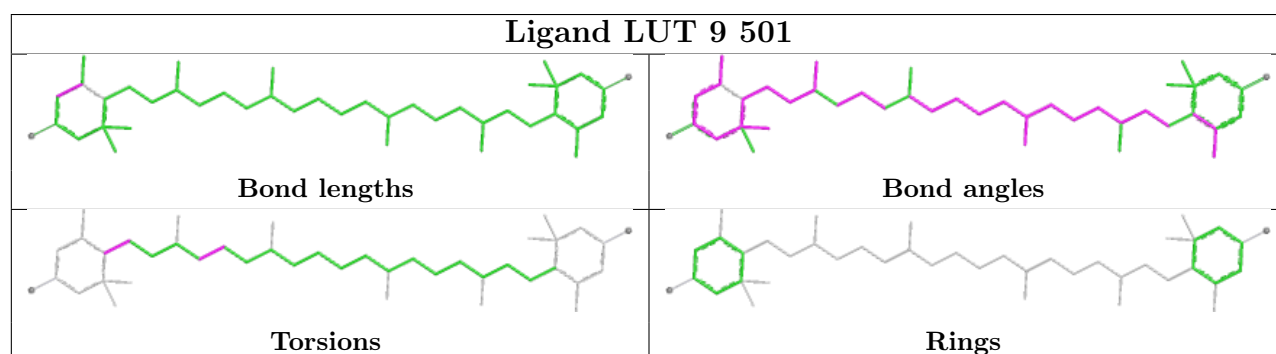
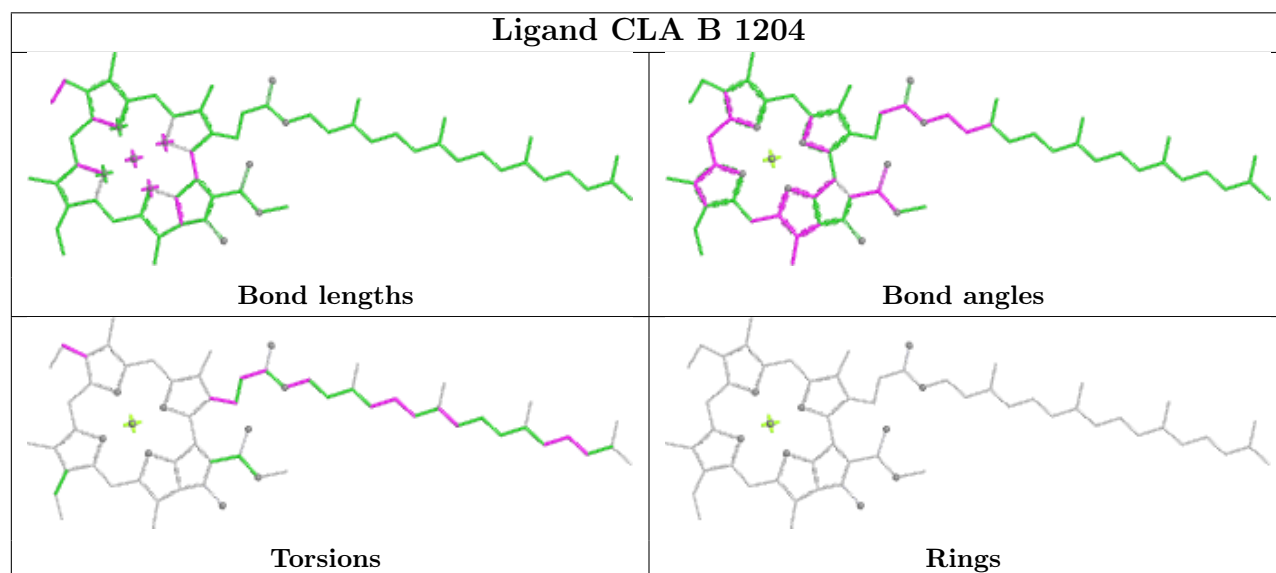
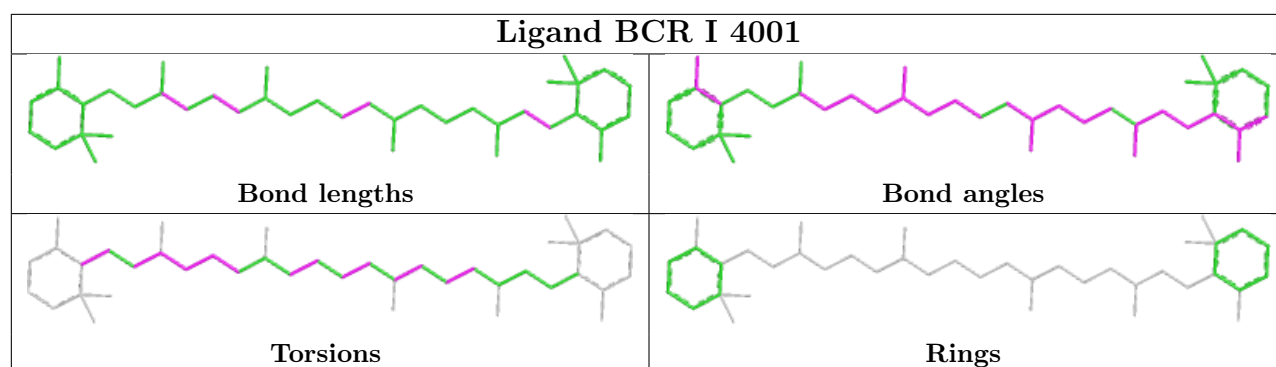


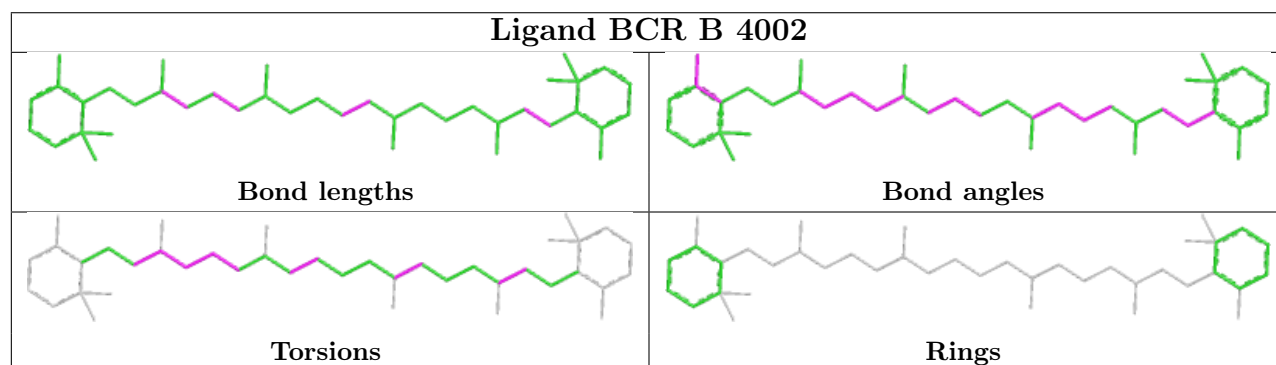
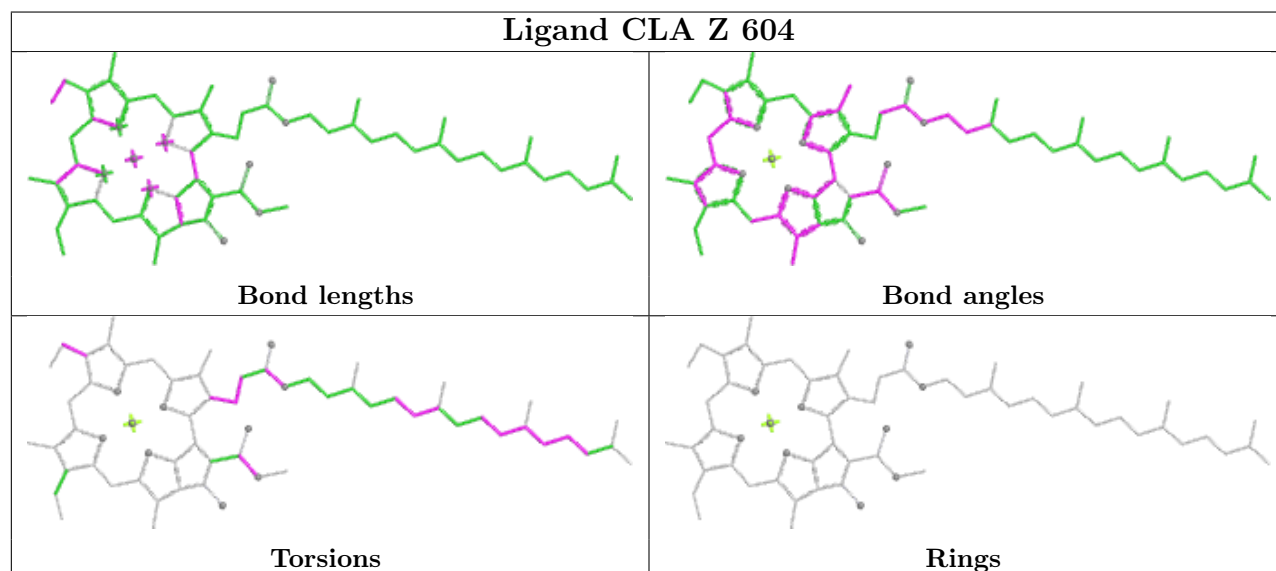
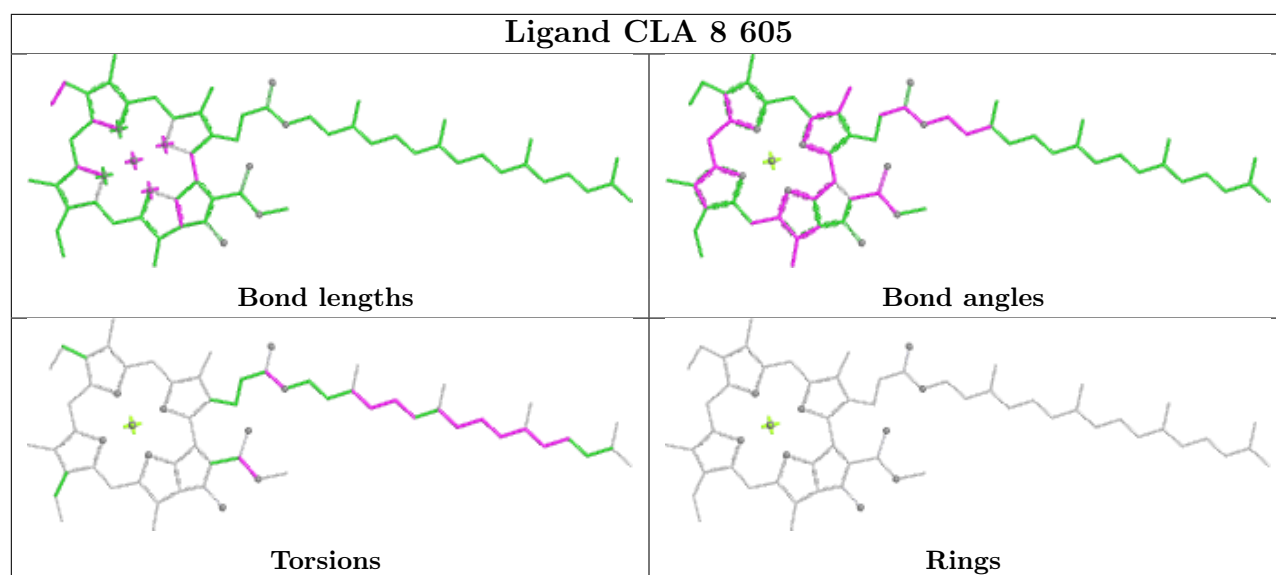
## Ligand CLA B 1238



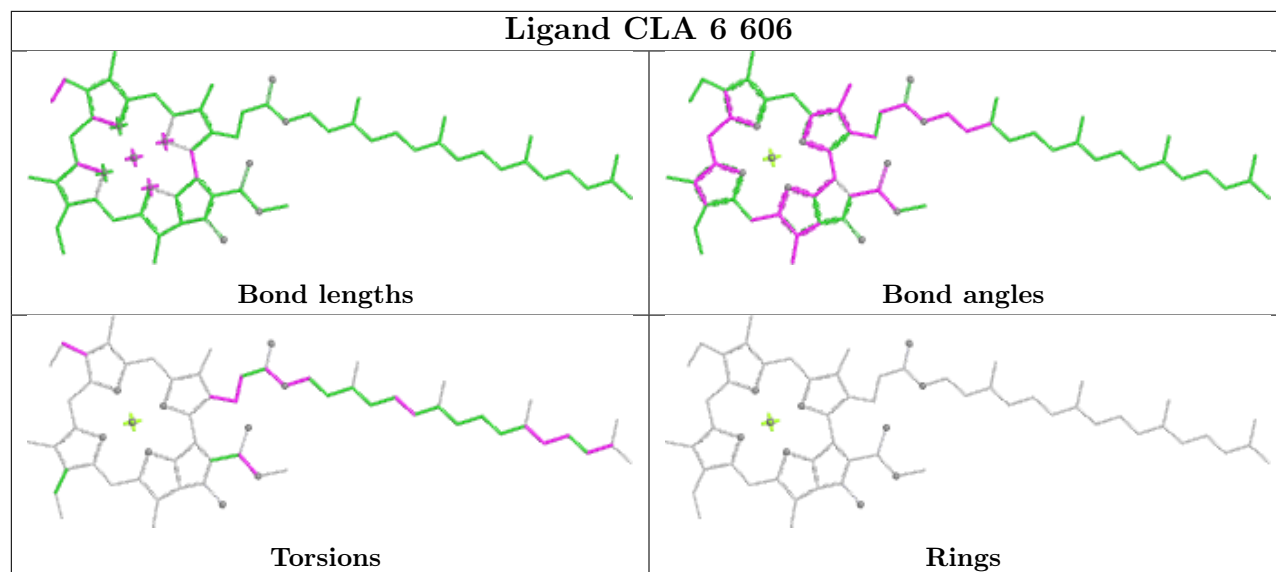
## Ligand LUT 2 503



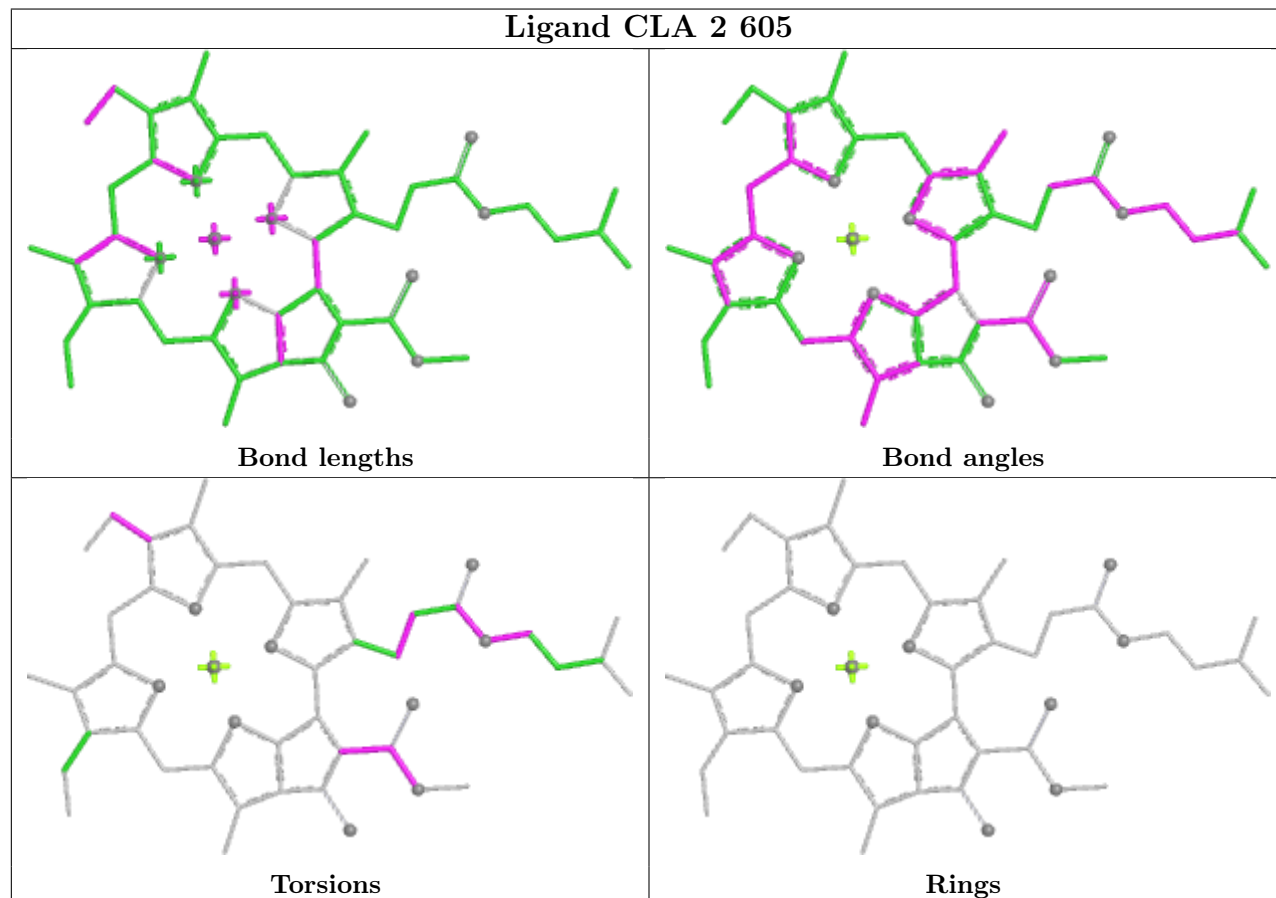




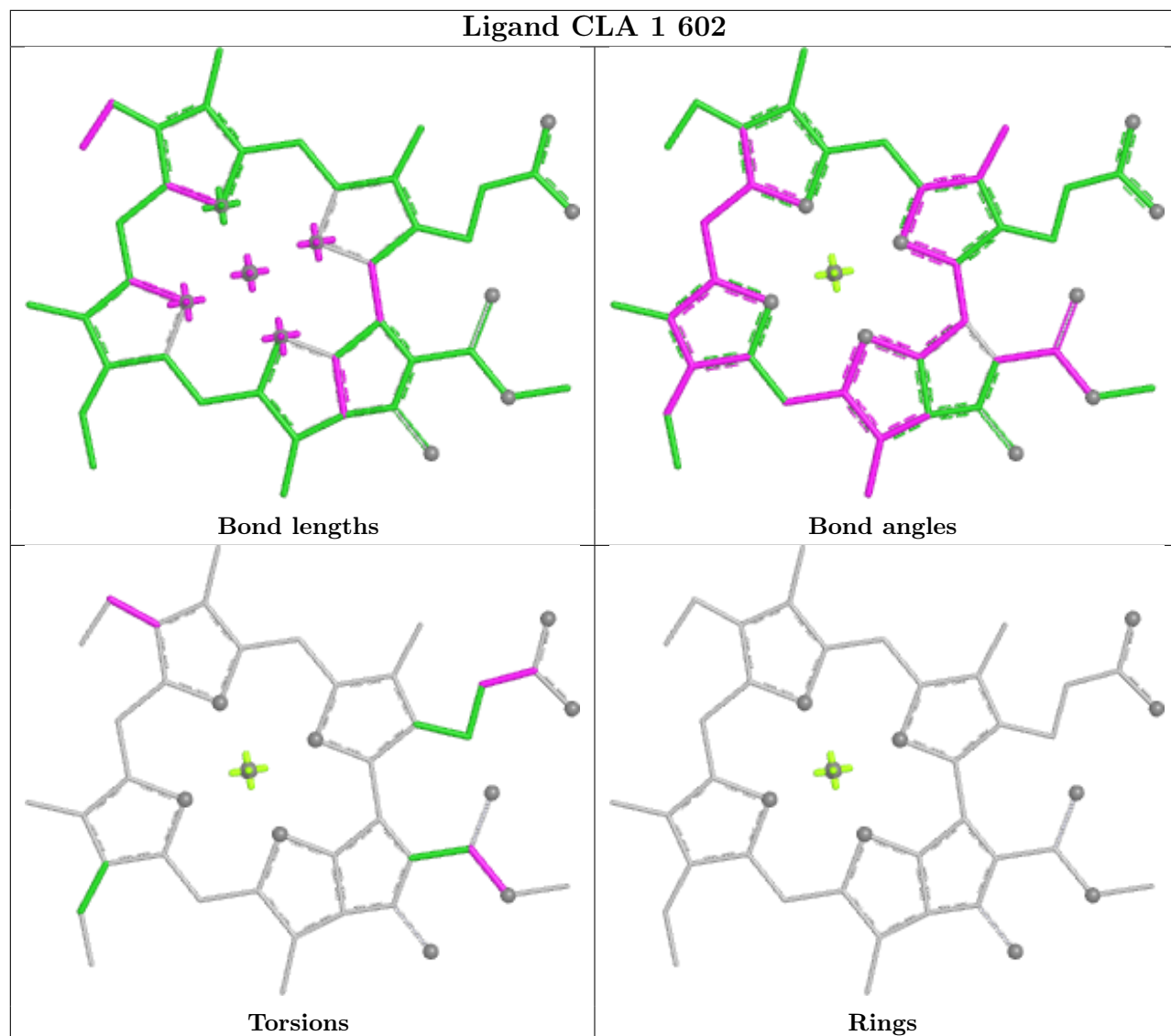
## Ligand CLA 6 606



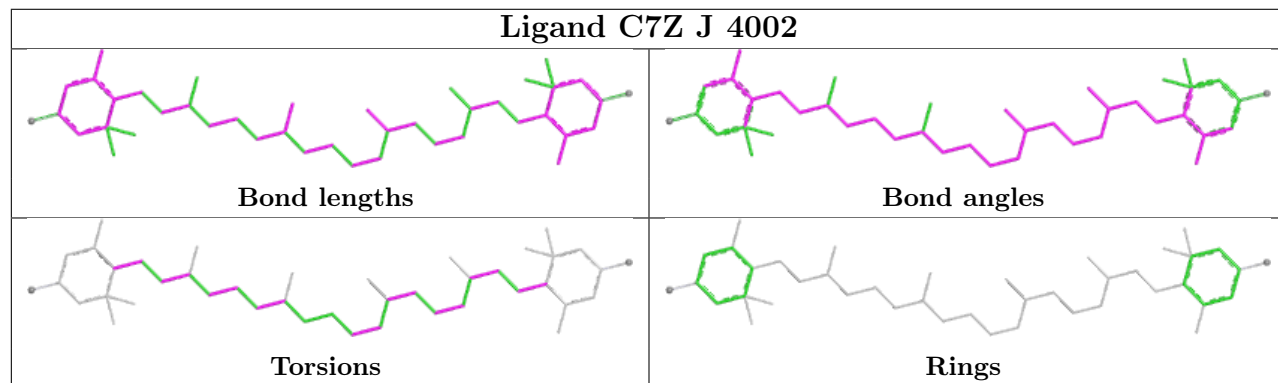
## Ligand CLA 2 605

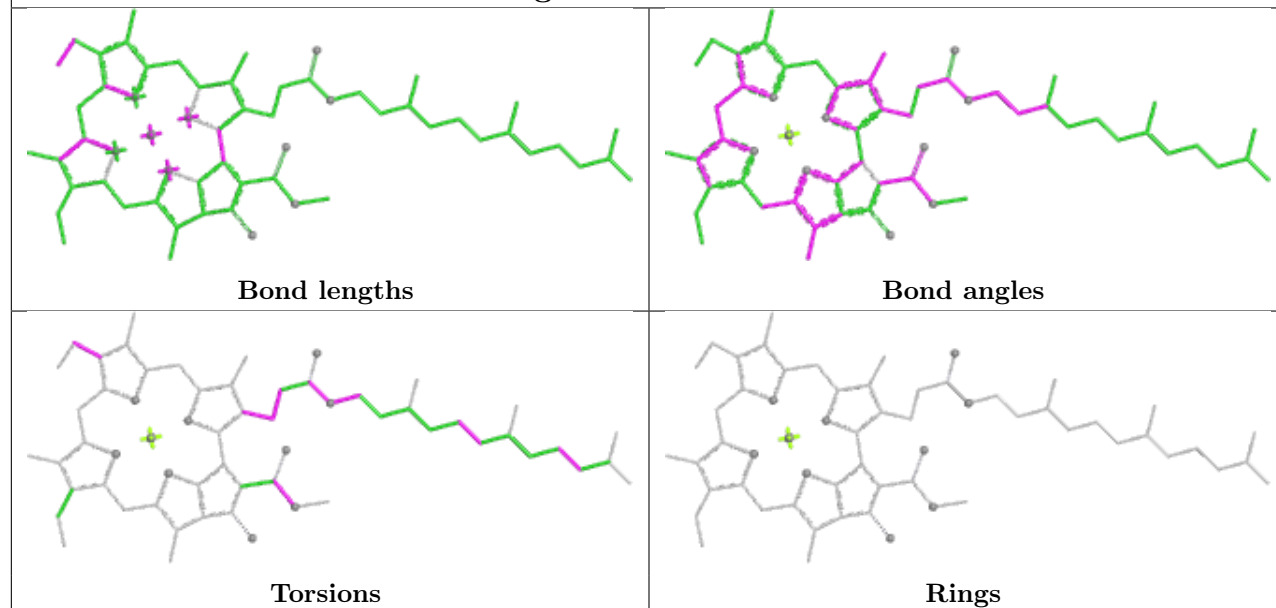
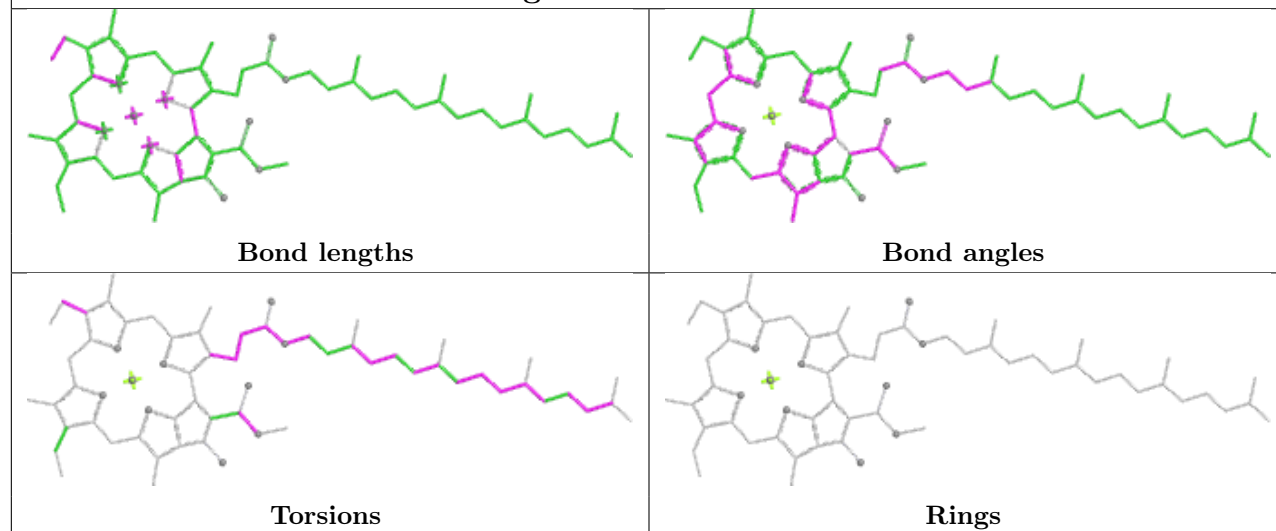


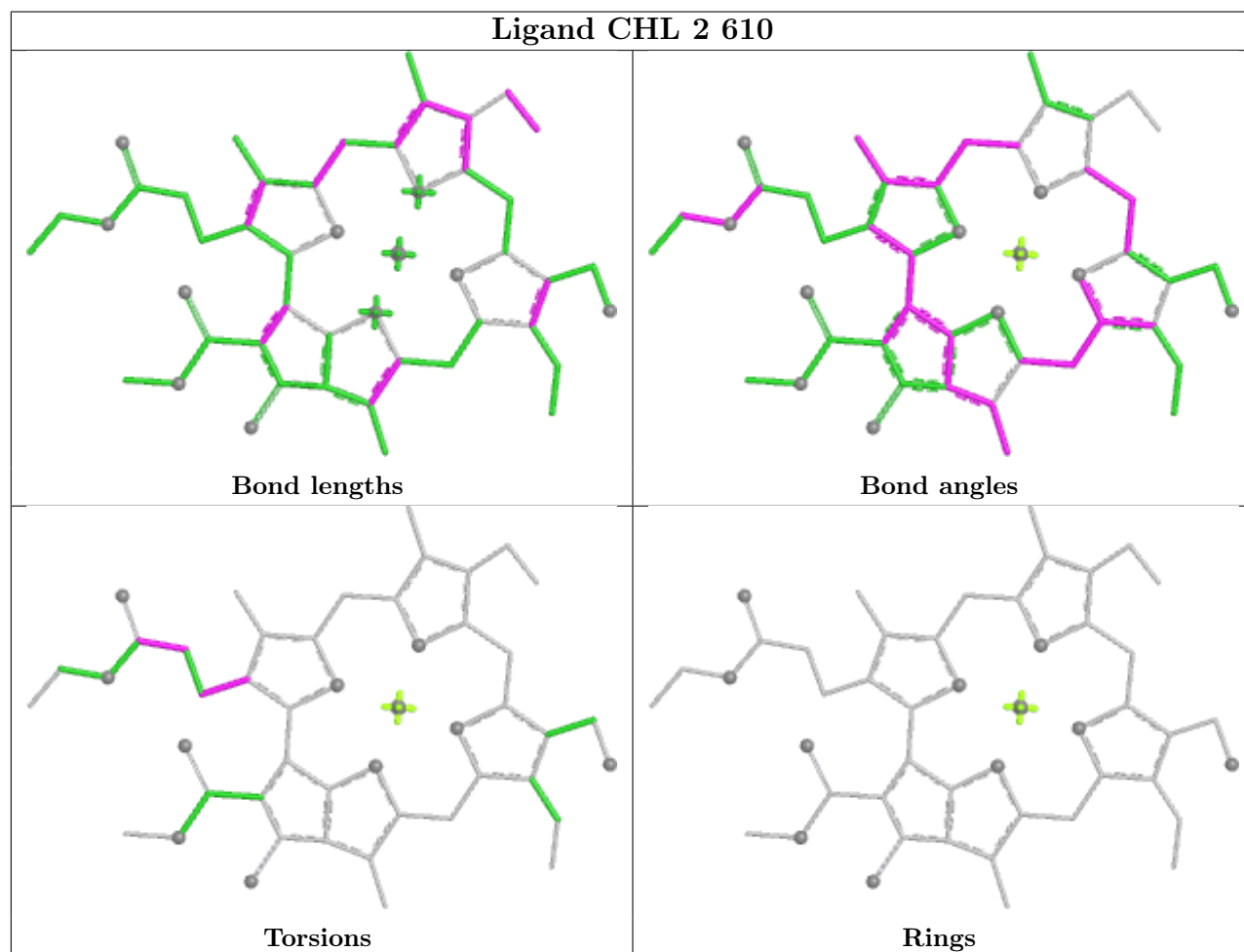
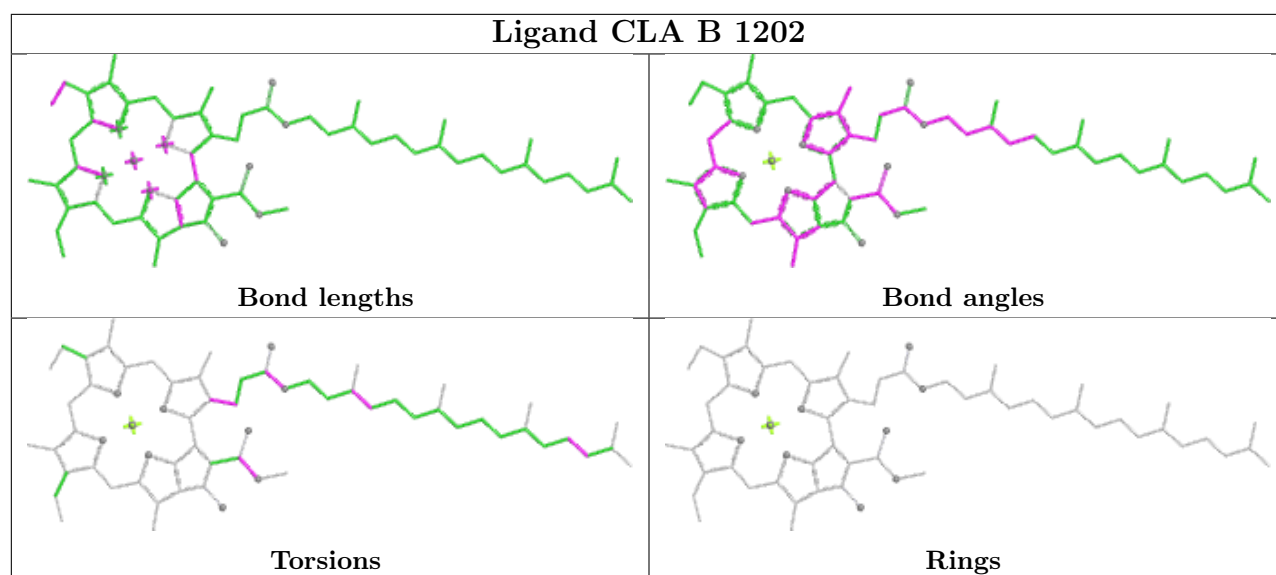
## Ligand CLA 1 602



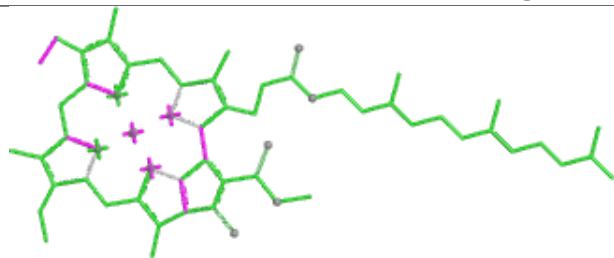
## Ligand C7Z J 4002



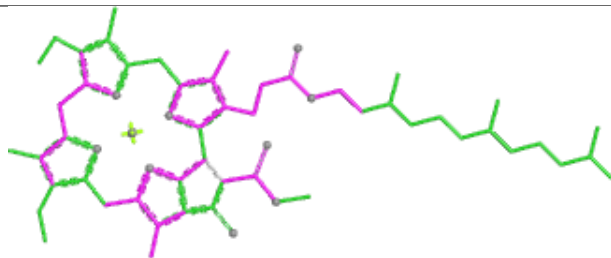
**Ligand CLA Z 601****Ligand CLA B 1216**



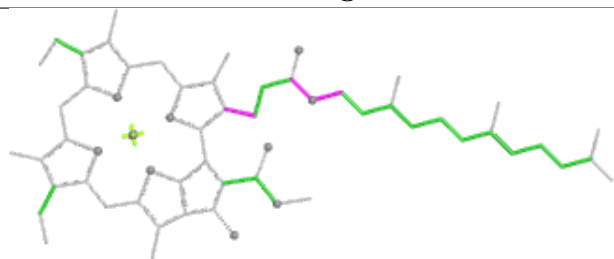
## Ligand CLA 3 604



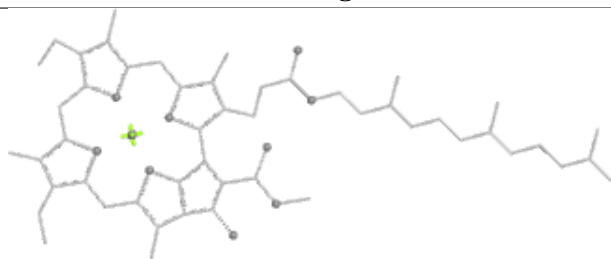
Bond lengths



Bond angles

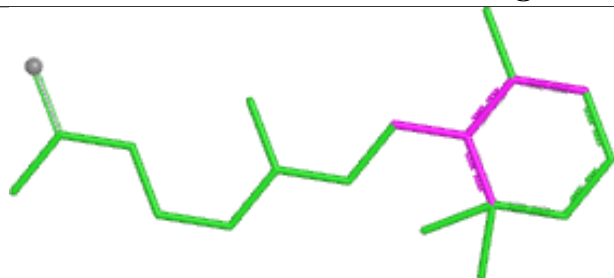


Torsions

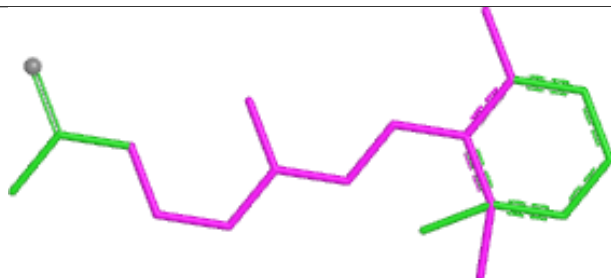


Rings

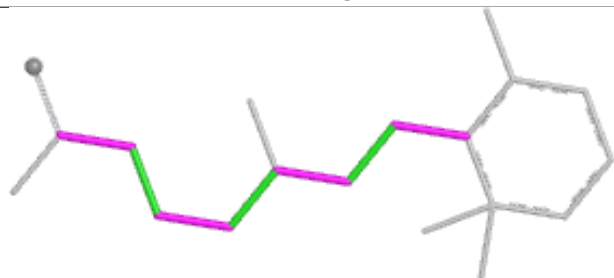
## Ligand QTB Z 504



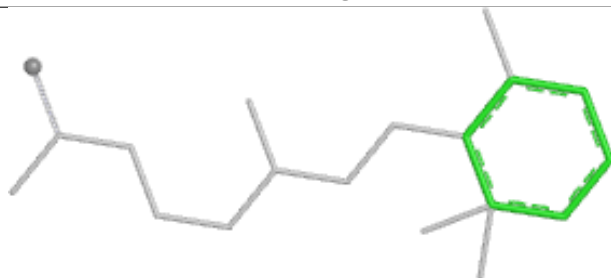
Bond lengths



Bond angles

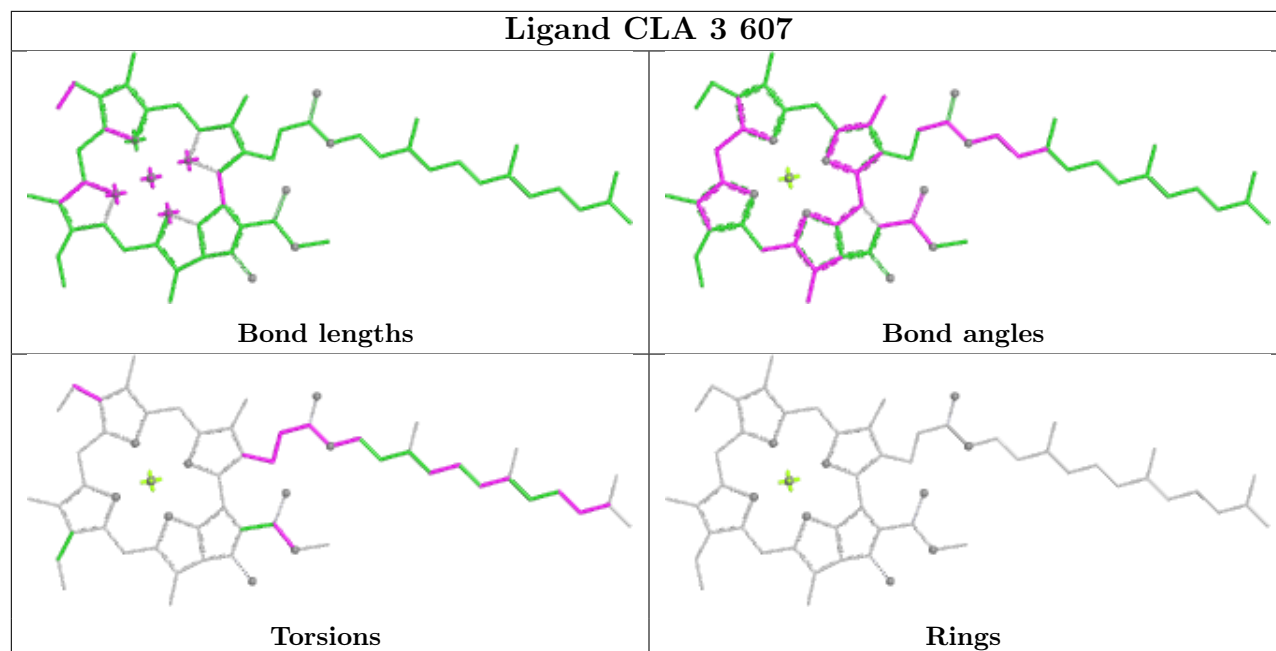


Torsions

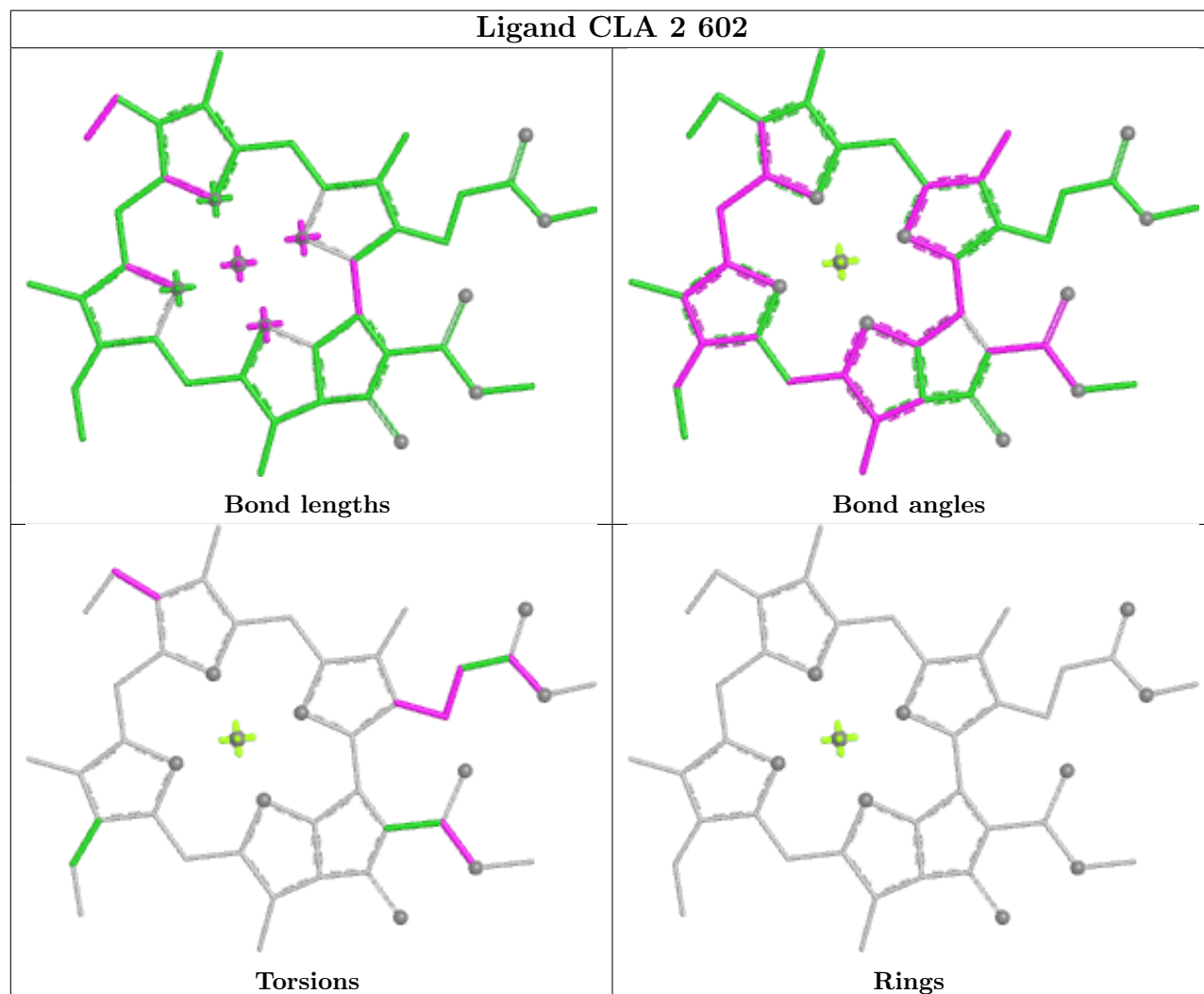


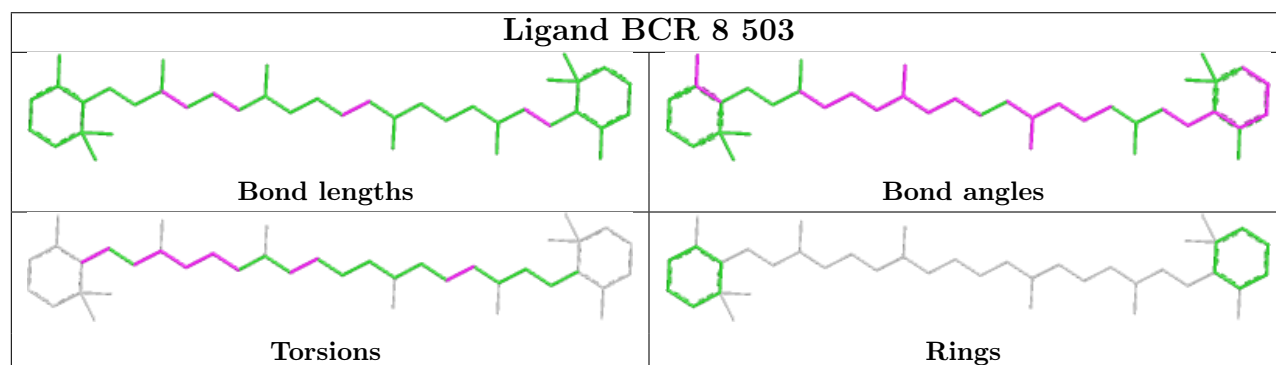
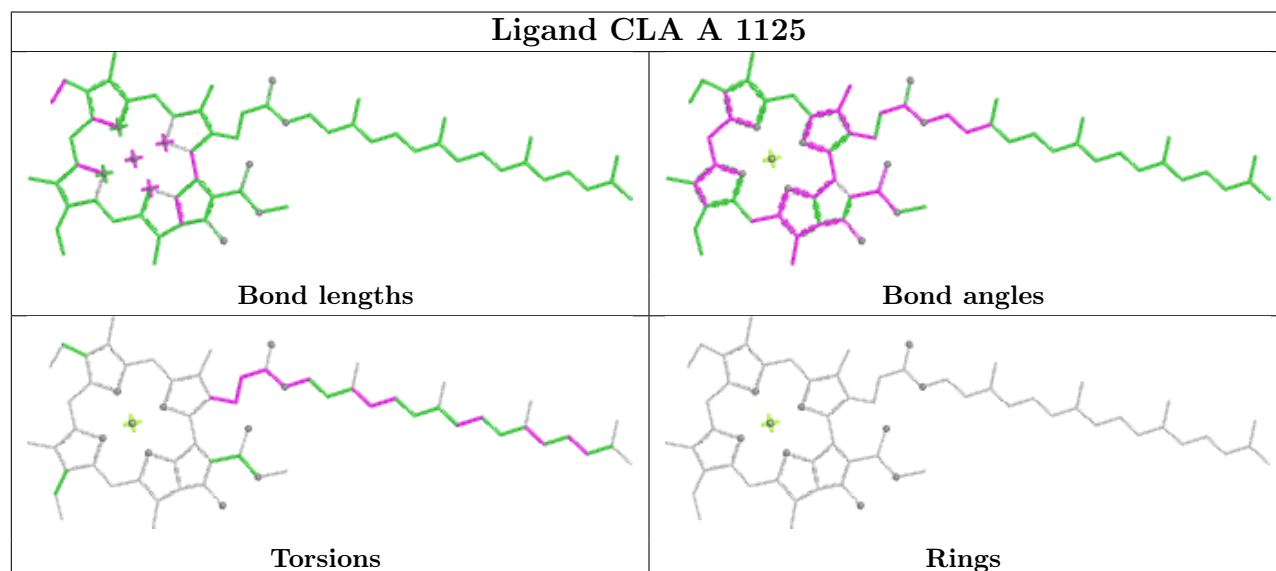
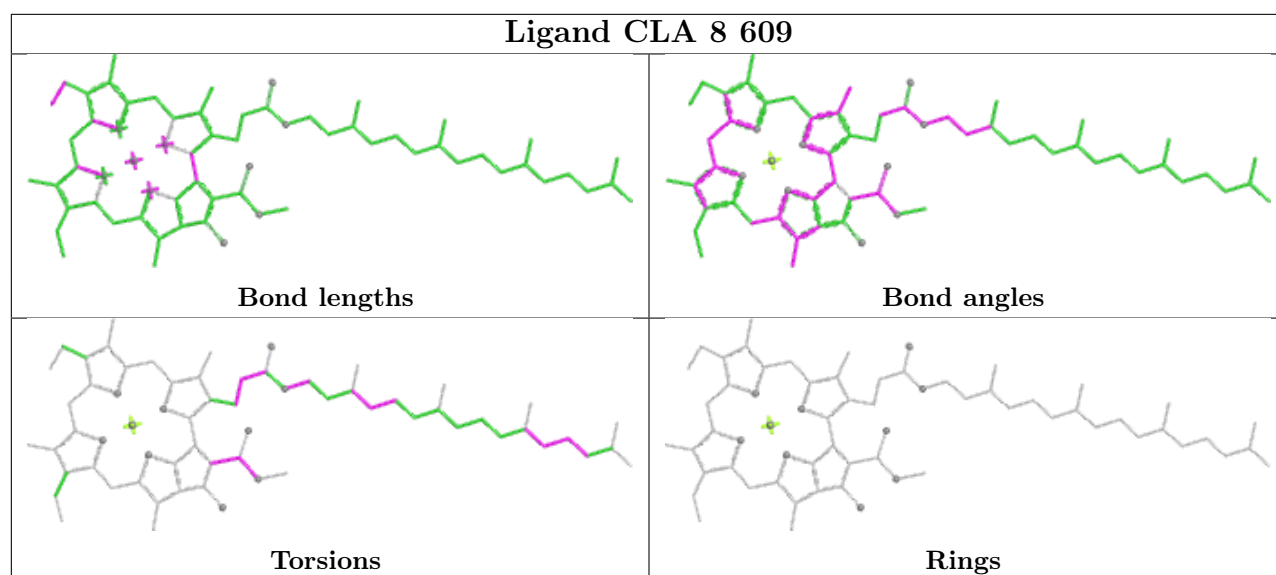
Rings

## Ligand CLA 3 607

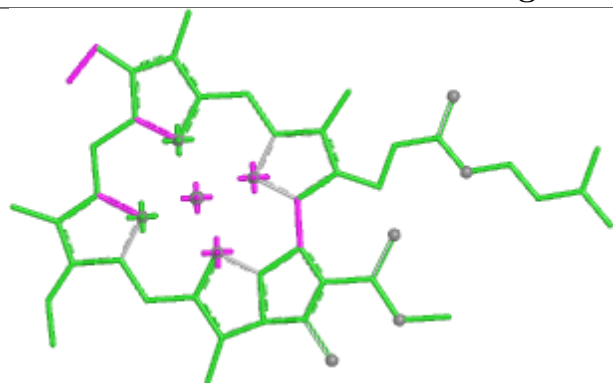


## Ligand CLA 2 602

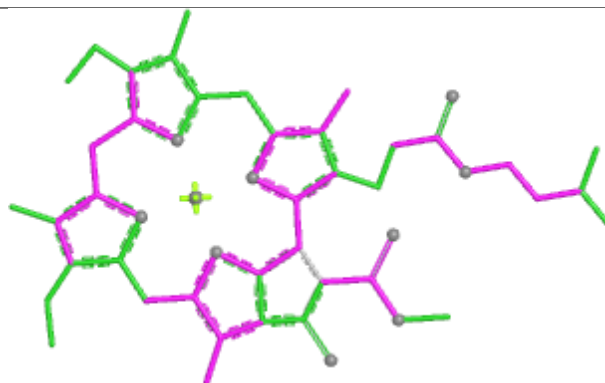




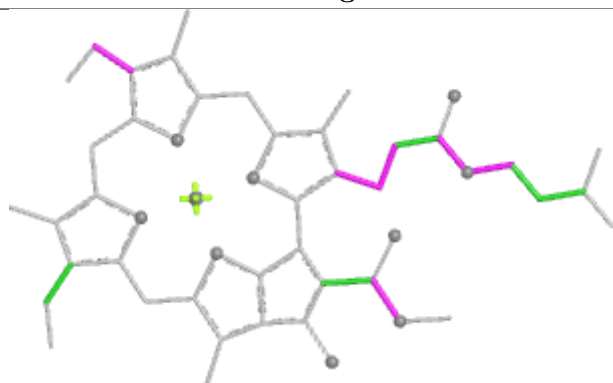
## Ligand CLA 5 615



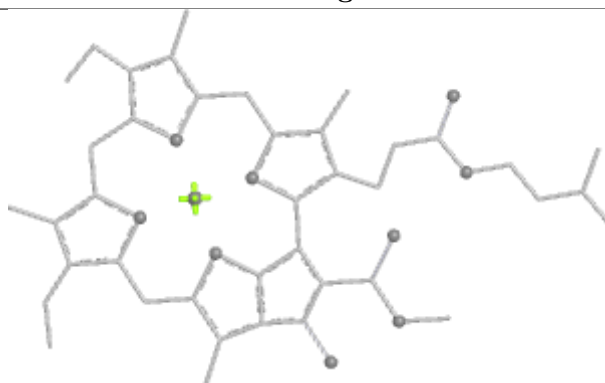
Bond lengths



Bond angles

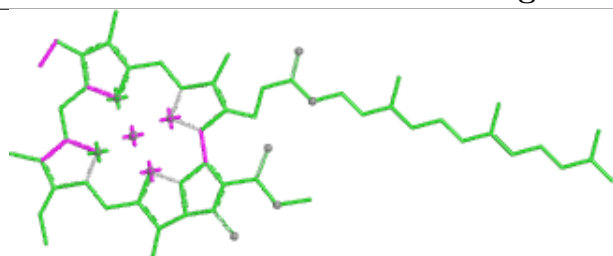


Torsions

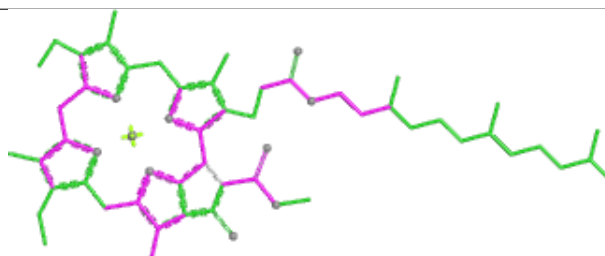


Rings

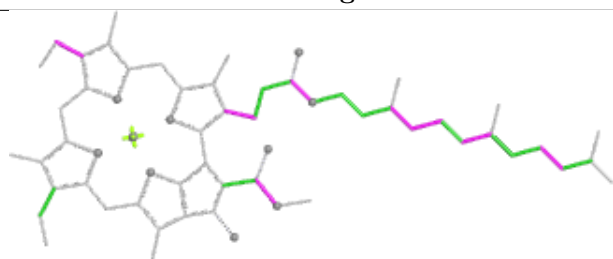
## Ligand CLA 5 601



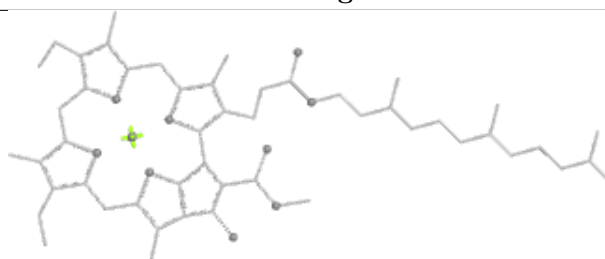
Bond lengths



Bond angles

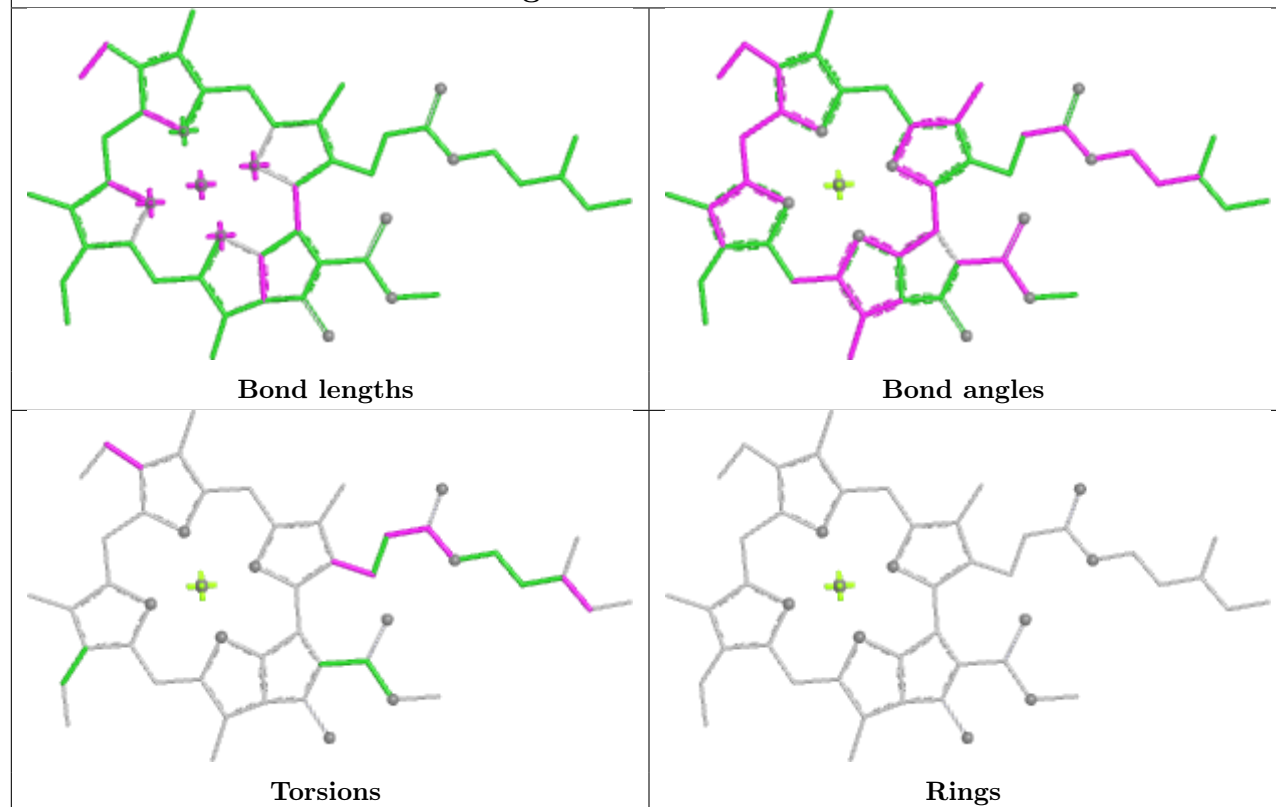


Torsions

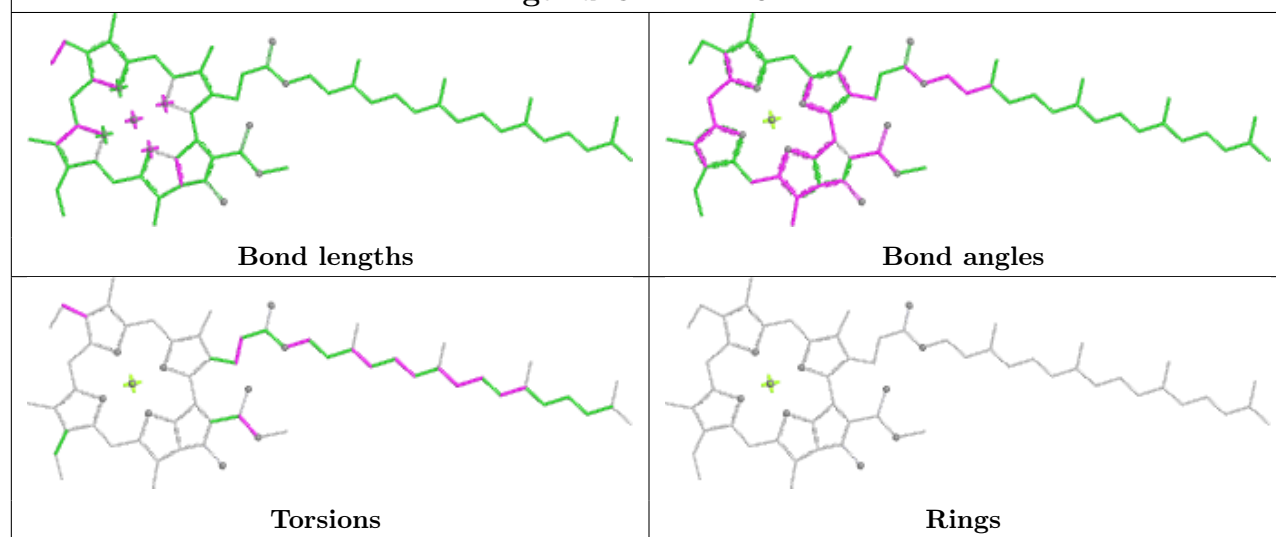


Rings

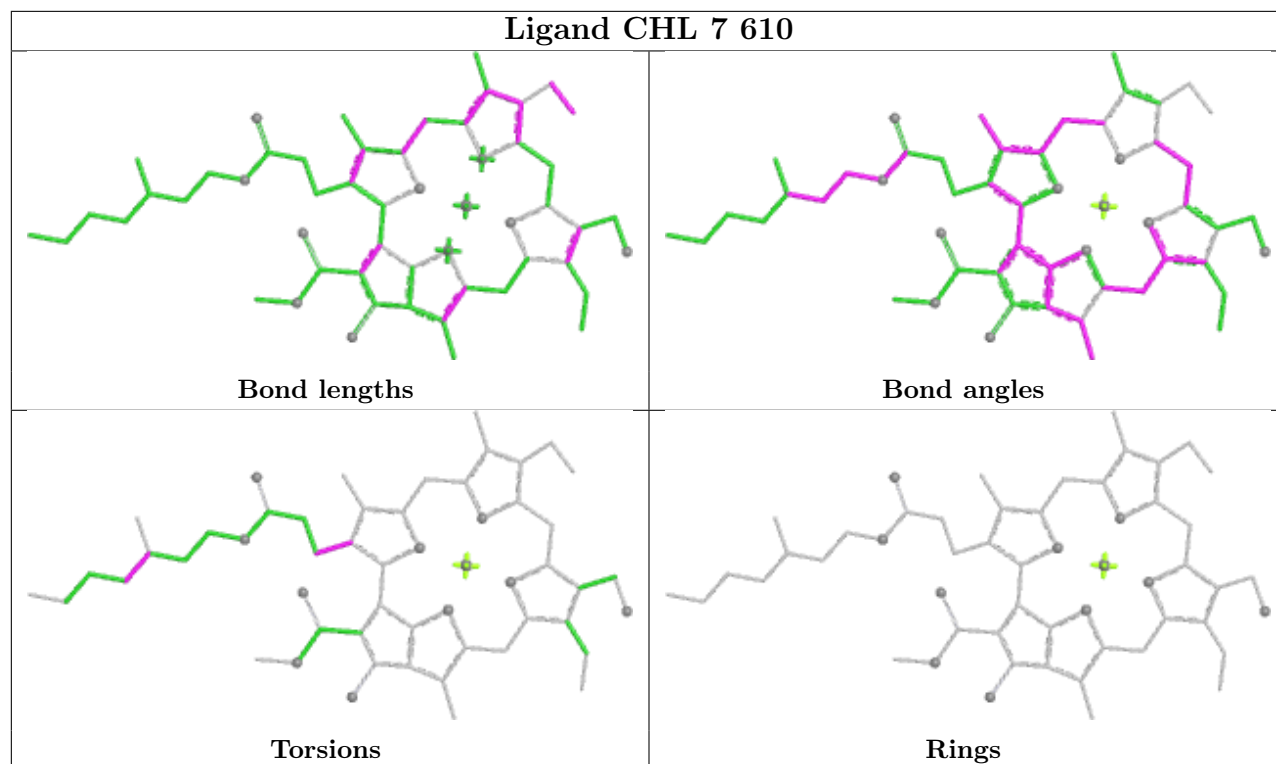
## Ligand CLA A 1135



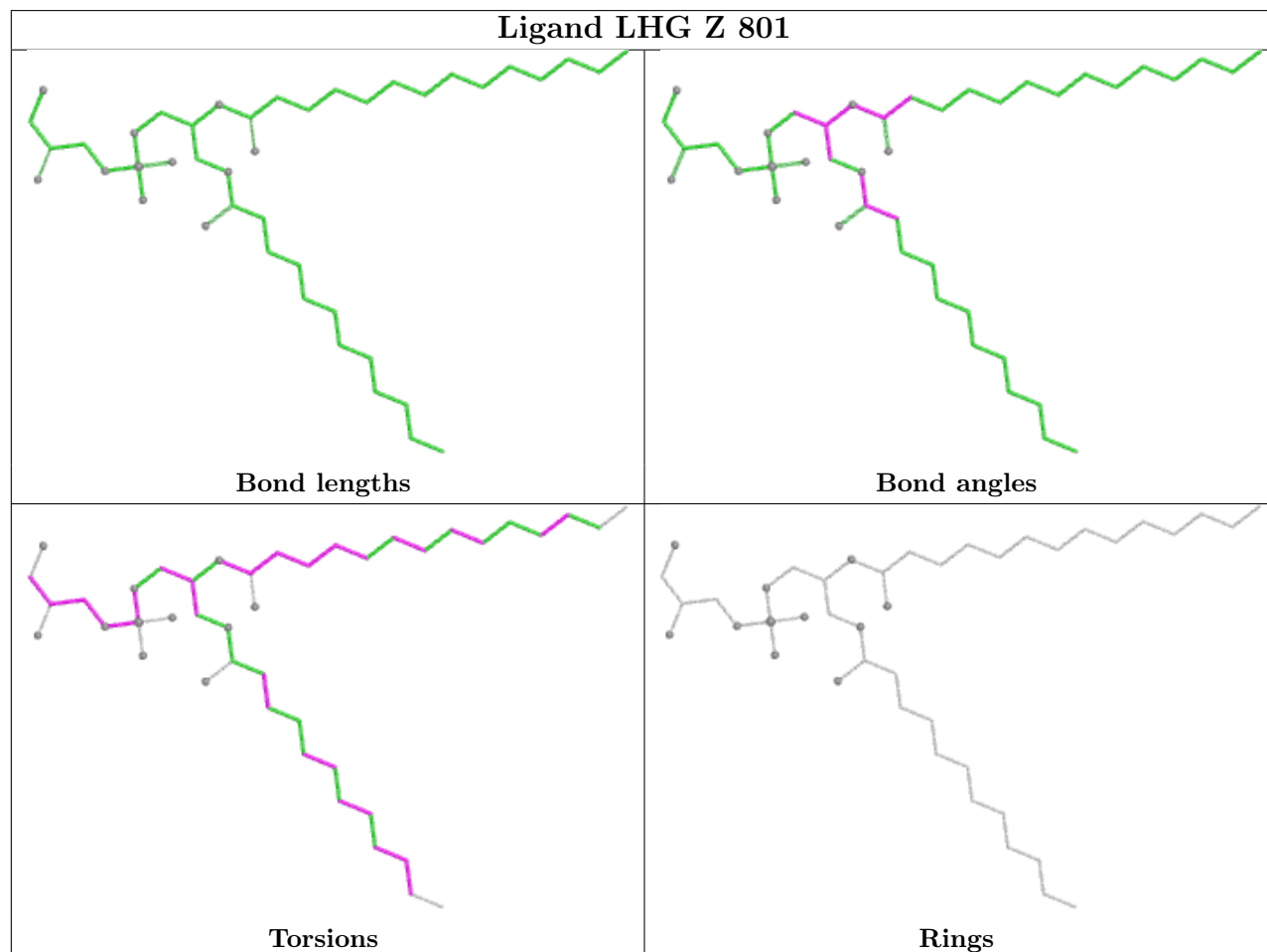
## Ligand CLA A 1012

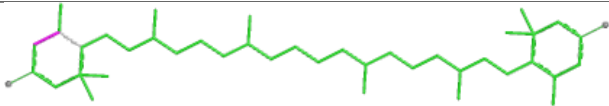
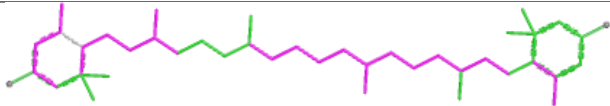
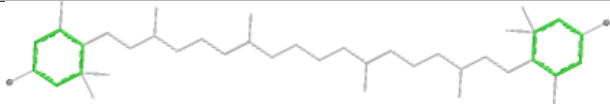


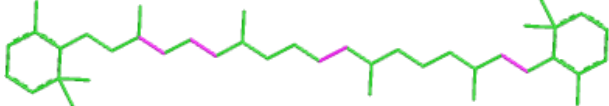
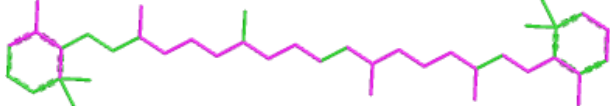
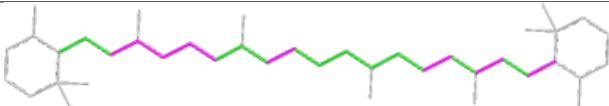
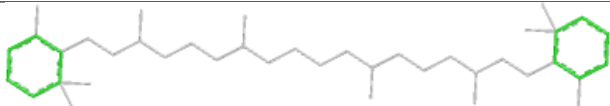
## Ligand CHL 7 610

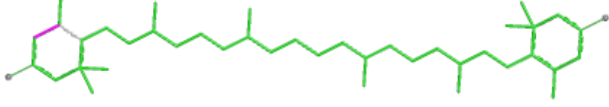
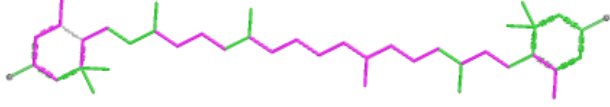
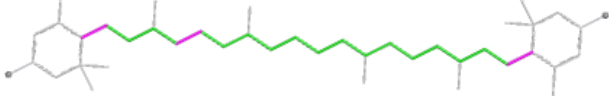
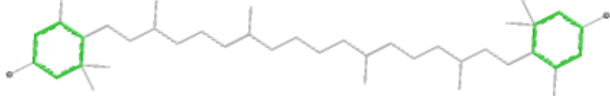


## Ligand LHG Z 801

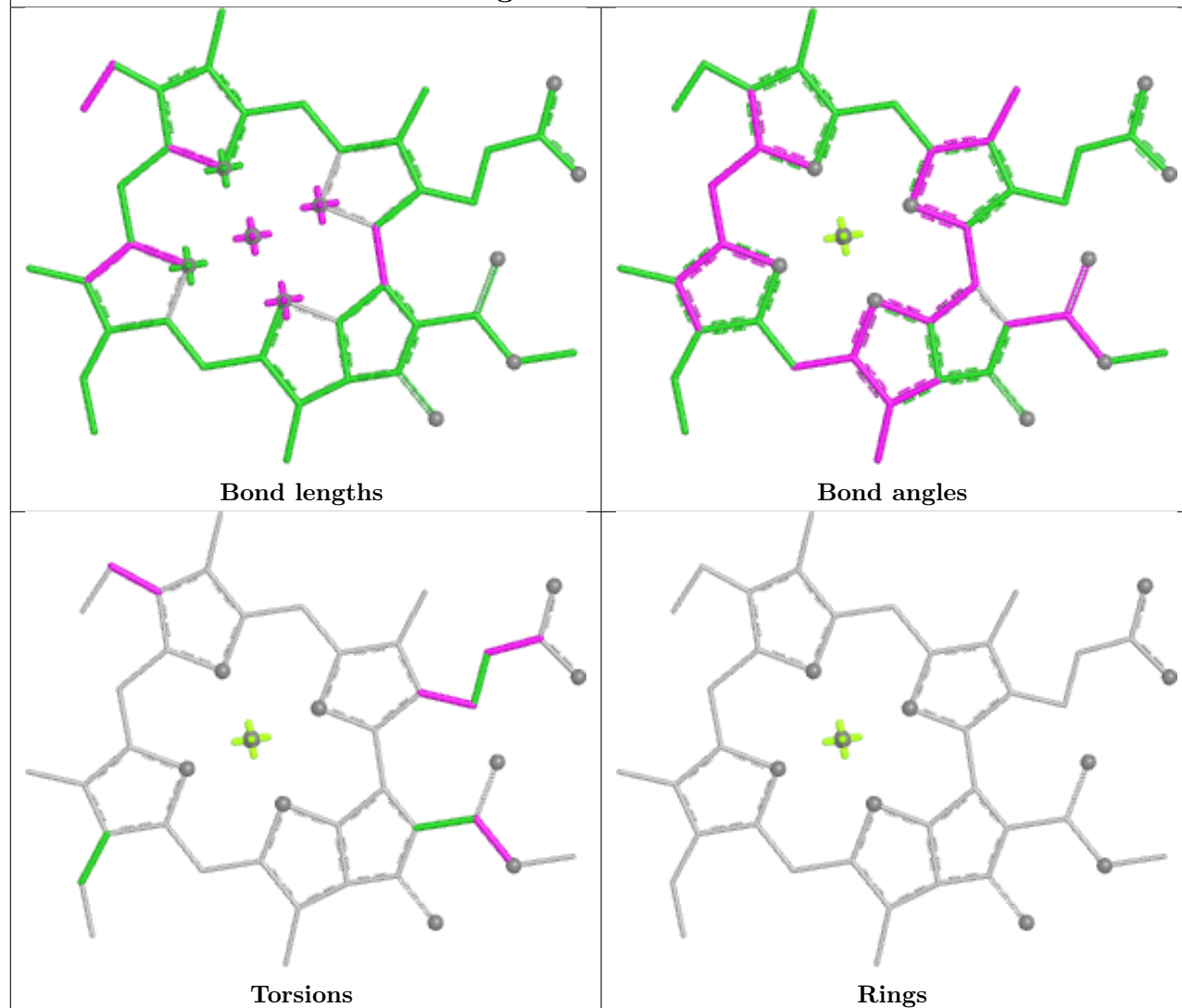


| Ligand LUT 6 501                                                                   |              |
|------------------------------------------------------------------------------------|--------------|
|   | Bond lengths |
|  | Bond angles  |
|   | Torsions     |
|  | Rings        |

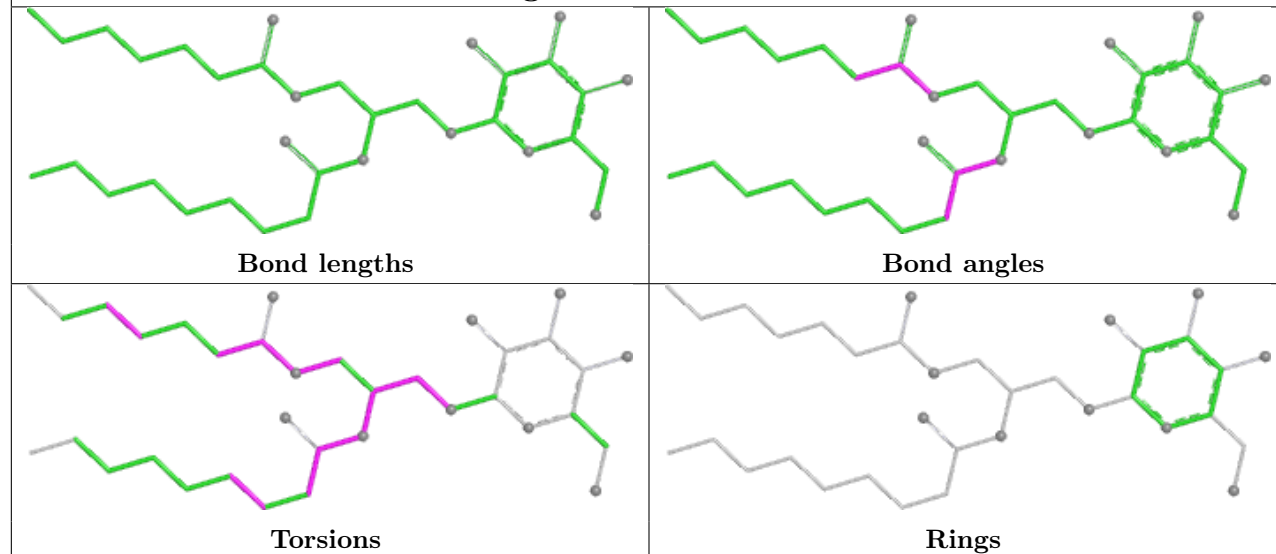
| Ligand BCR 7 504                                                                   |              |
|------------------------------------------------------------------------------------|--------------|
|   | Bond lengths |
|  | Bond angles  |
|   | Torsions     |
|  | Rings        |

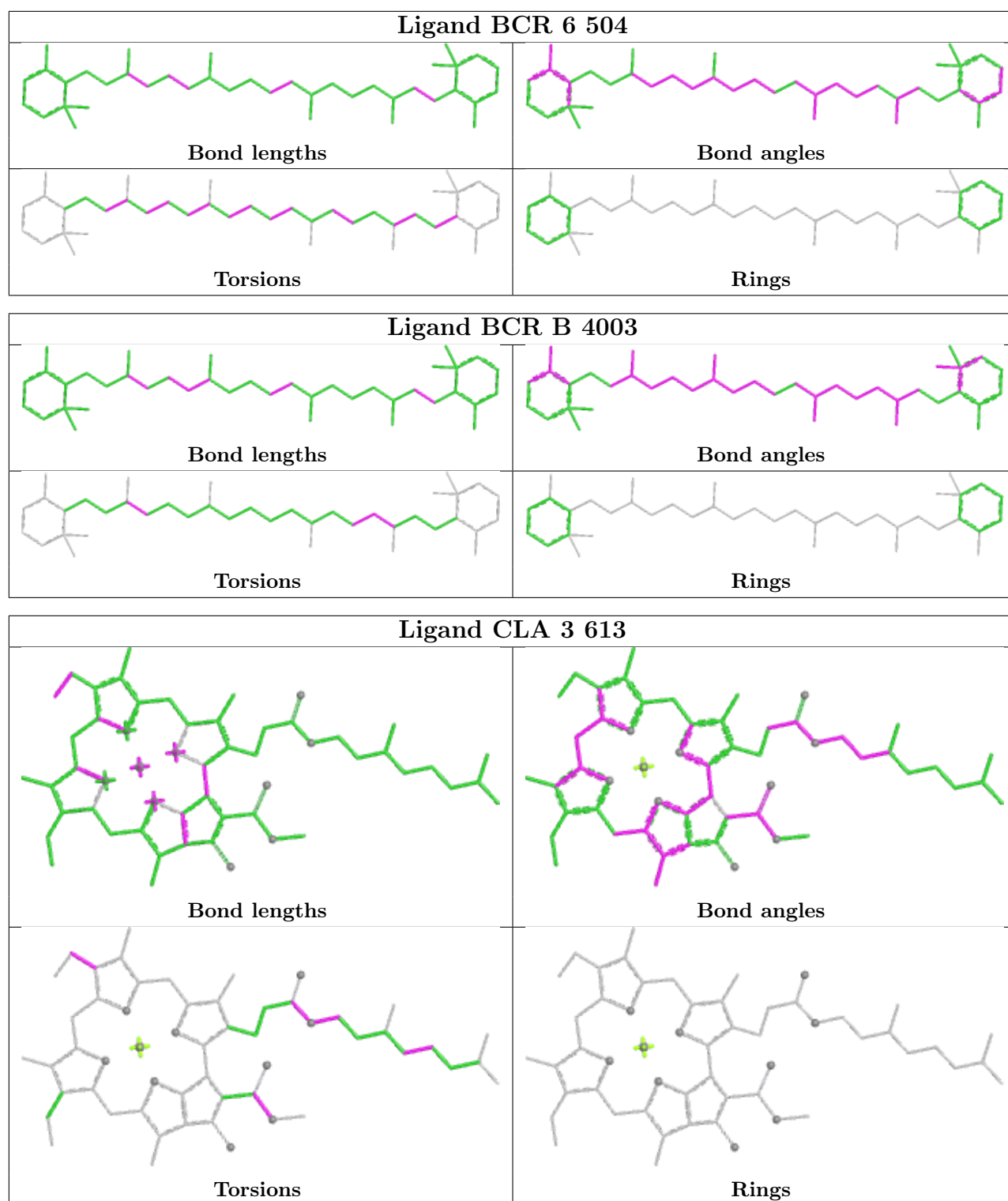
| Ligand LUT 7 501                                                                     |              |
|--------------------------------------------------------------------------------------|--------------|
|    | Bond lengths |
|   | Bond angles  |
|   | Torsions     |
|  | Rings        |

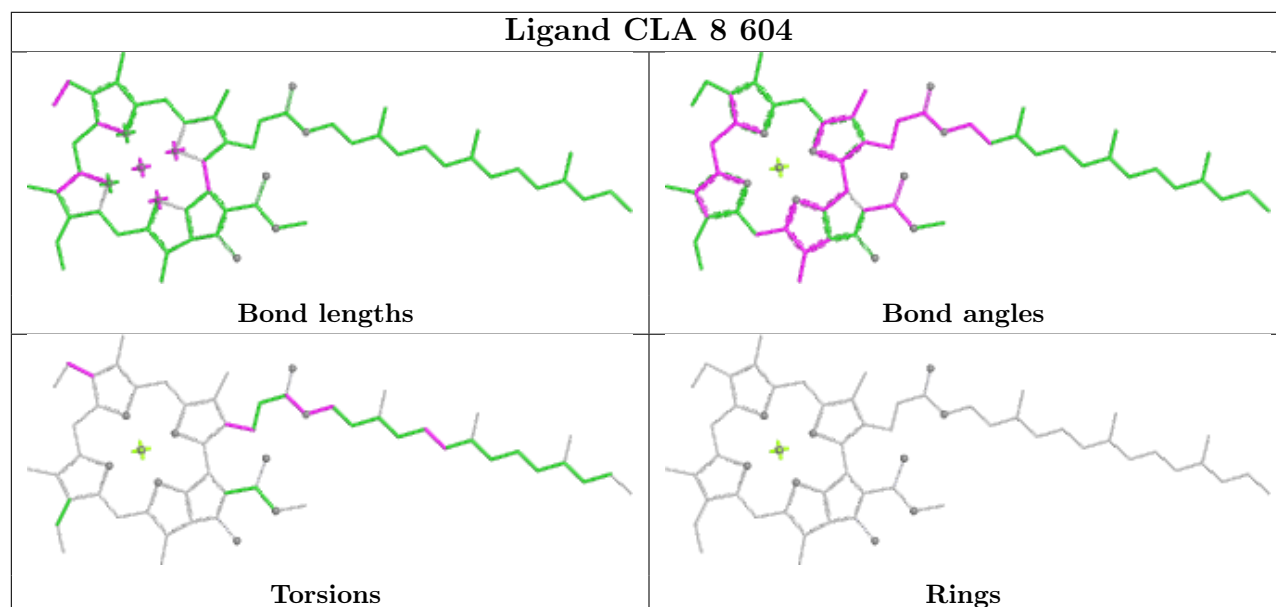
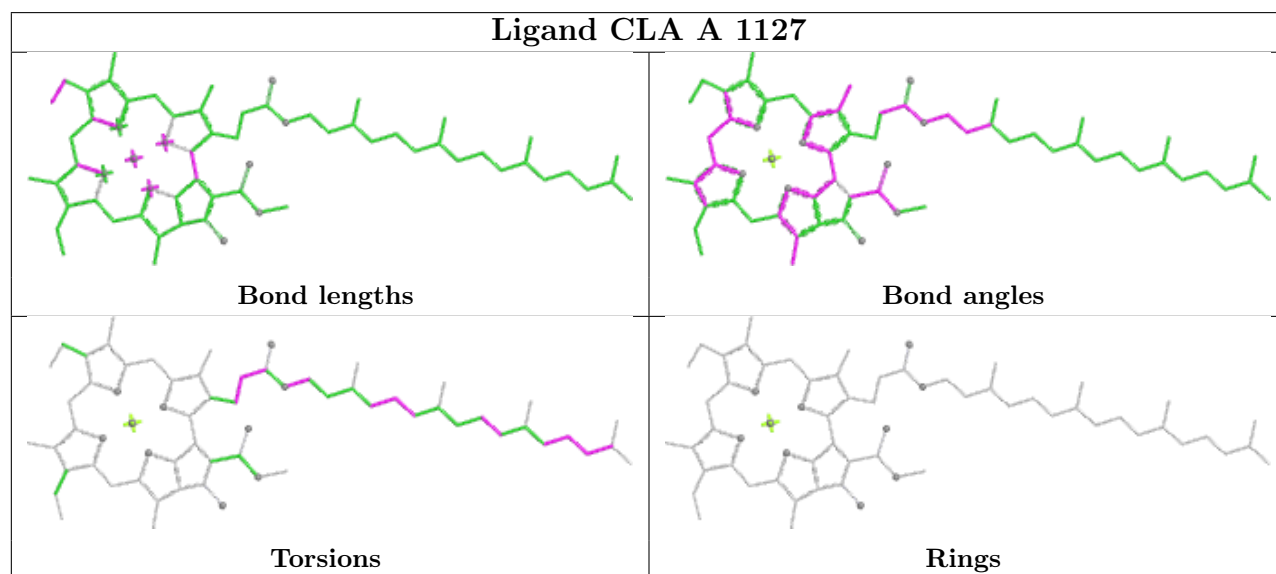
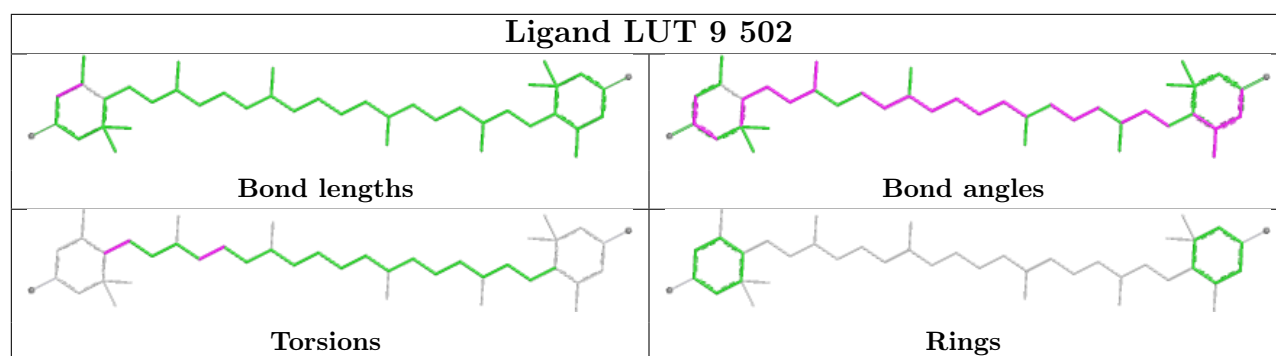
## Ligand CLA 3 608



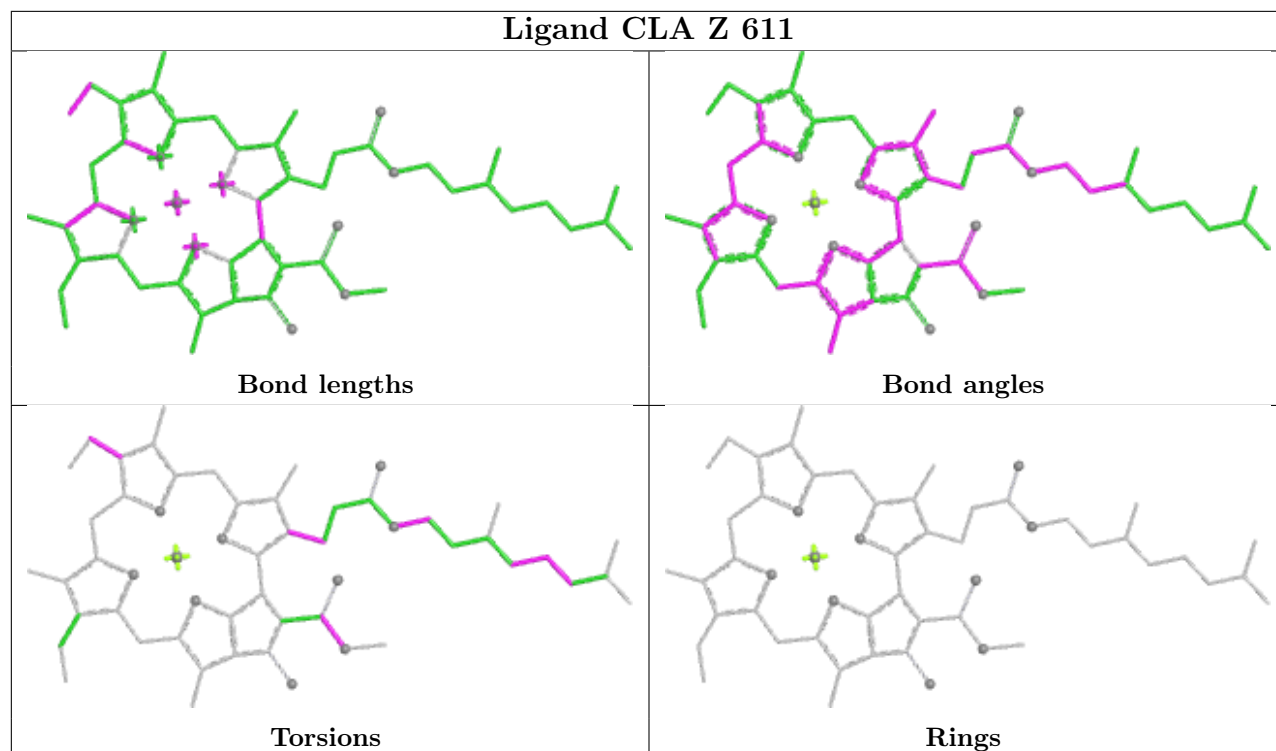
## Ligand LMG J 5001



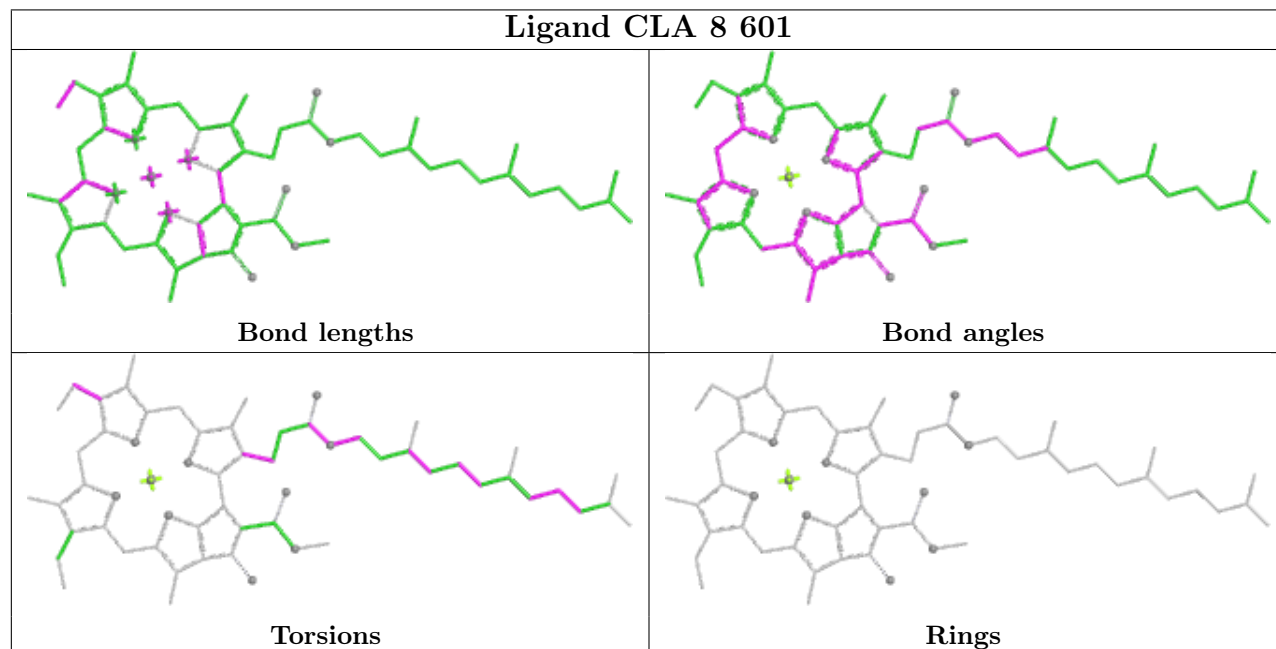


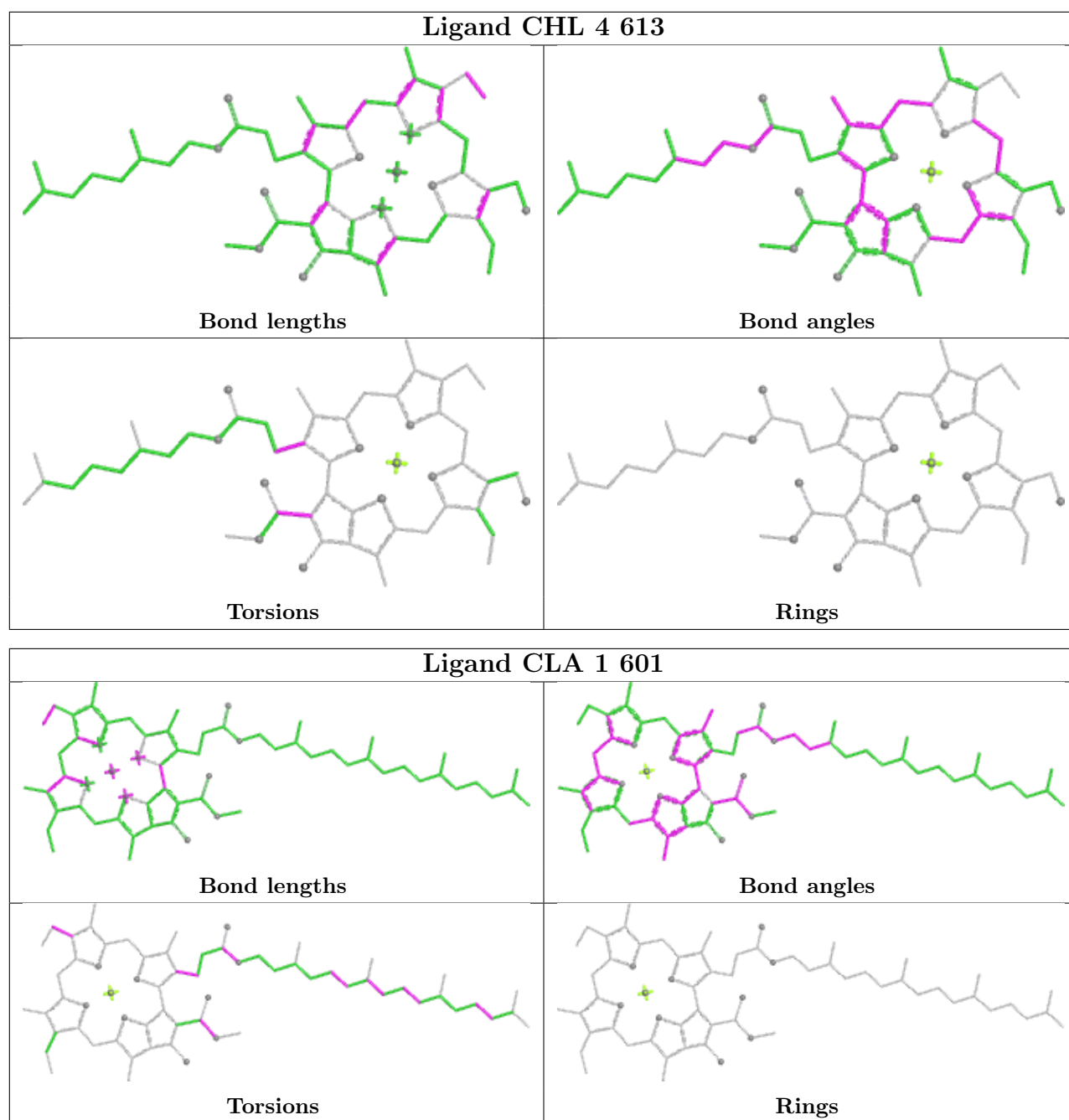


## Ligand CLA Z 611

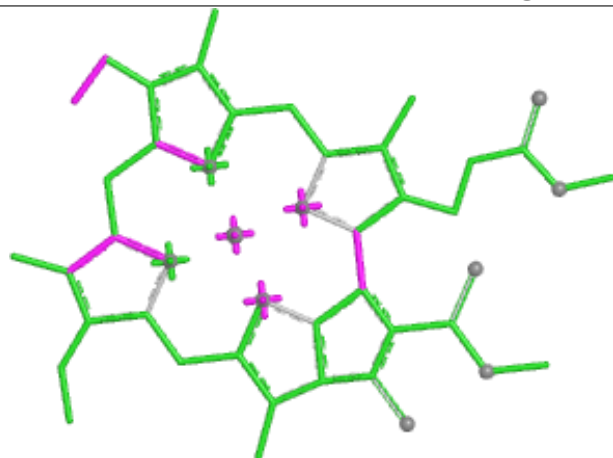


## Ligand CLA 8 601

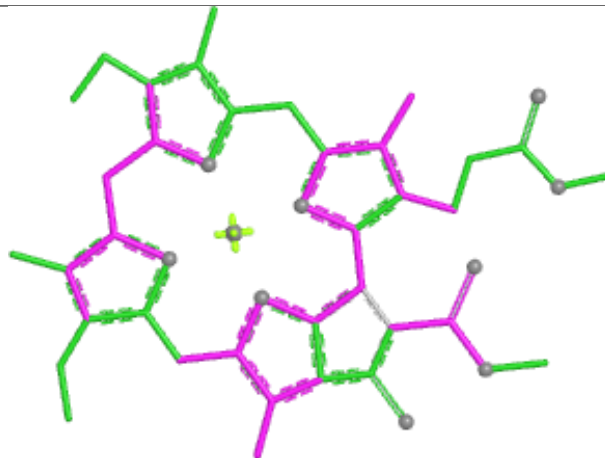




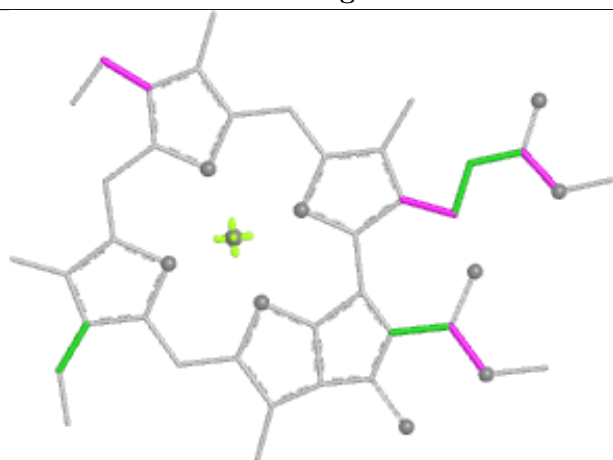
## Ligand CLA 9 609



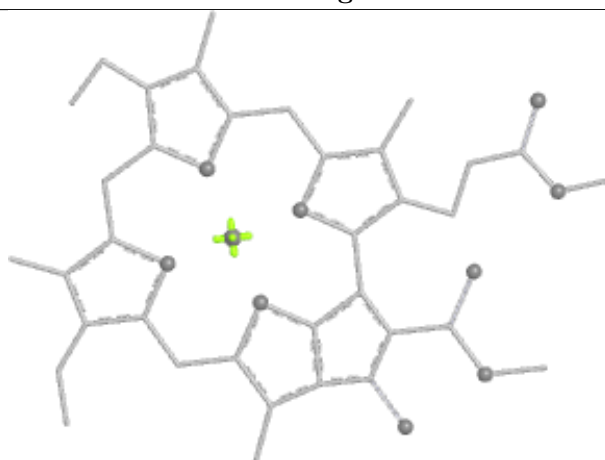
Bond lengths



Bond angles

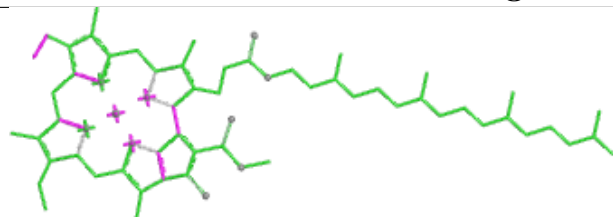


Torsions

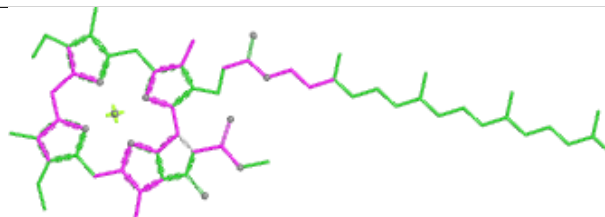


Rings

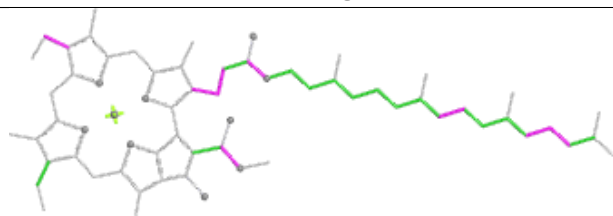
## Ligand CLA B 1239



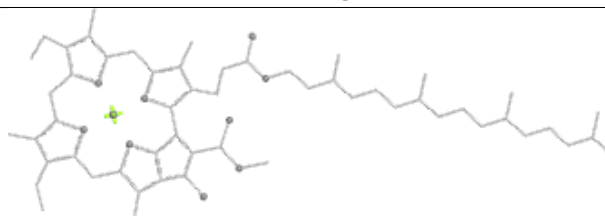
Bond lengths



Bond angles

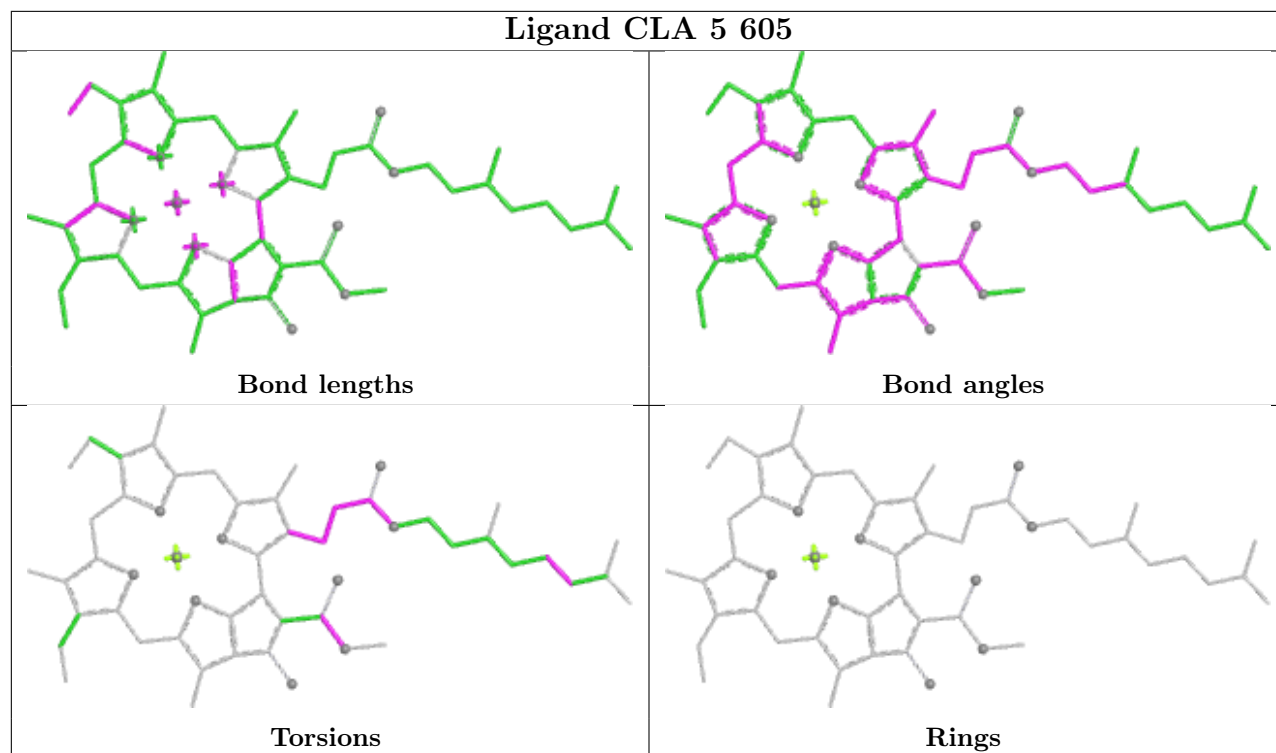


Torsions

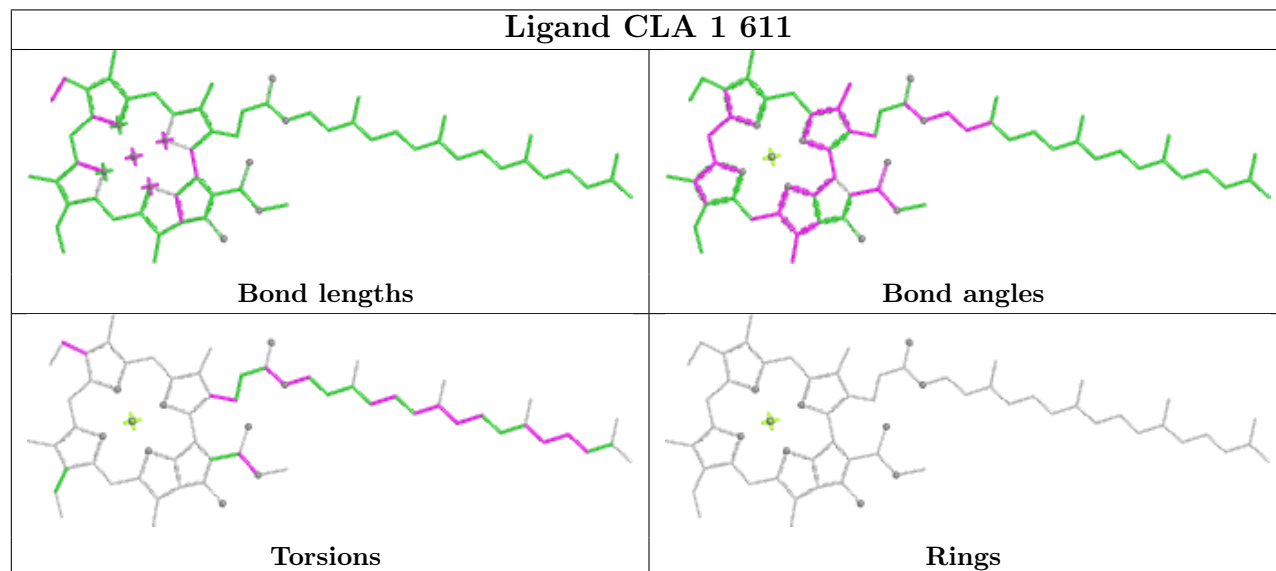


Rings

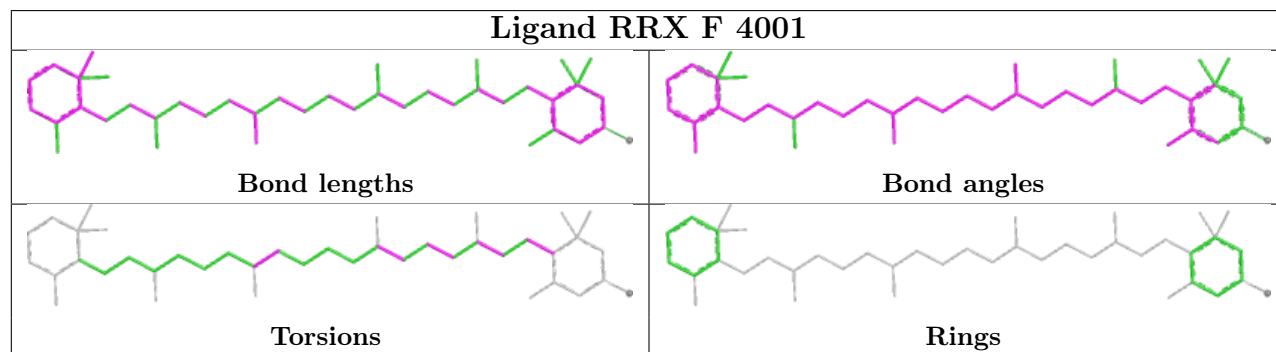
## Ligand CLA 5 605



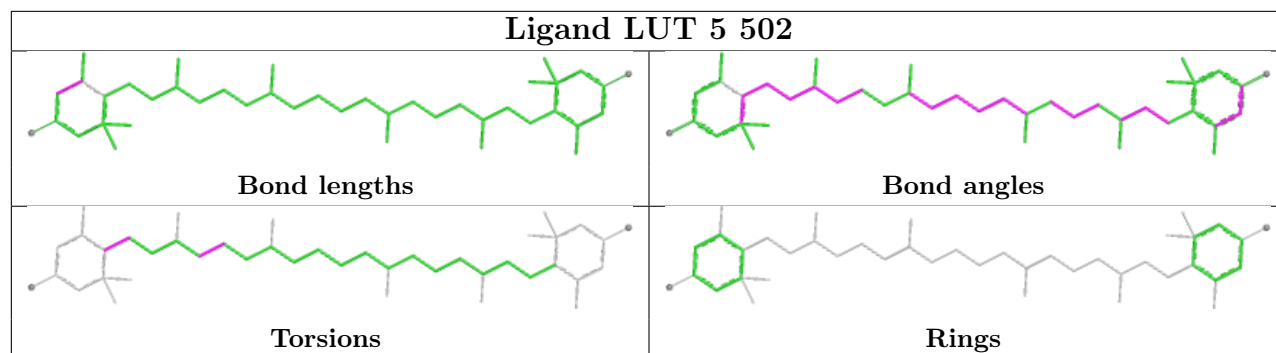
## Ligand CLA 1 611



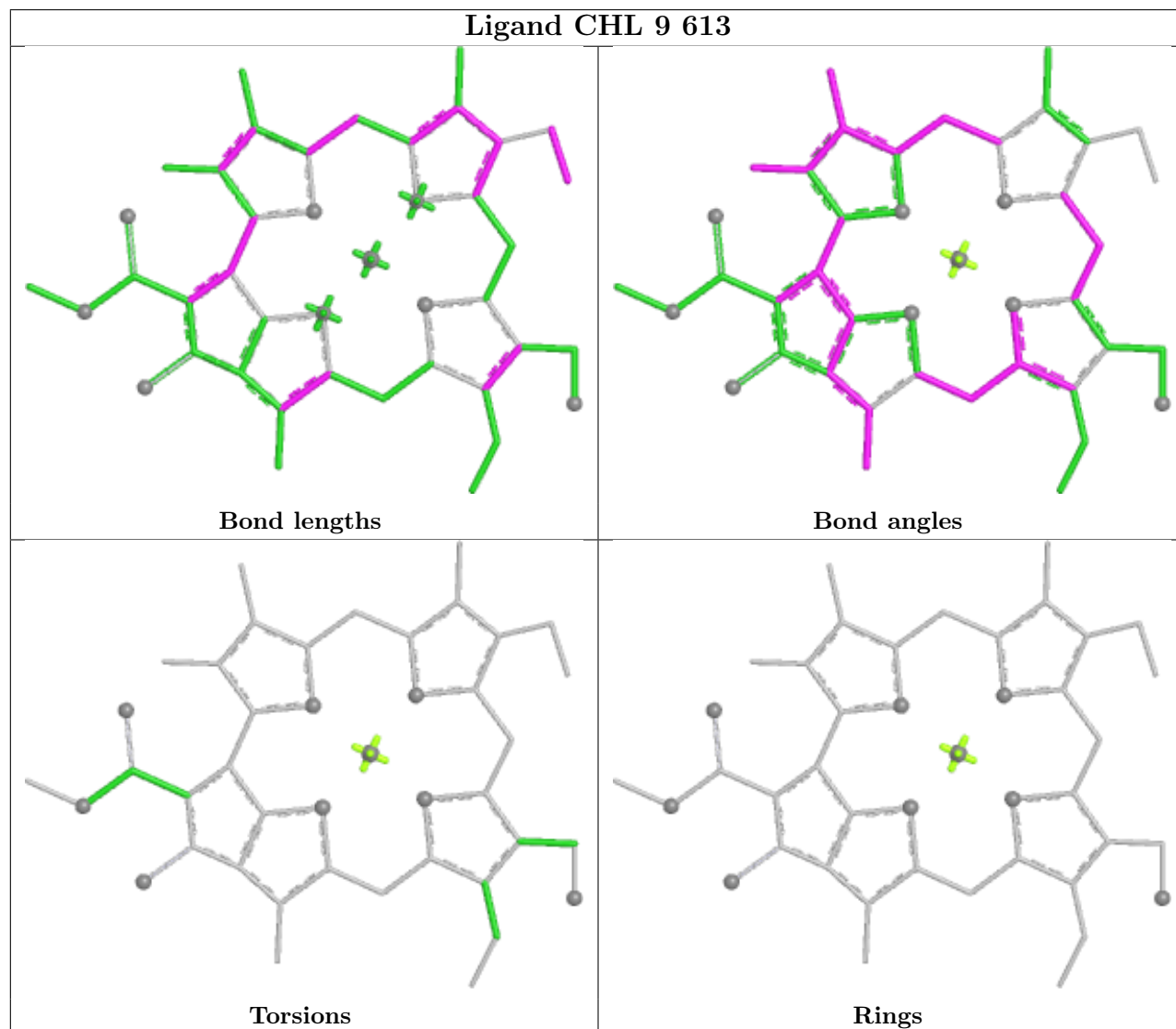
## Ligand RRX F 4001

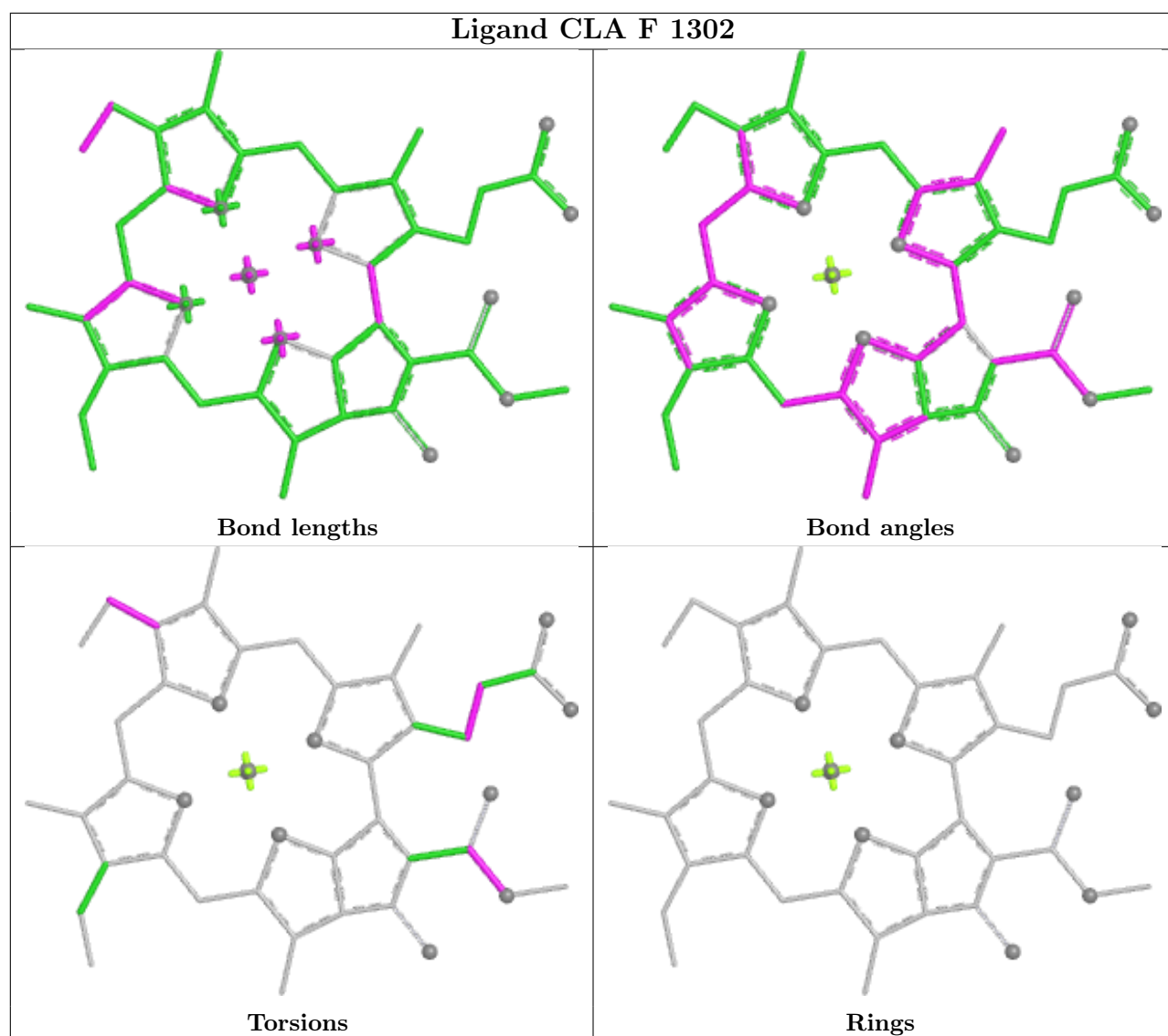


## Ligand LUT 5 502

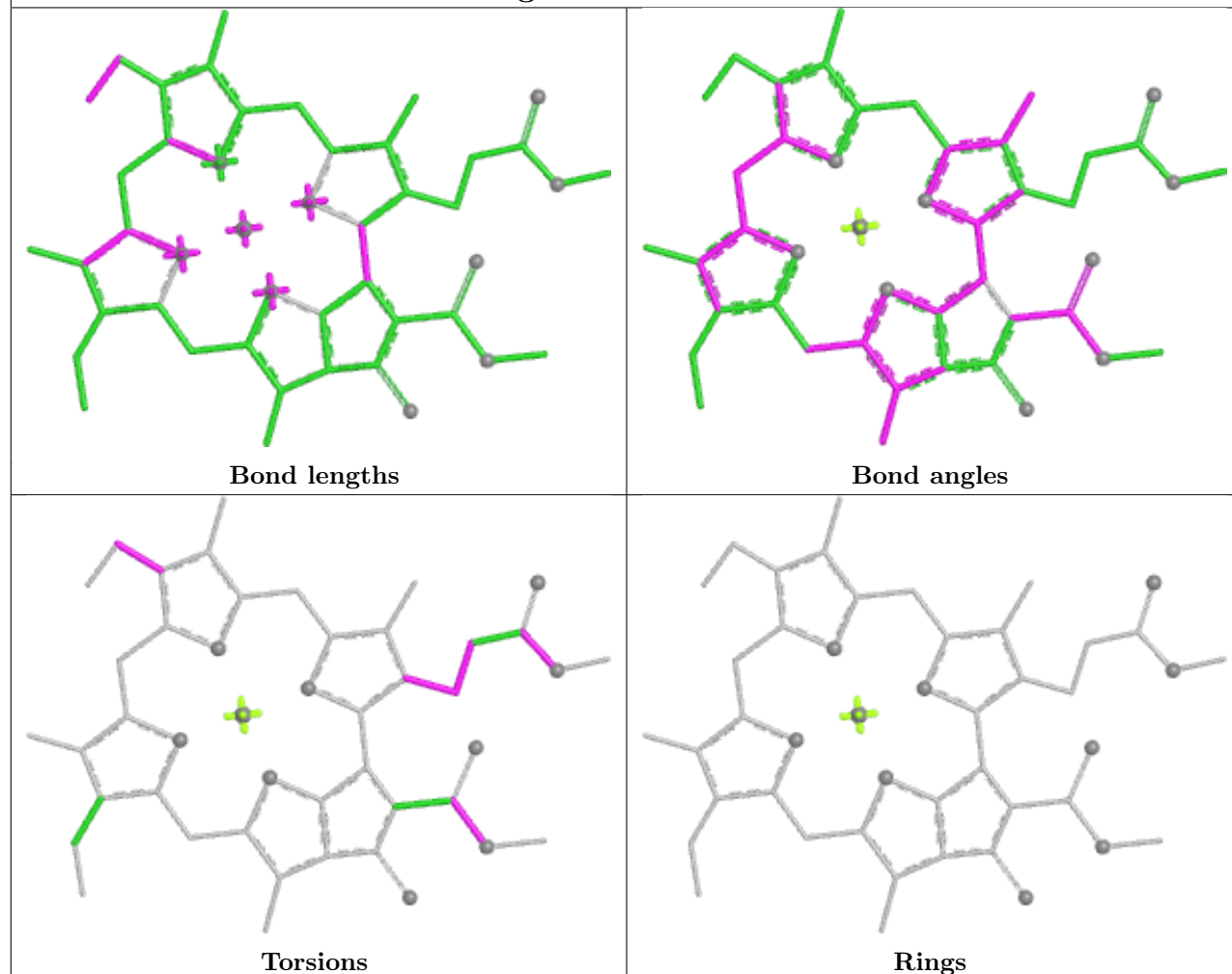


## Ligand CHL 9 613

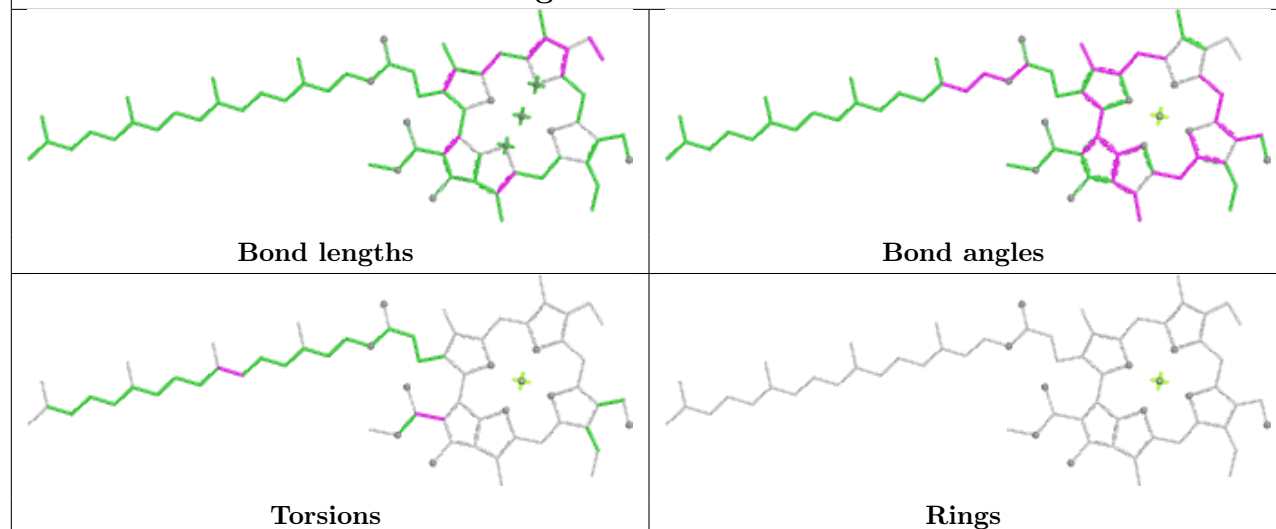




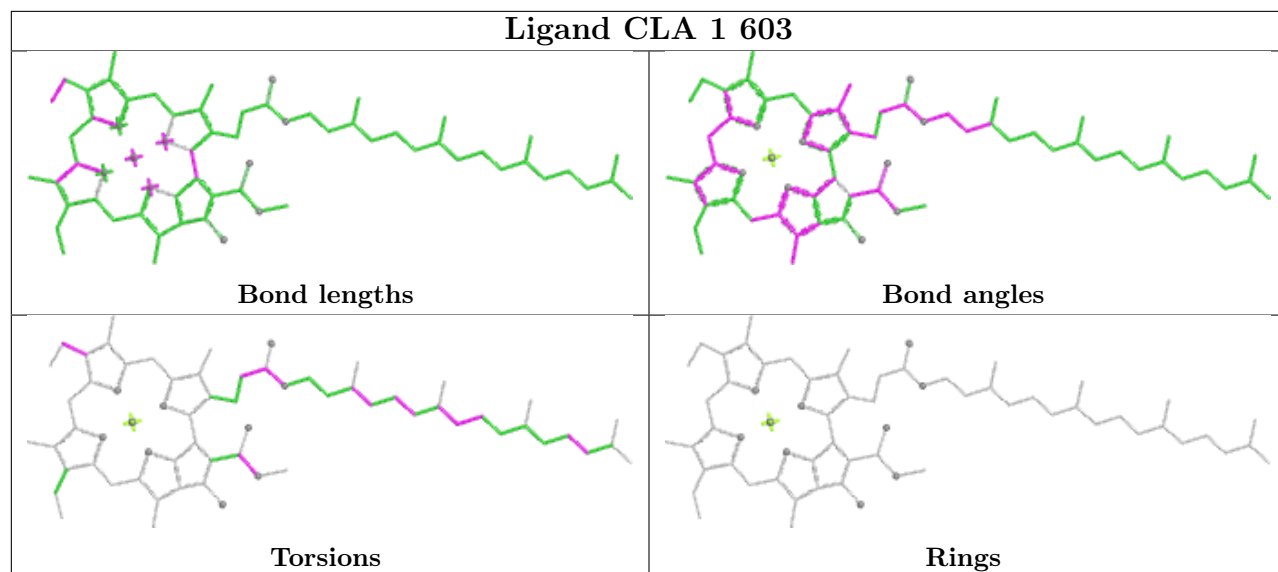
## Ligand CLA 3 618



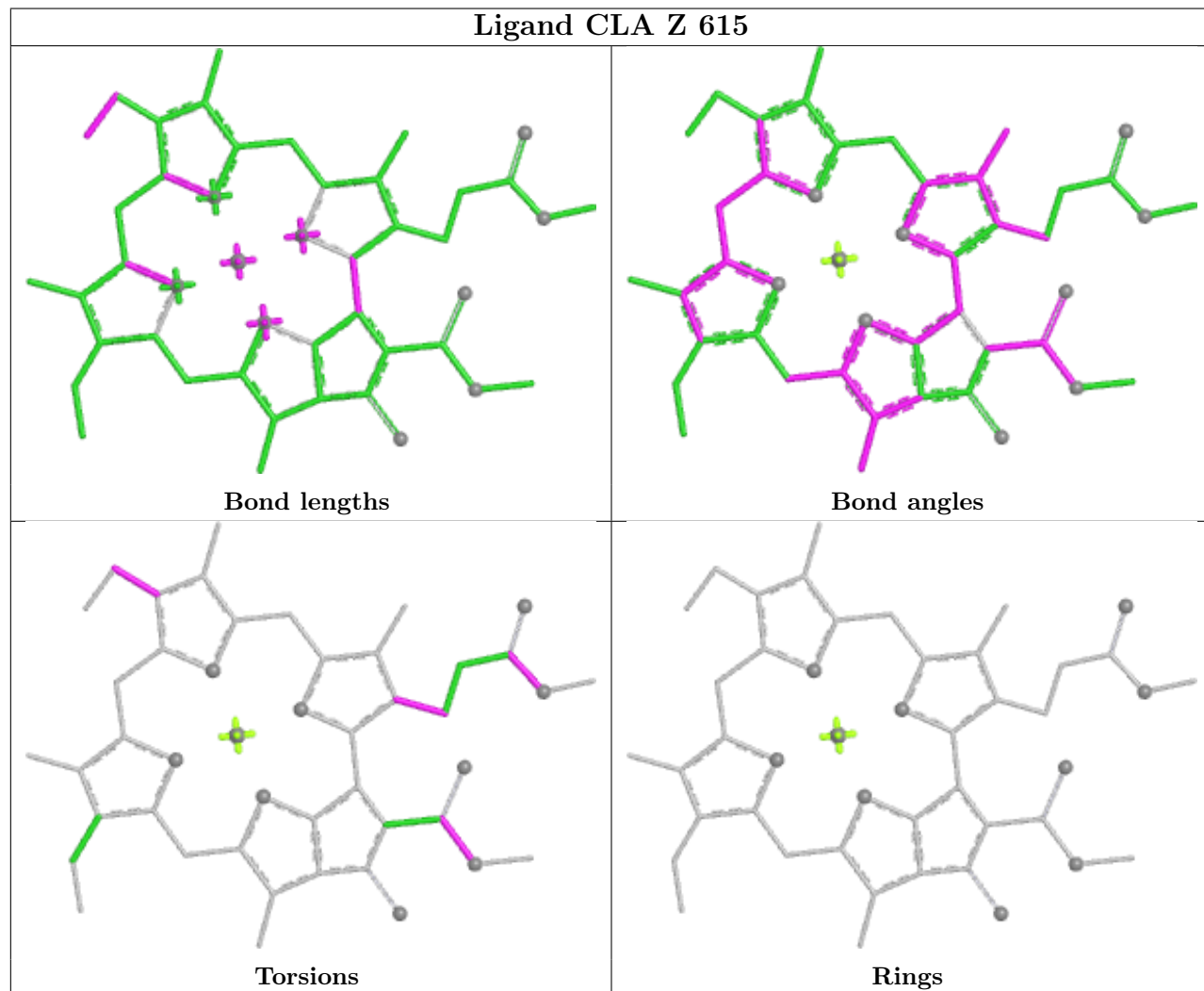
## Ligand CHL 3 611

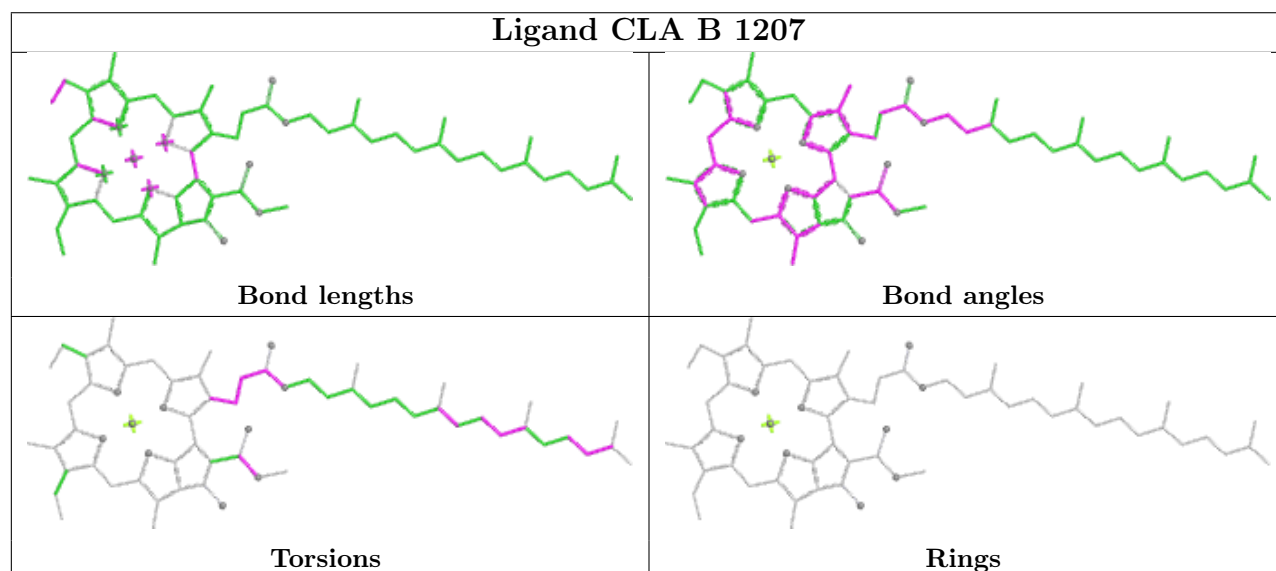
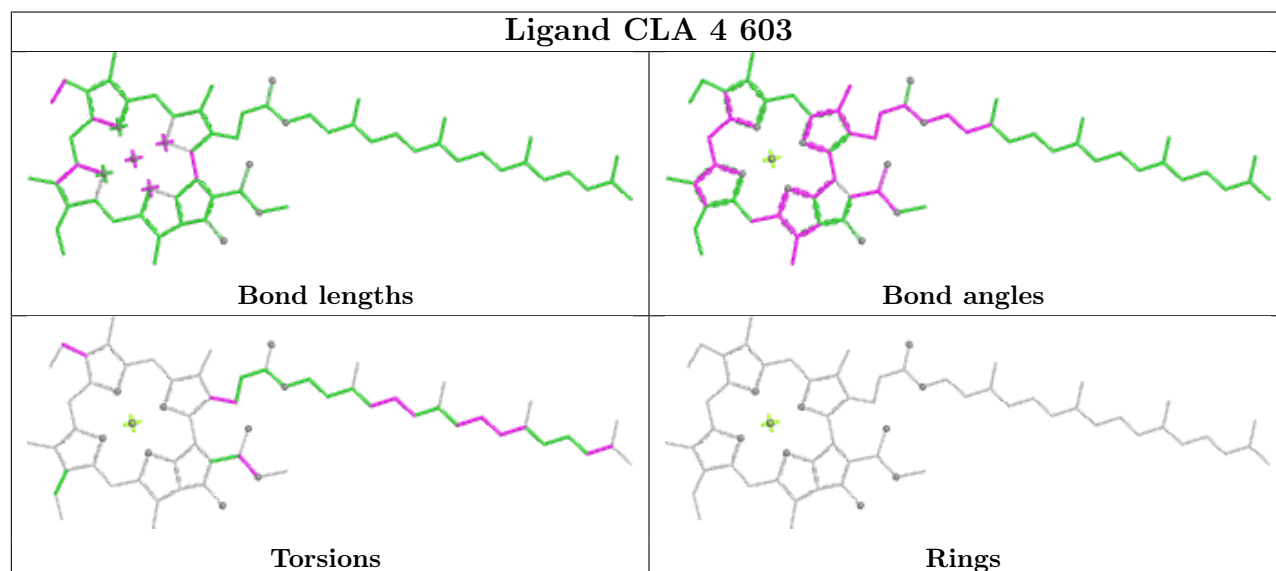
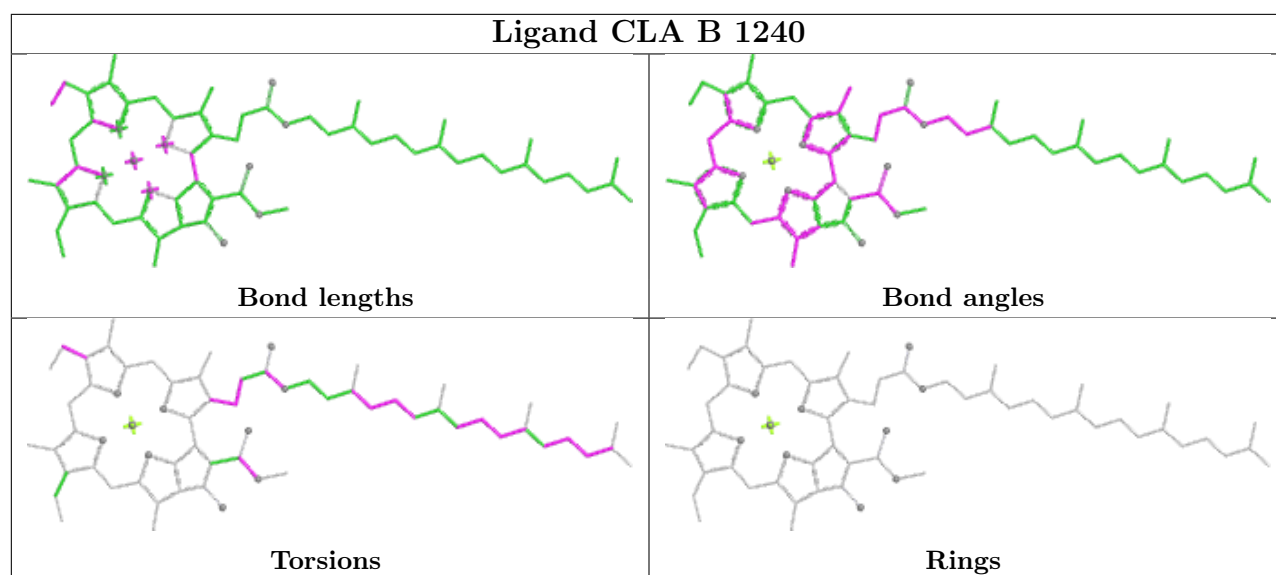


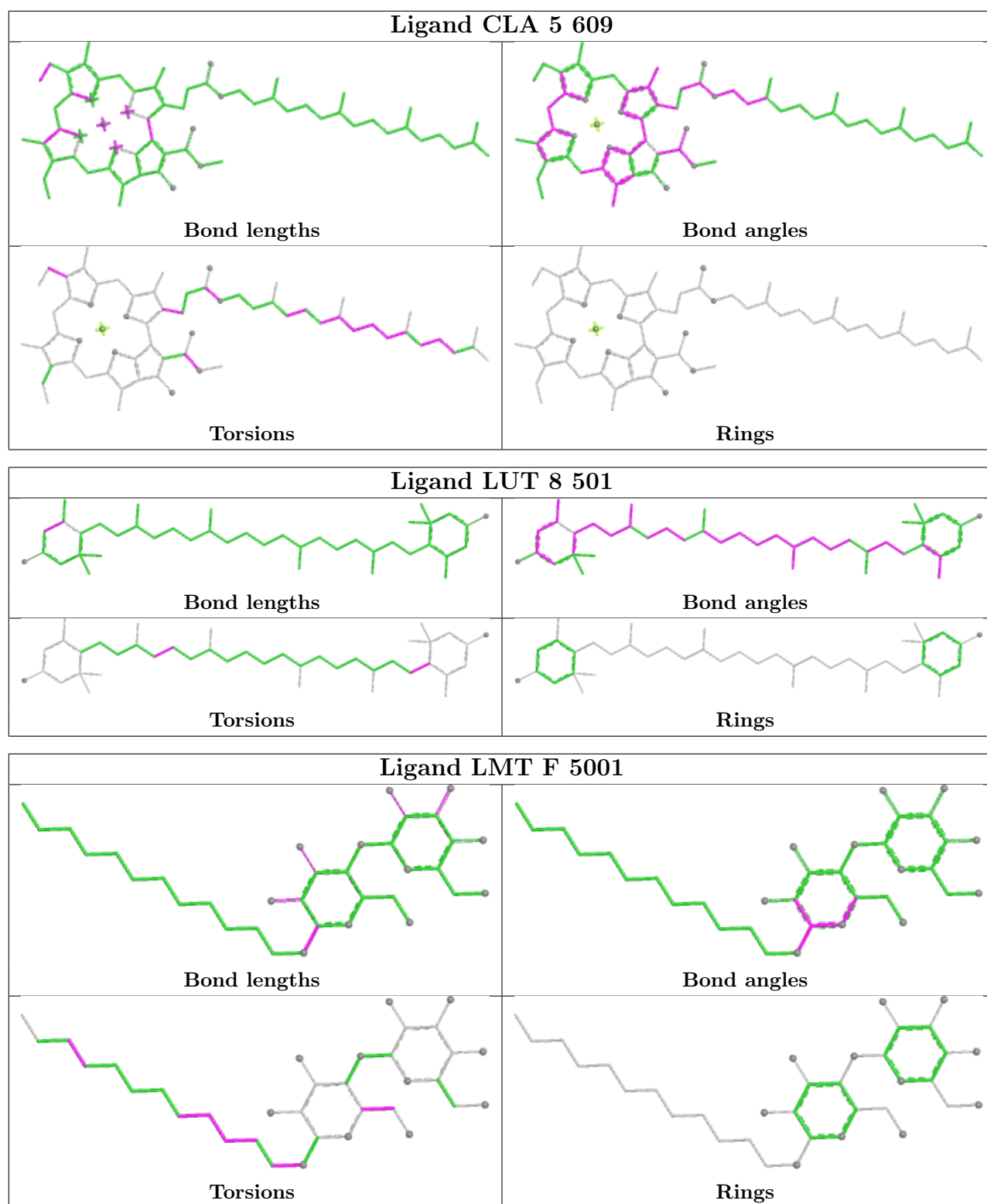
## Ligand CLA 1 603

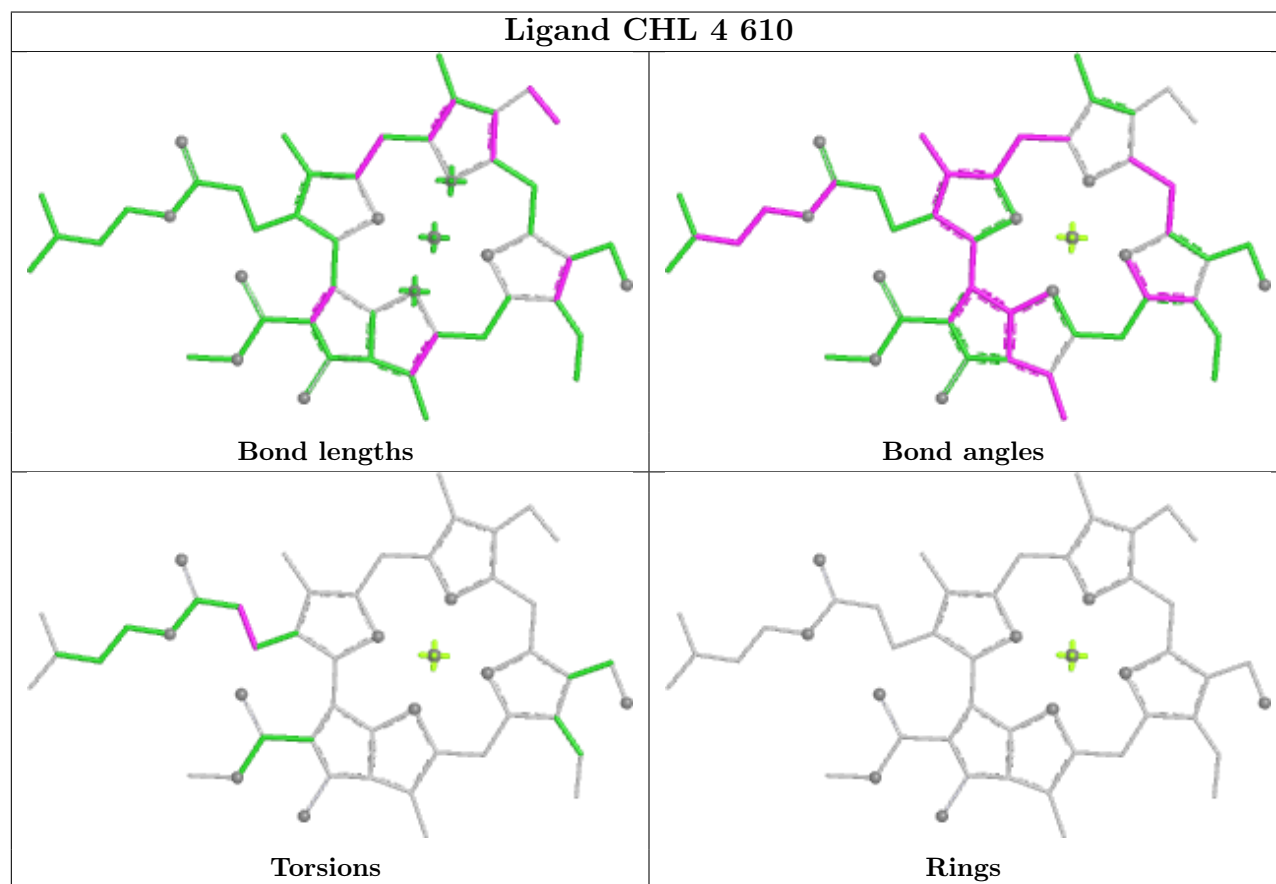
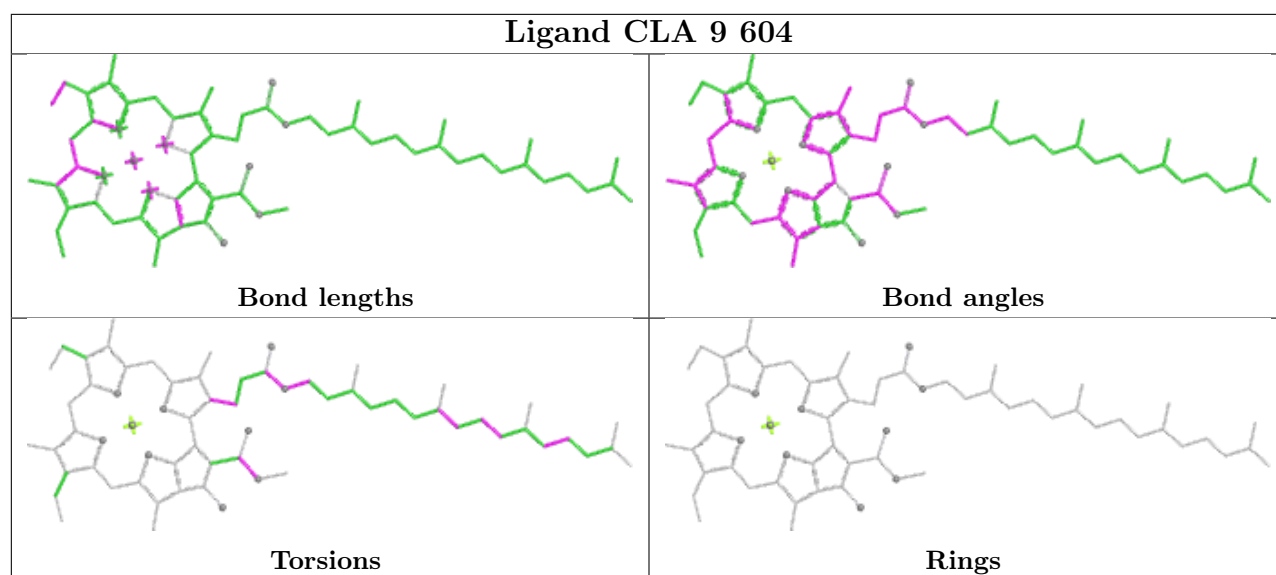


## Ligand CLA Z 615

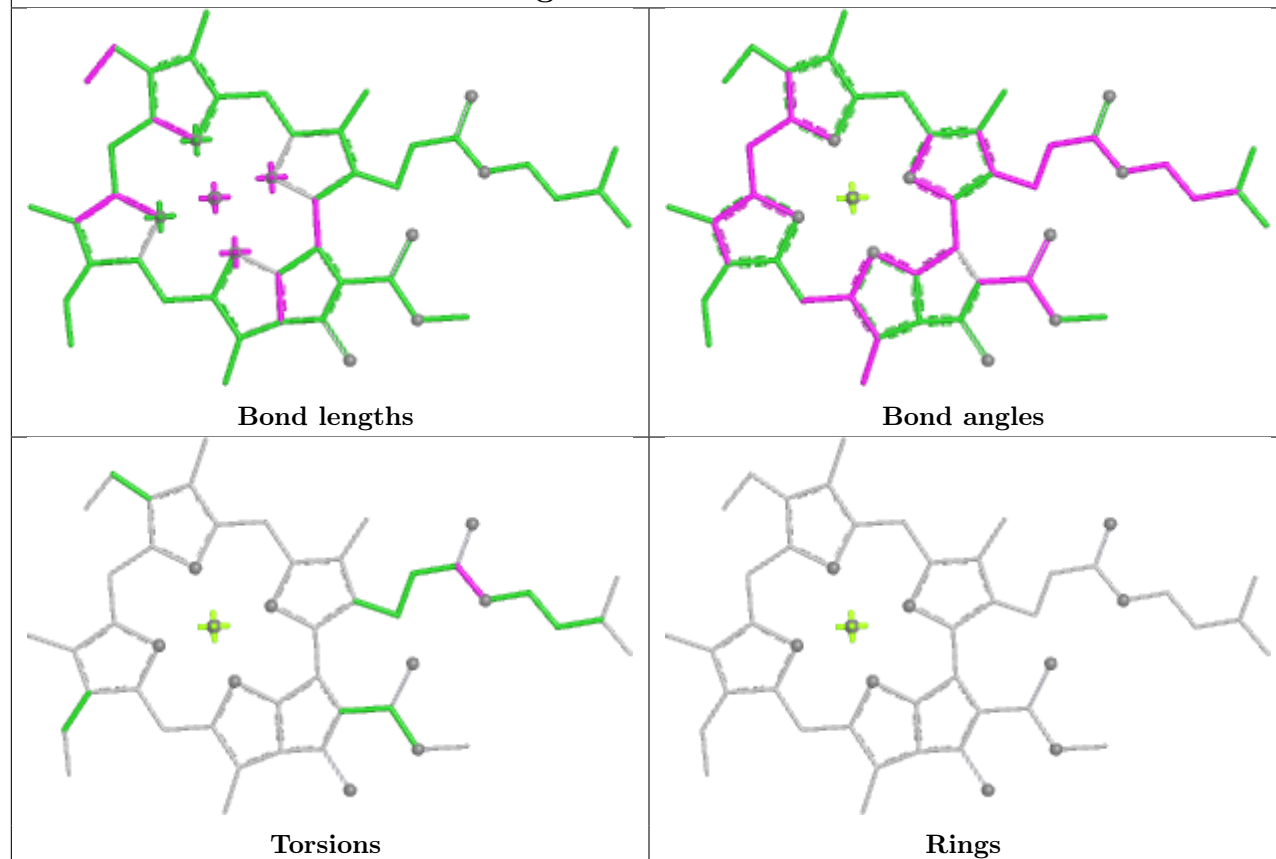




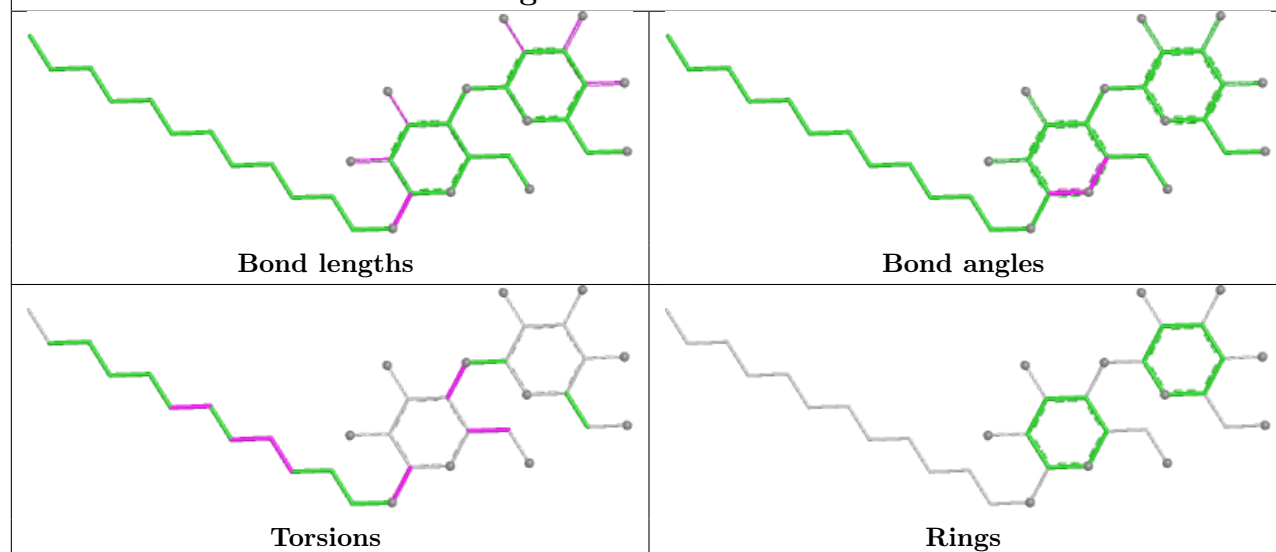


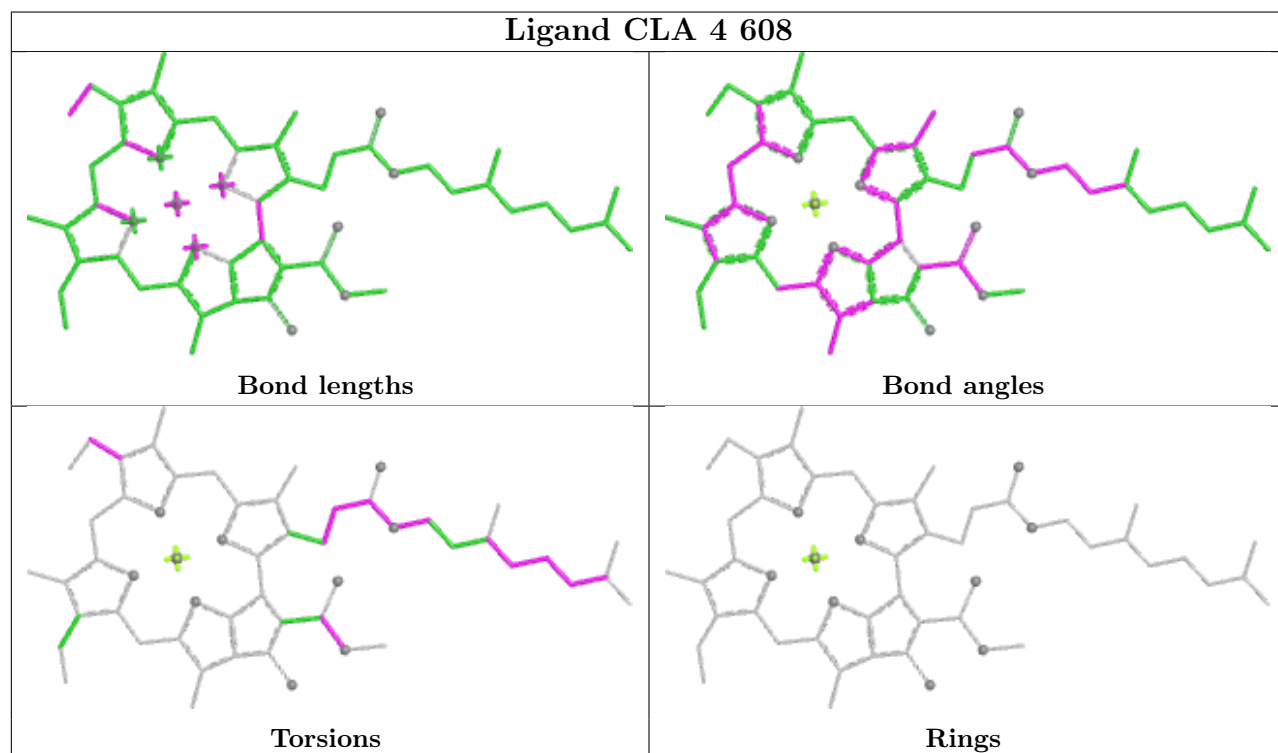
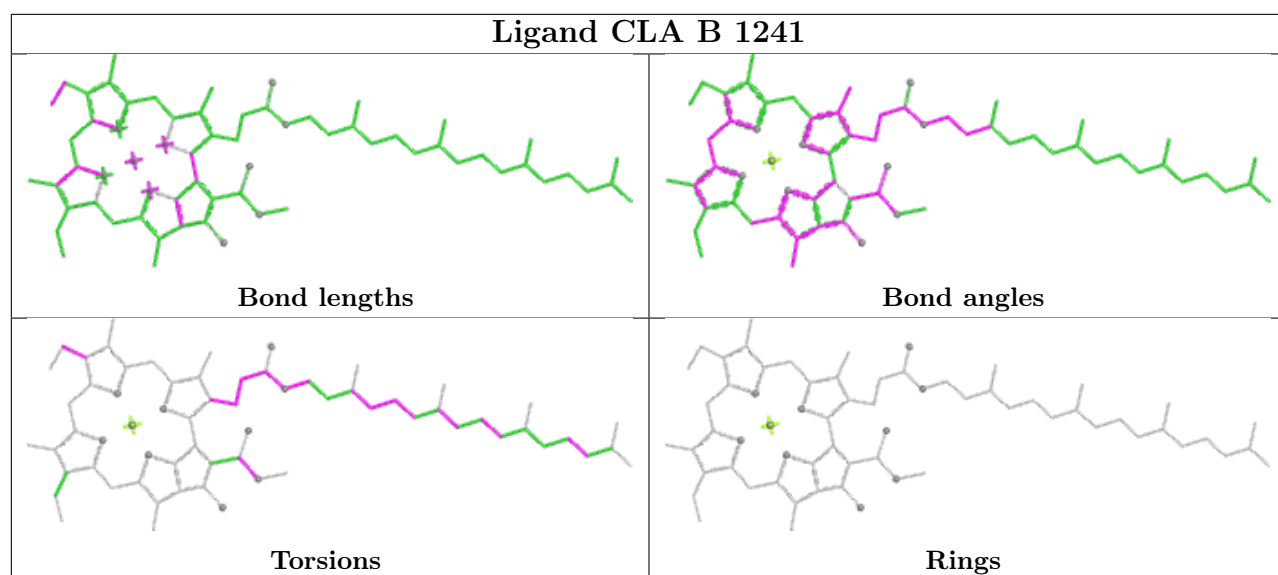


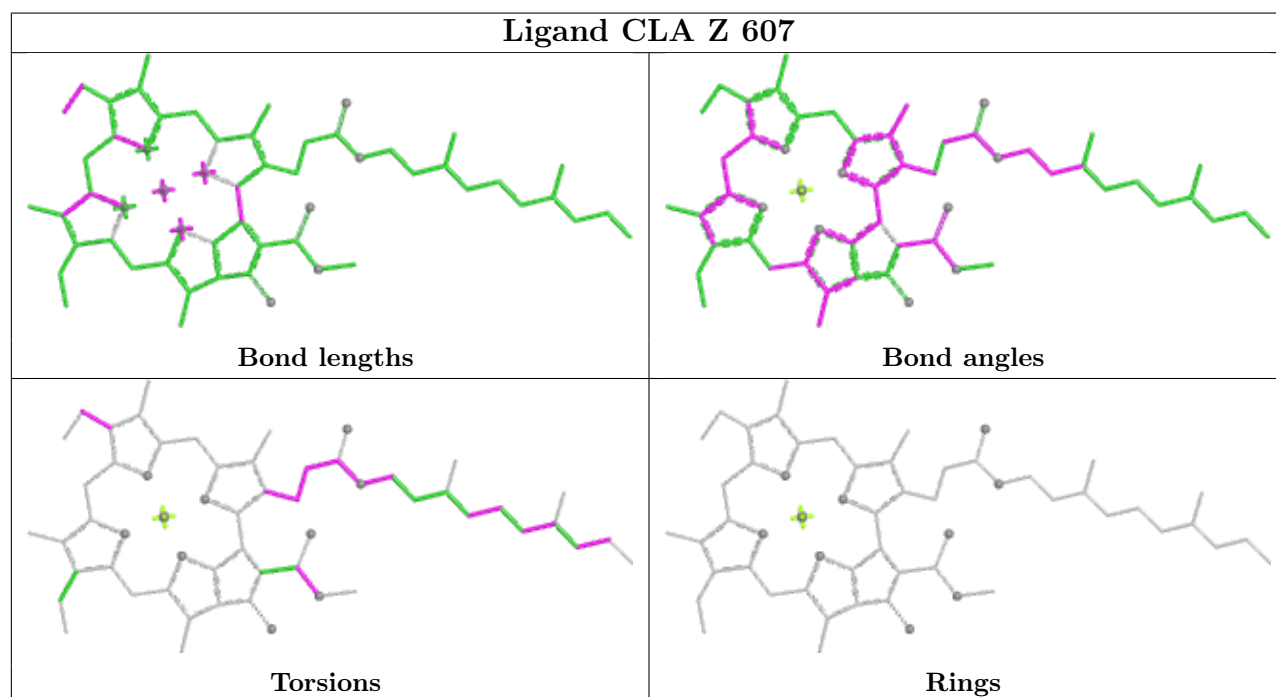
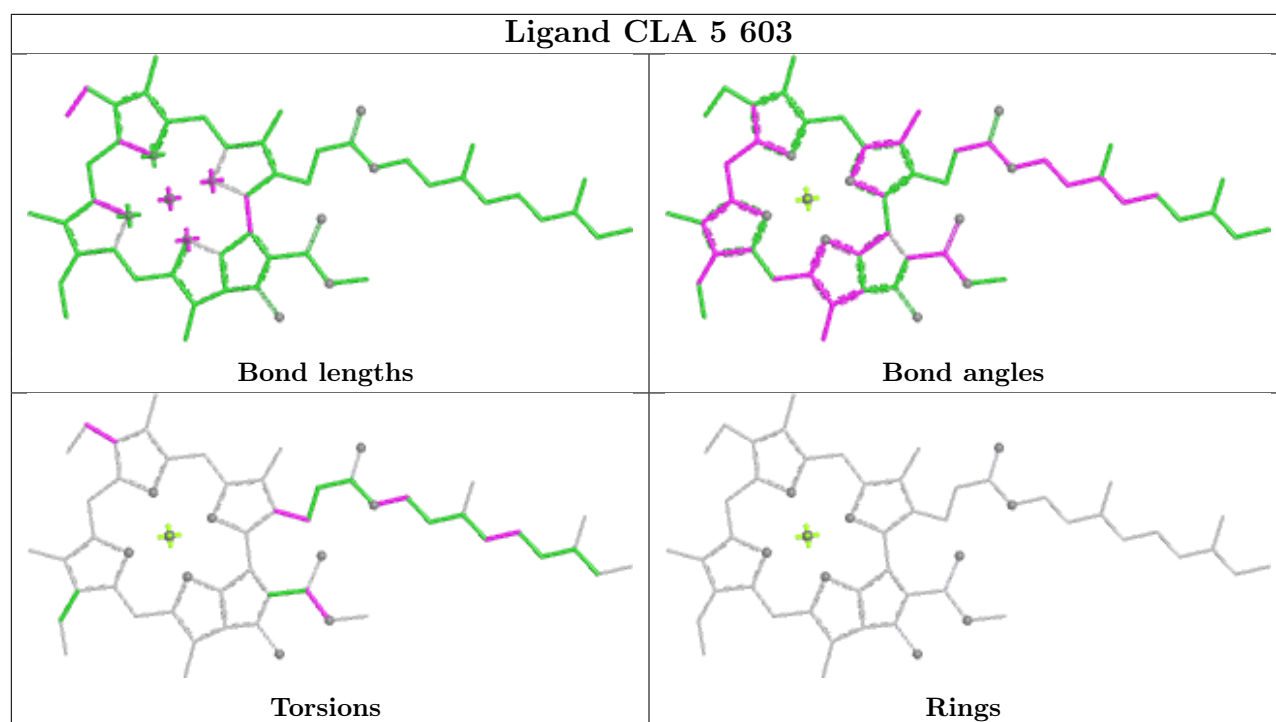
## Ligand CLA 9 612



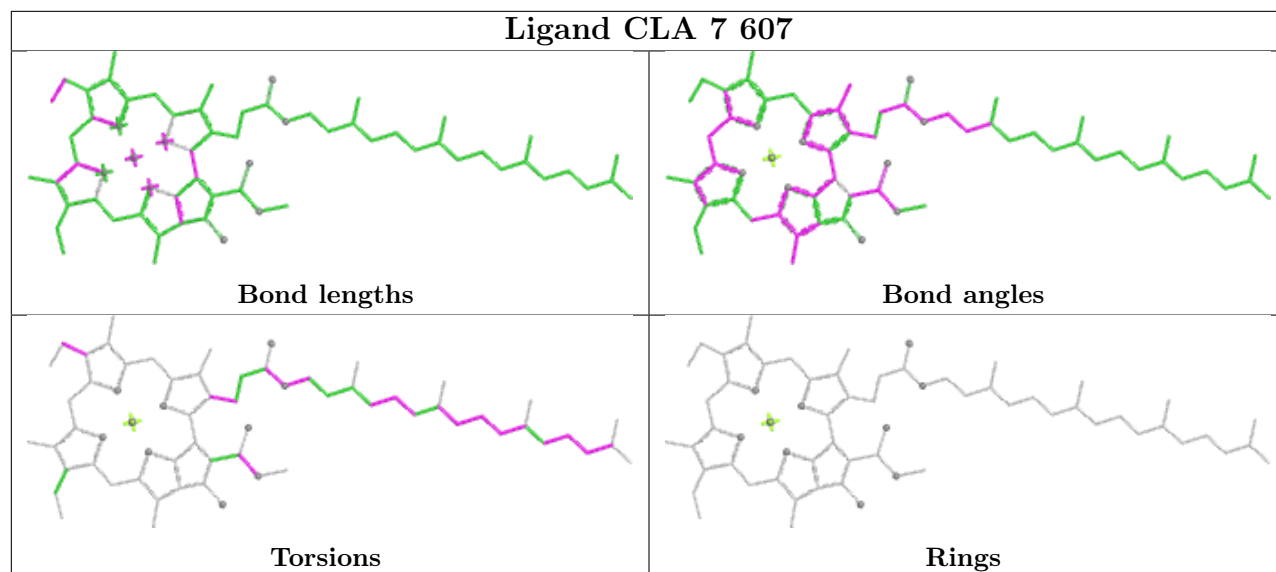
## Ligand LMT A 5006



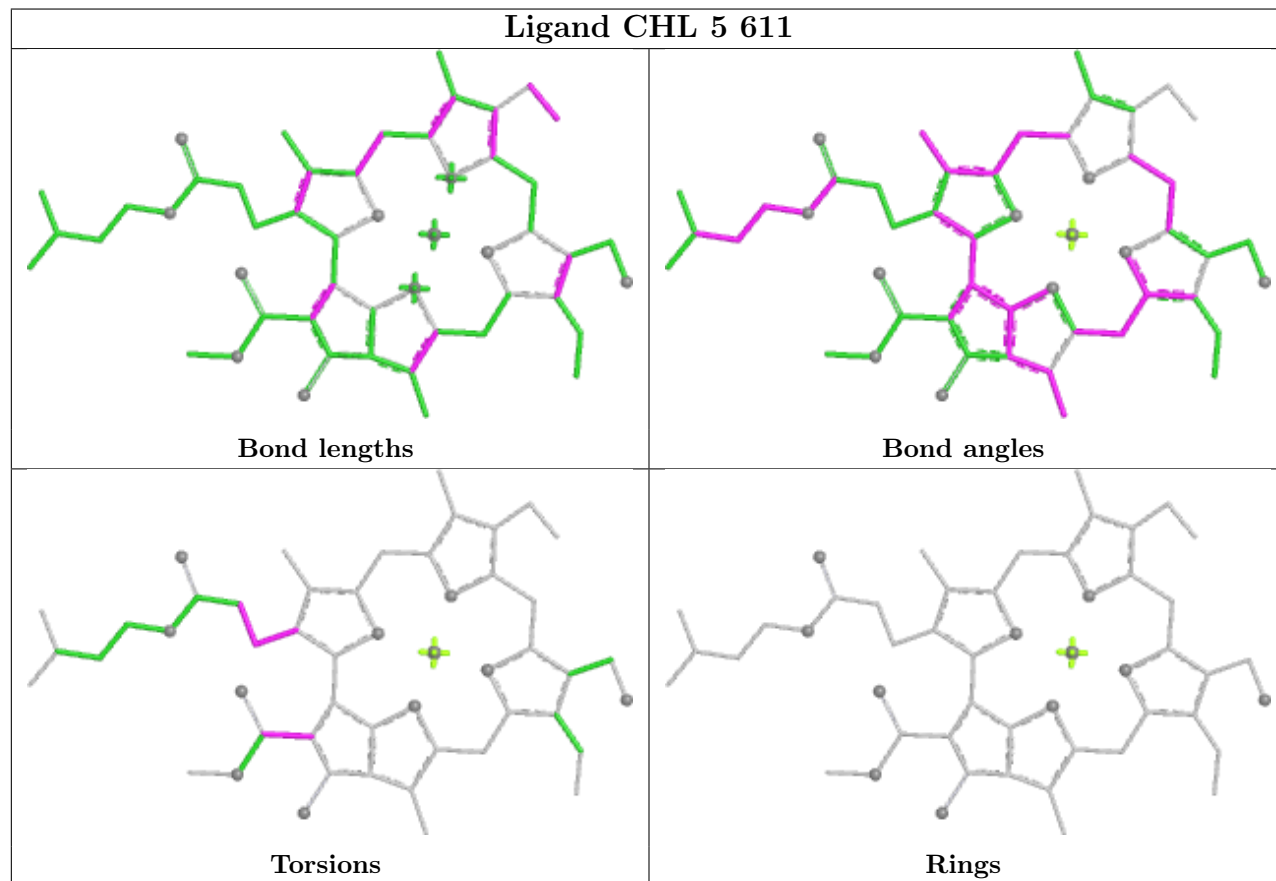


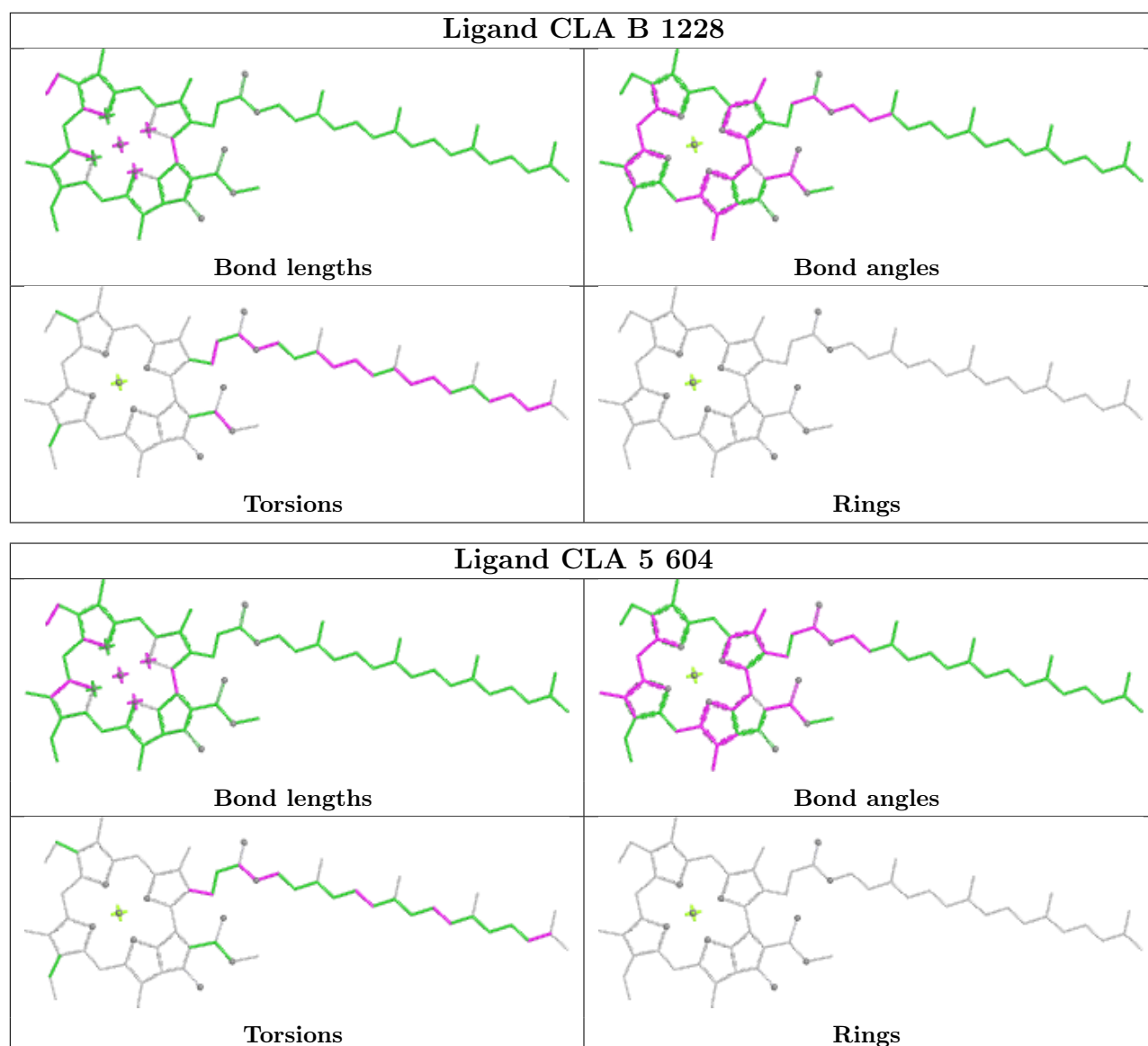


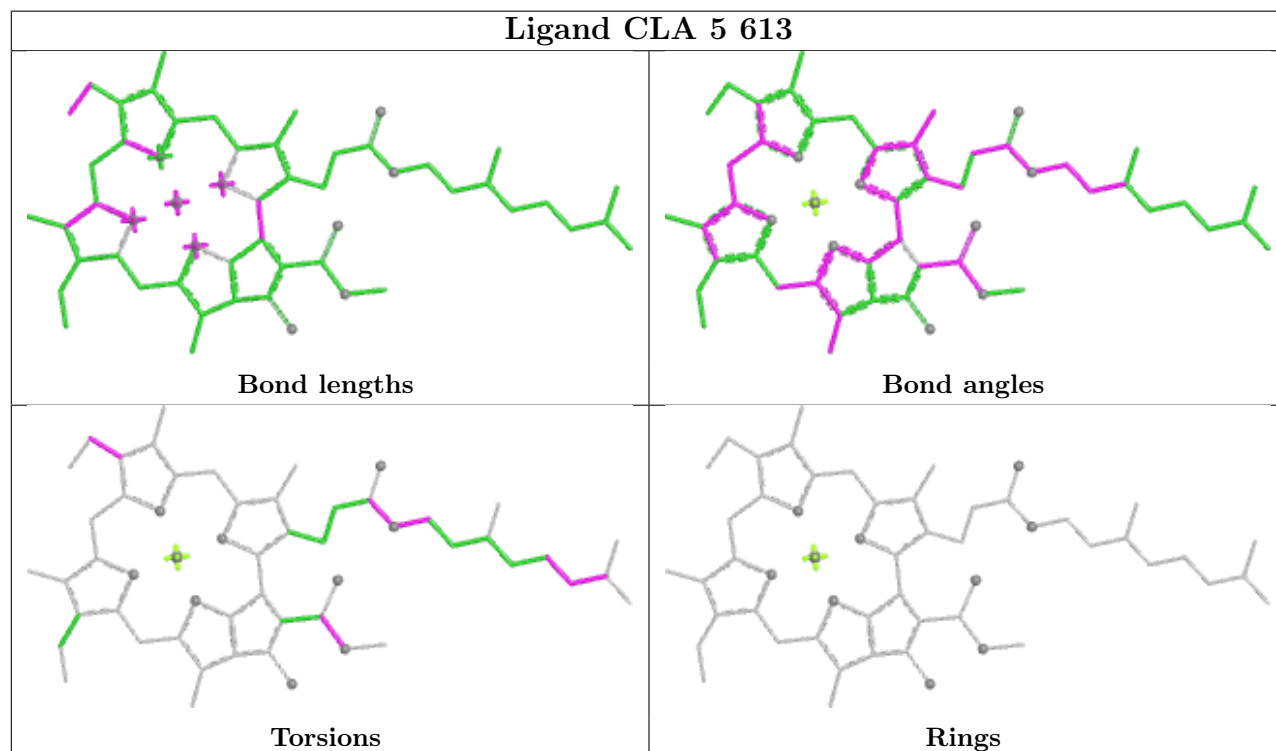
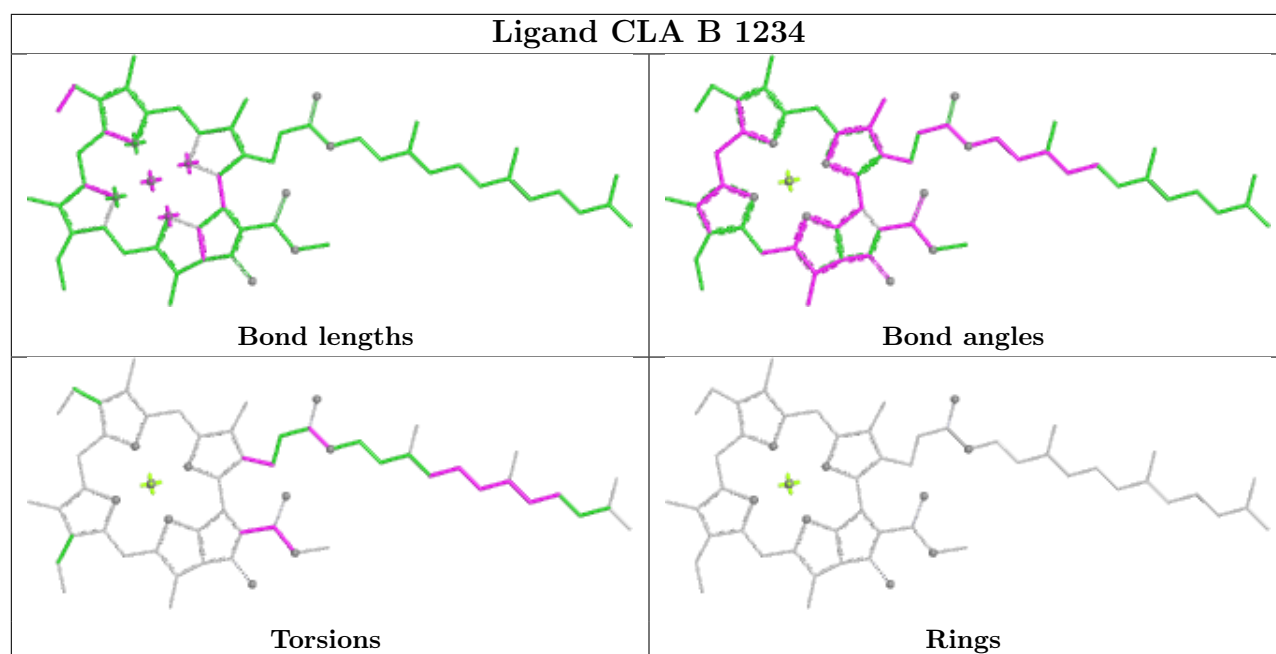
## Ligand CLA 7 607



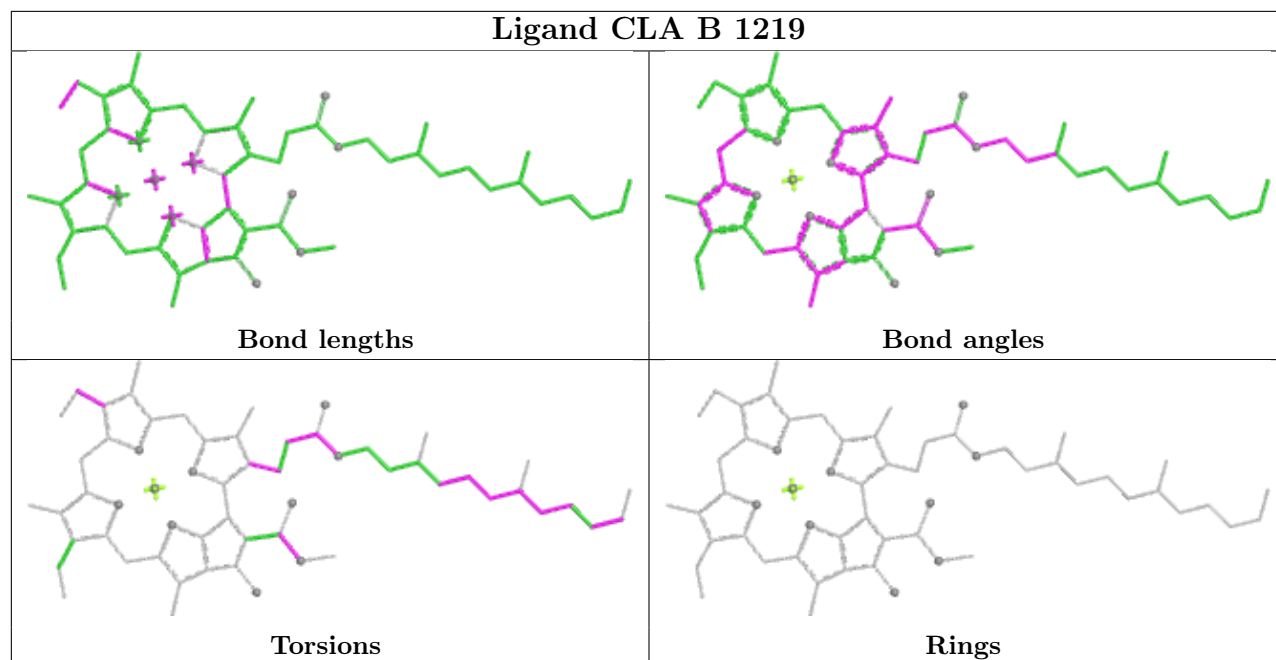
## Ligand CHL 5 611



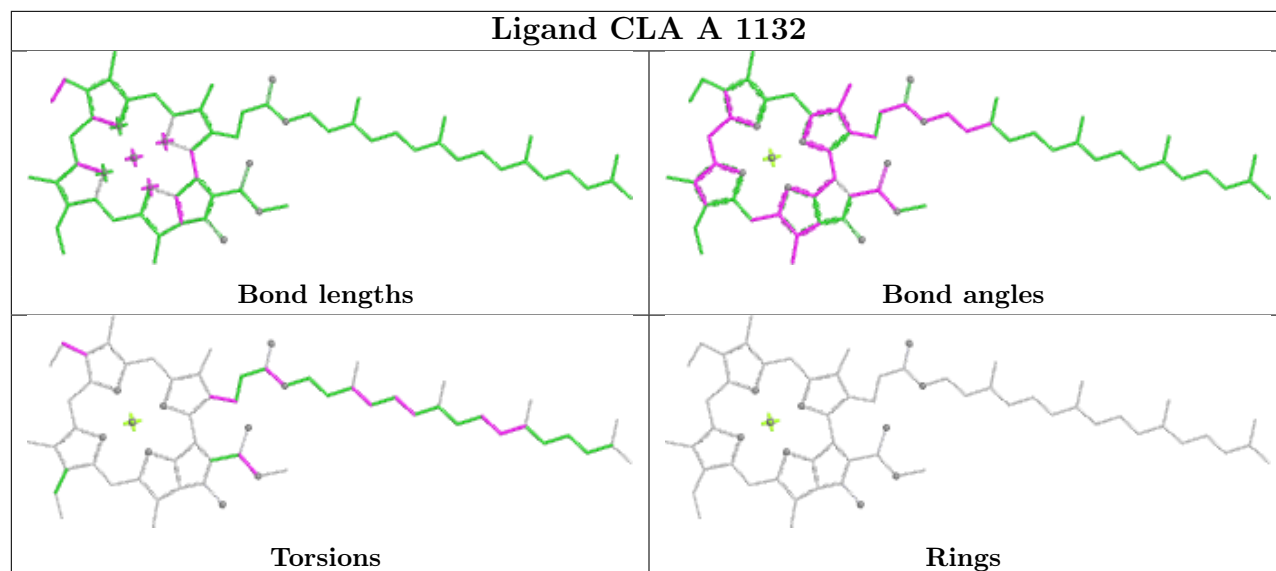


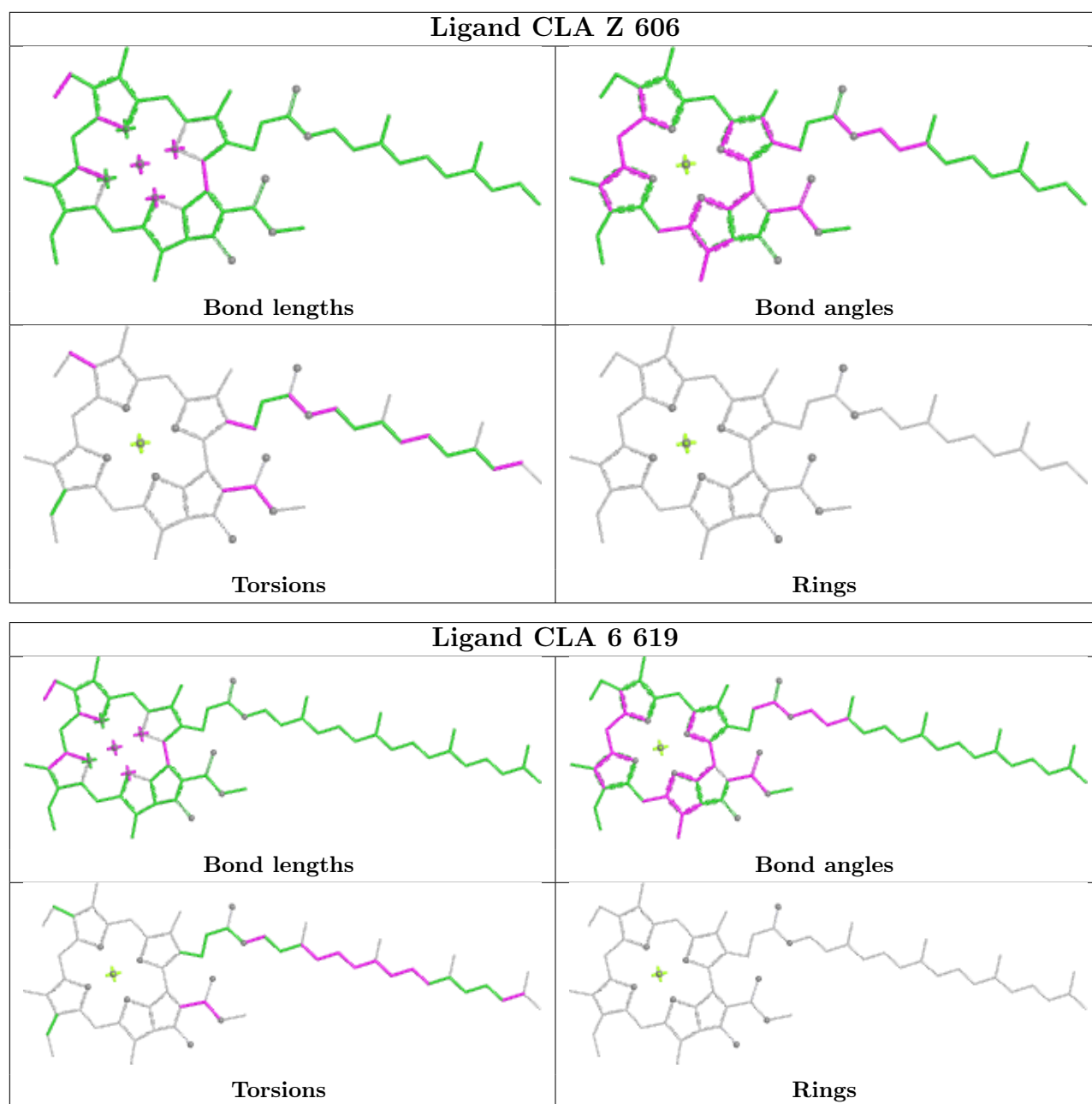


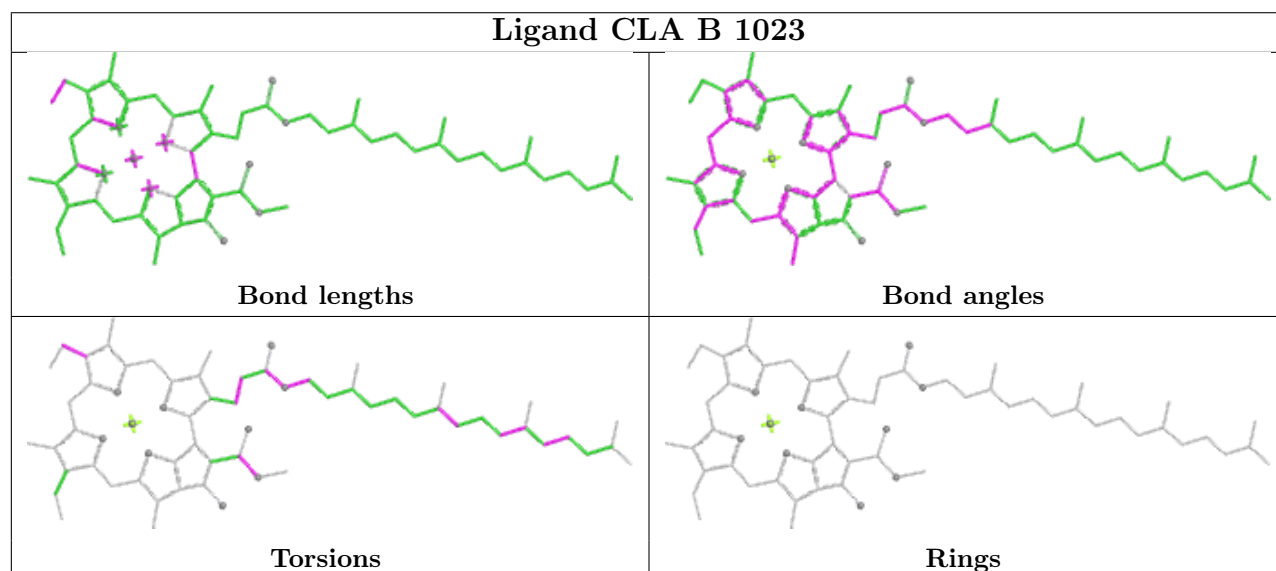
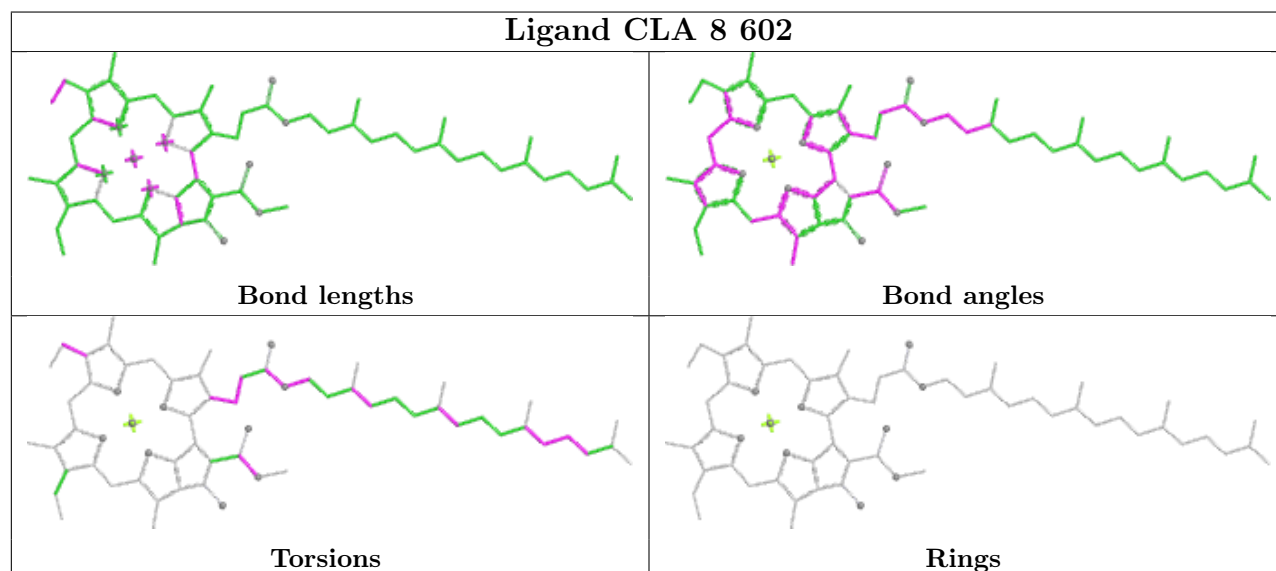
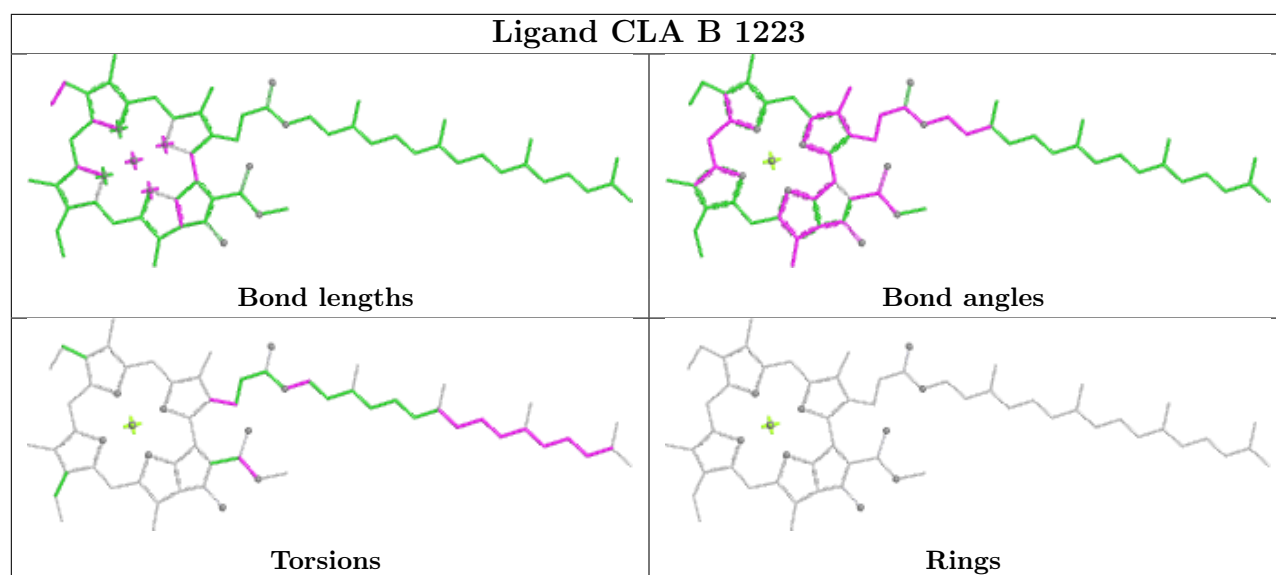
## Ligand CLA B 1219

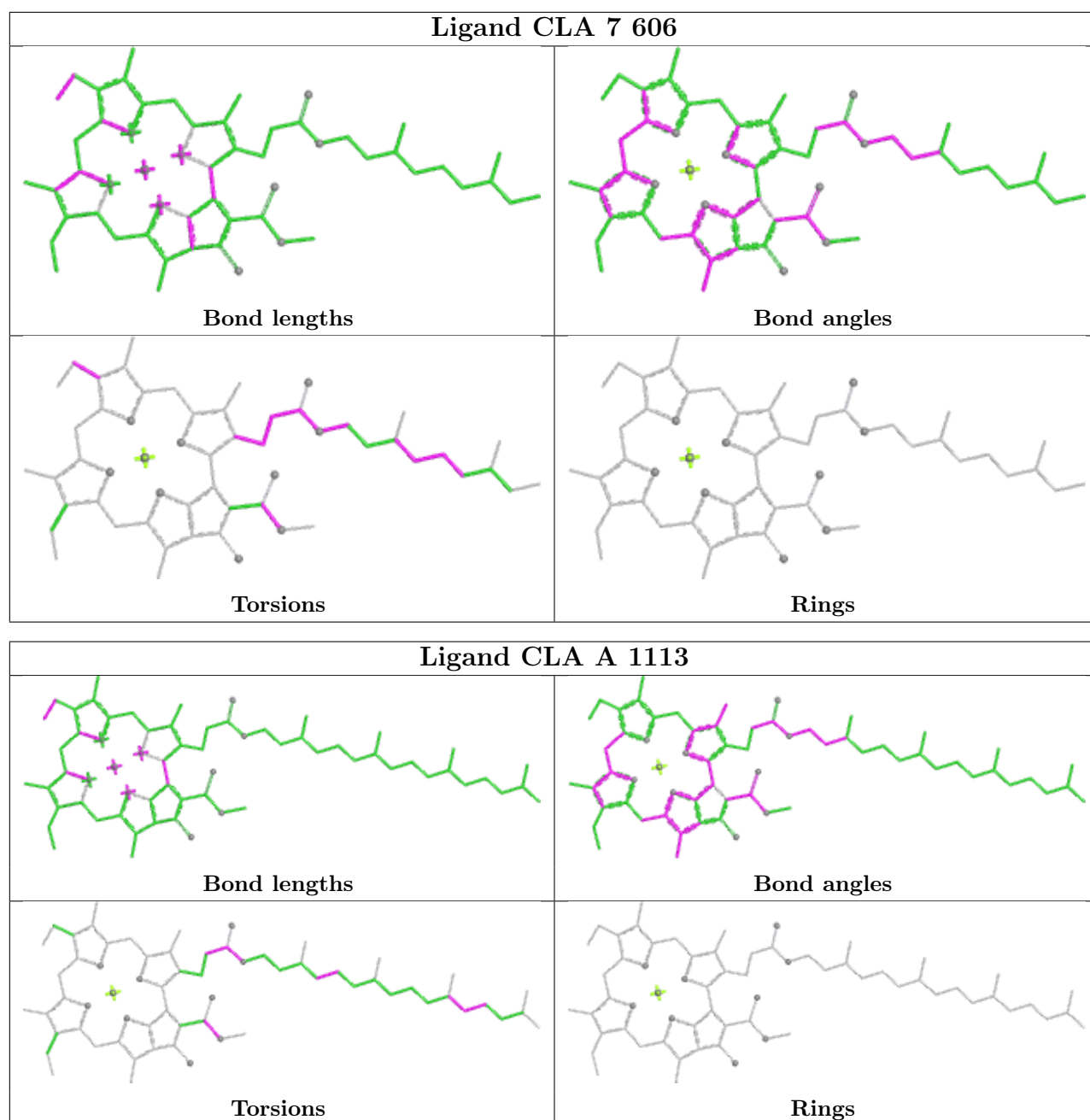


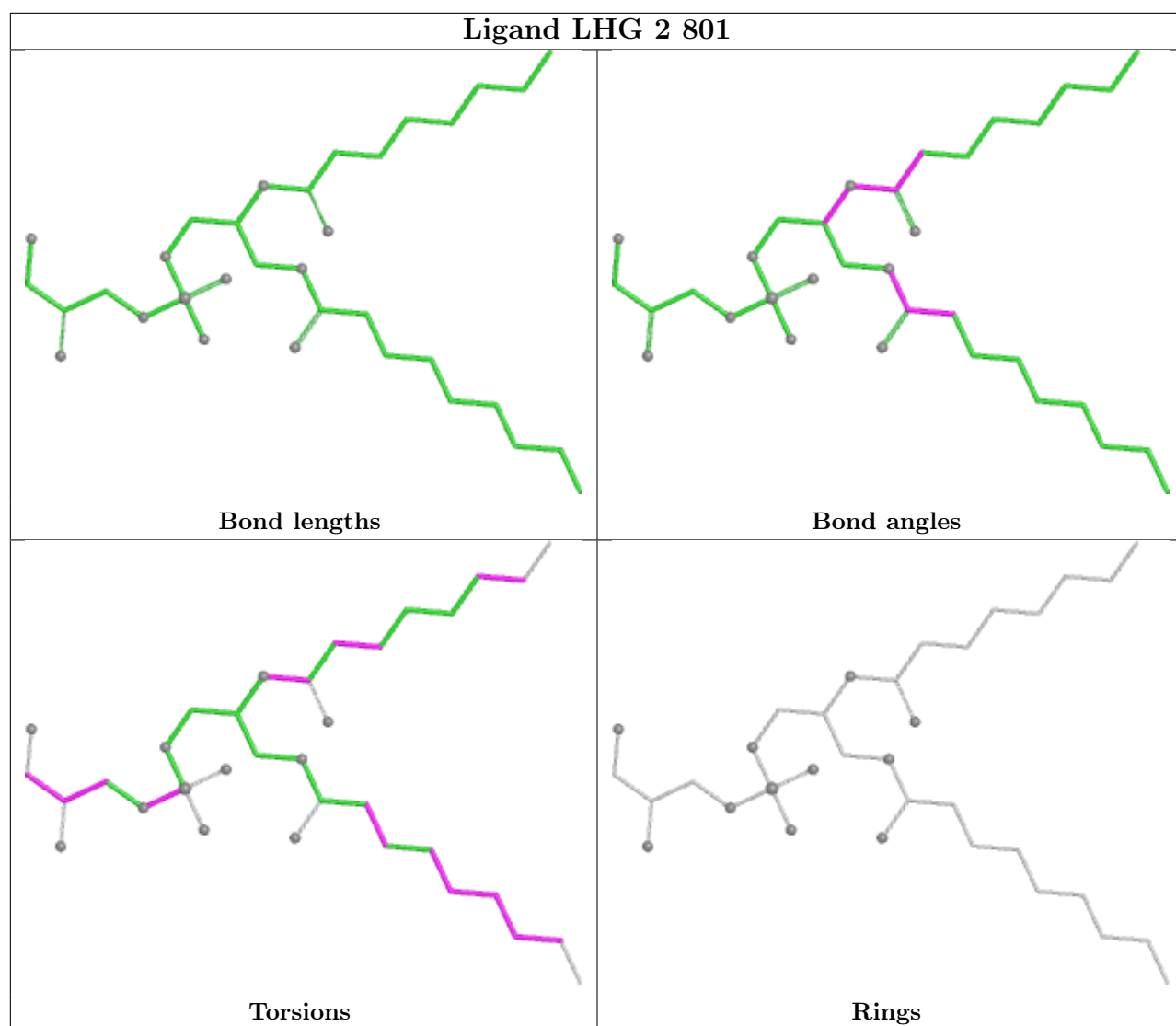
## Ligand CLA A 1132

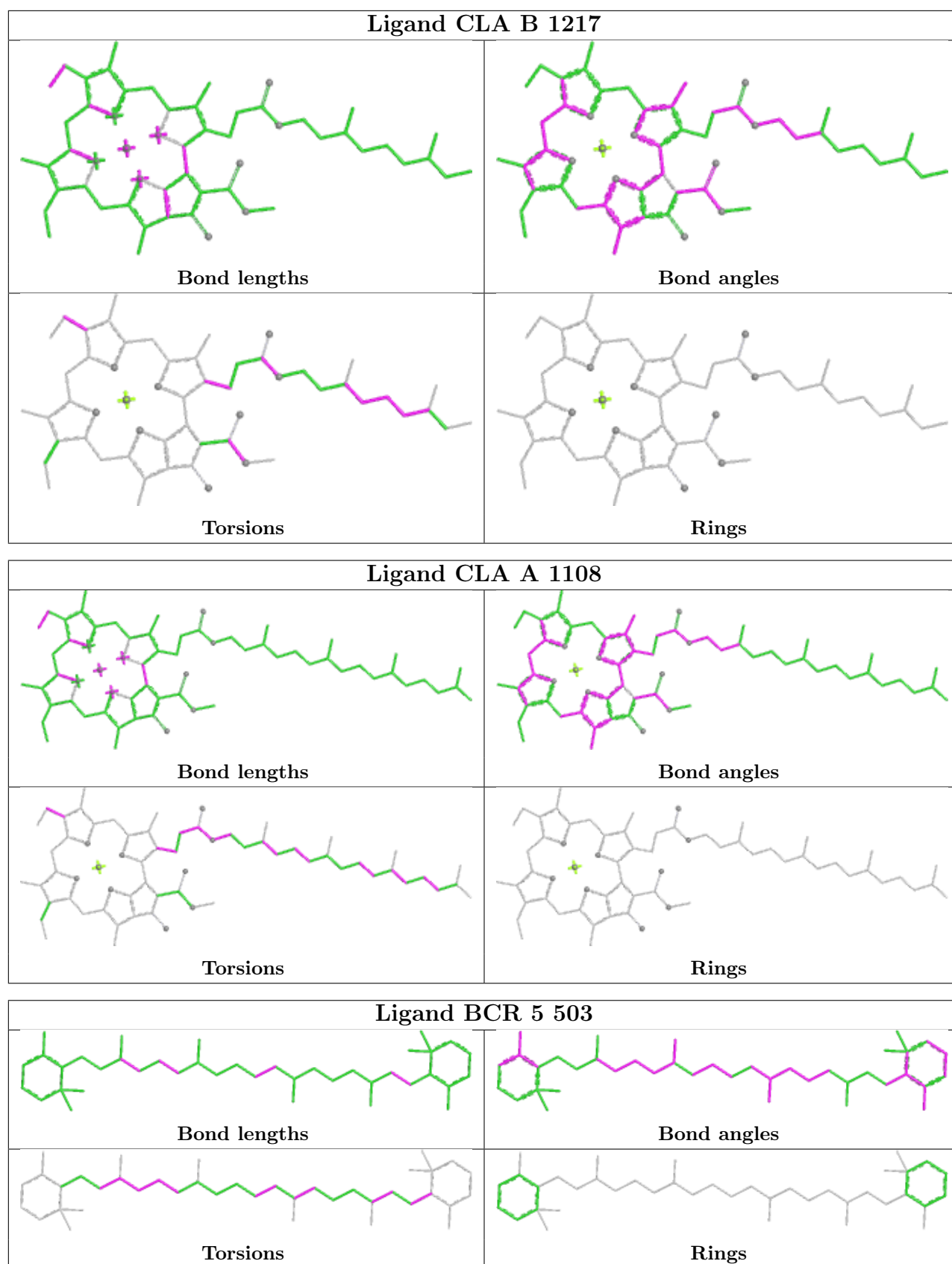


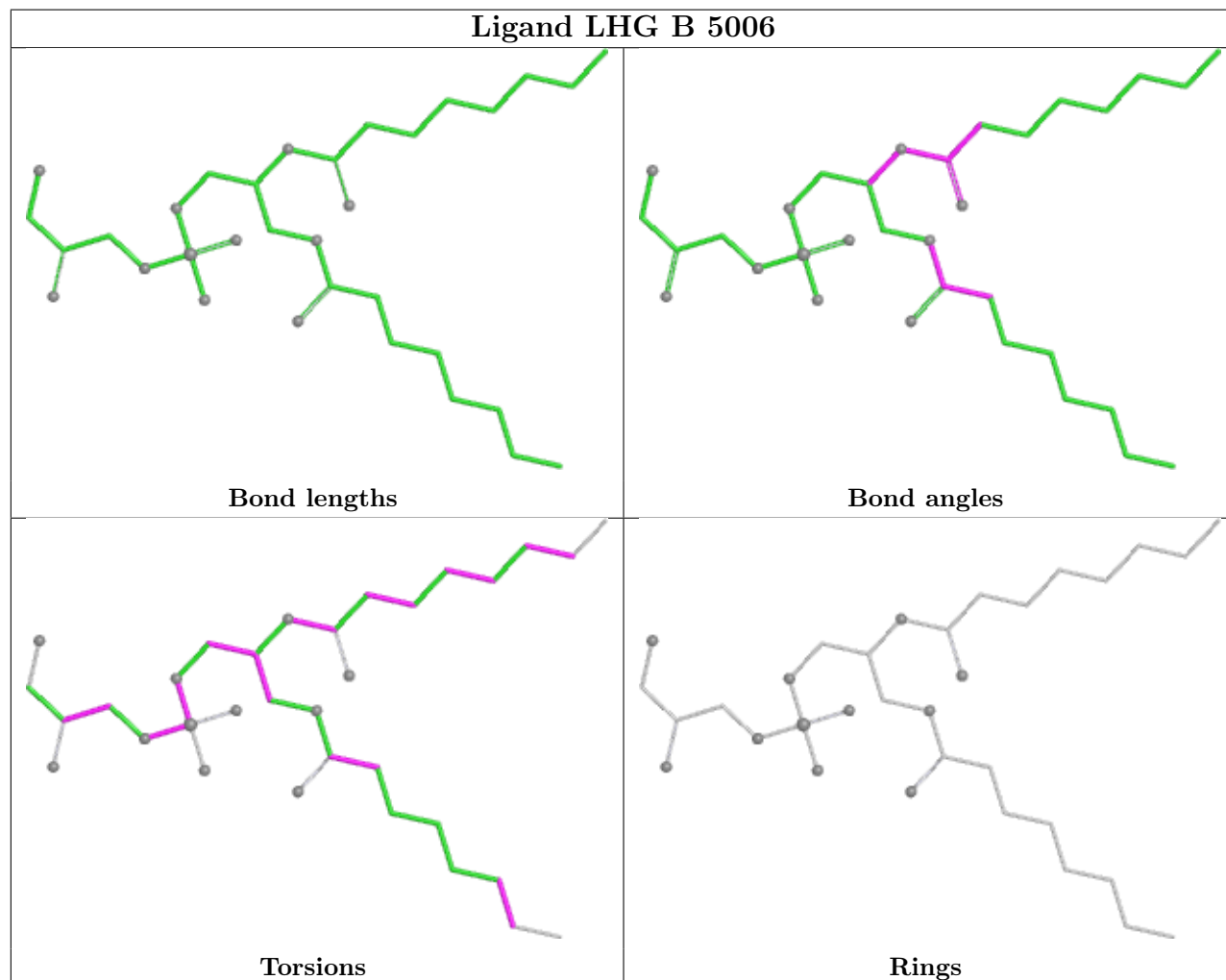
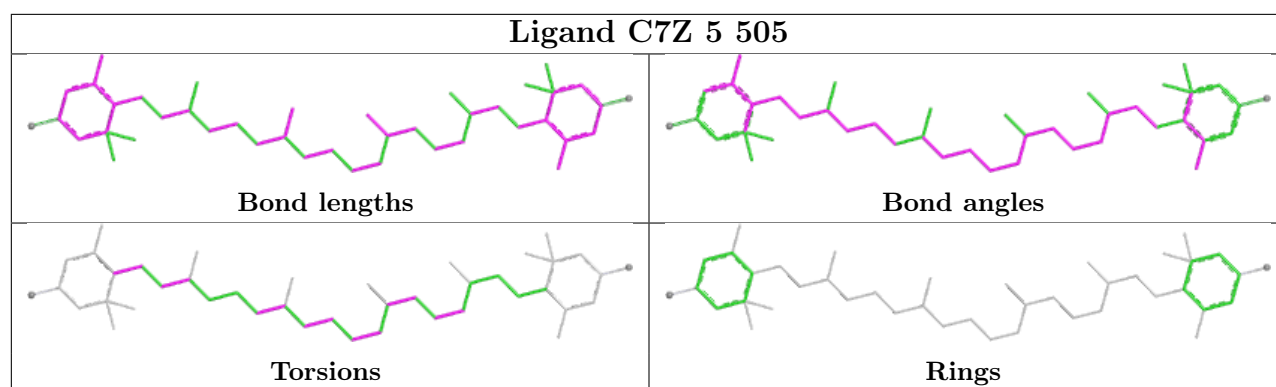




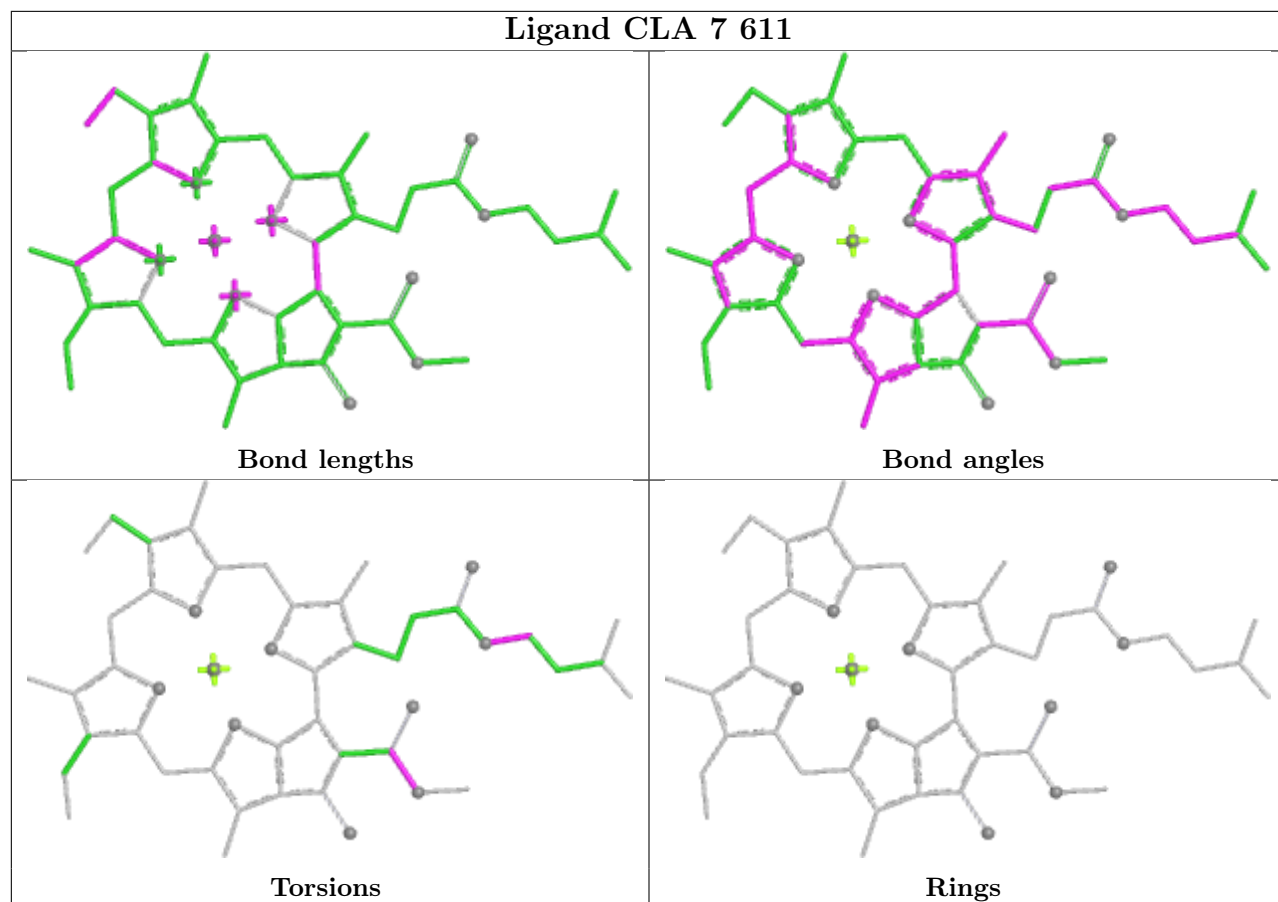


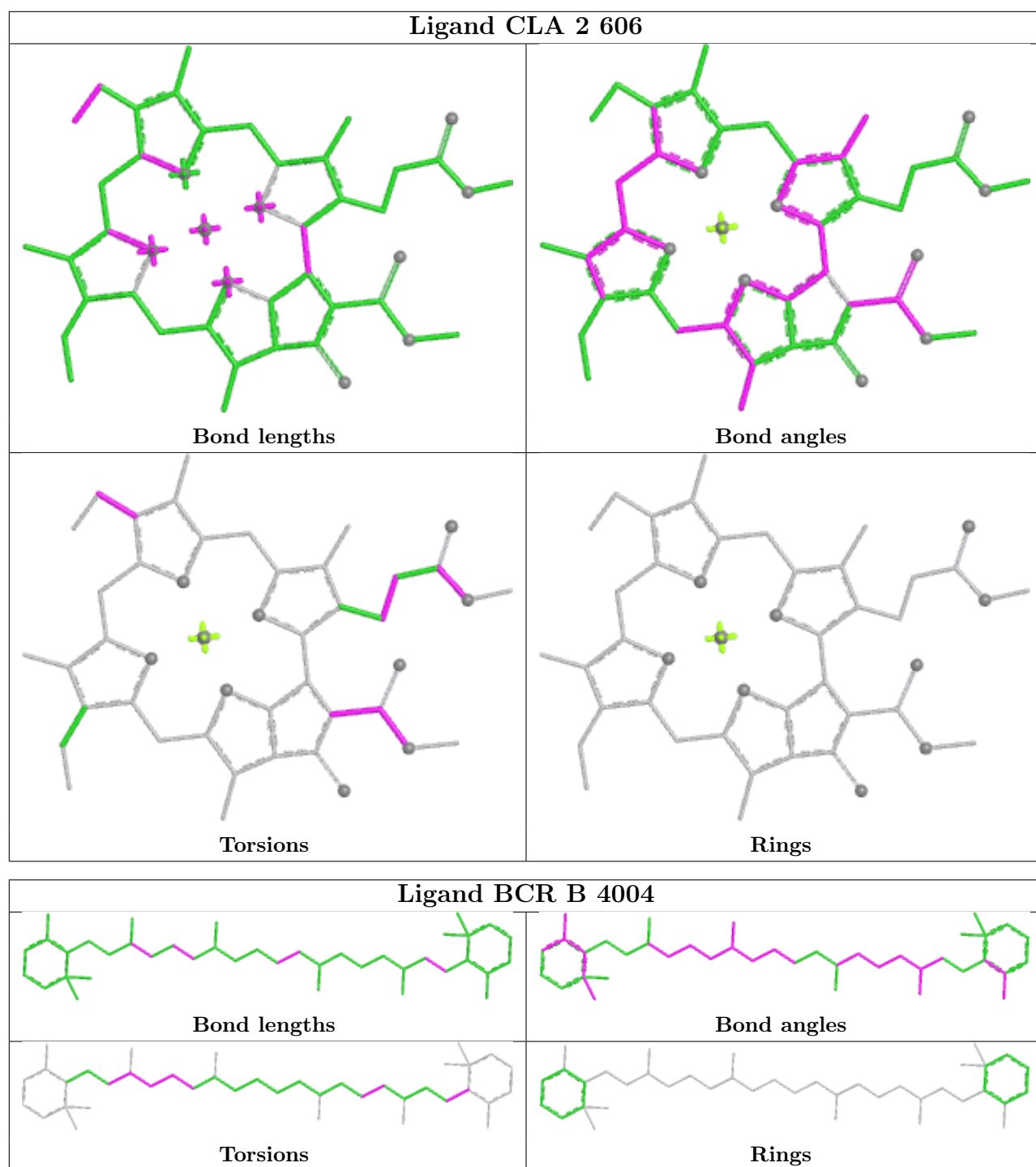


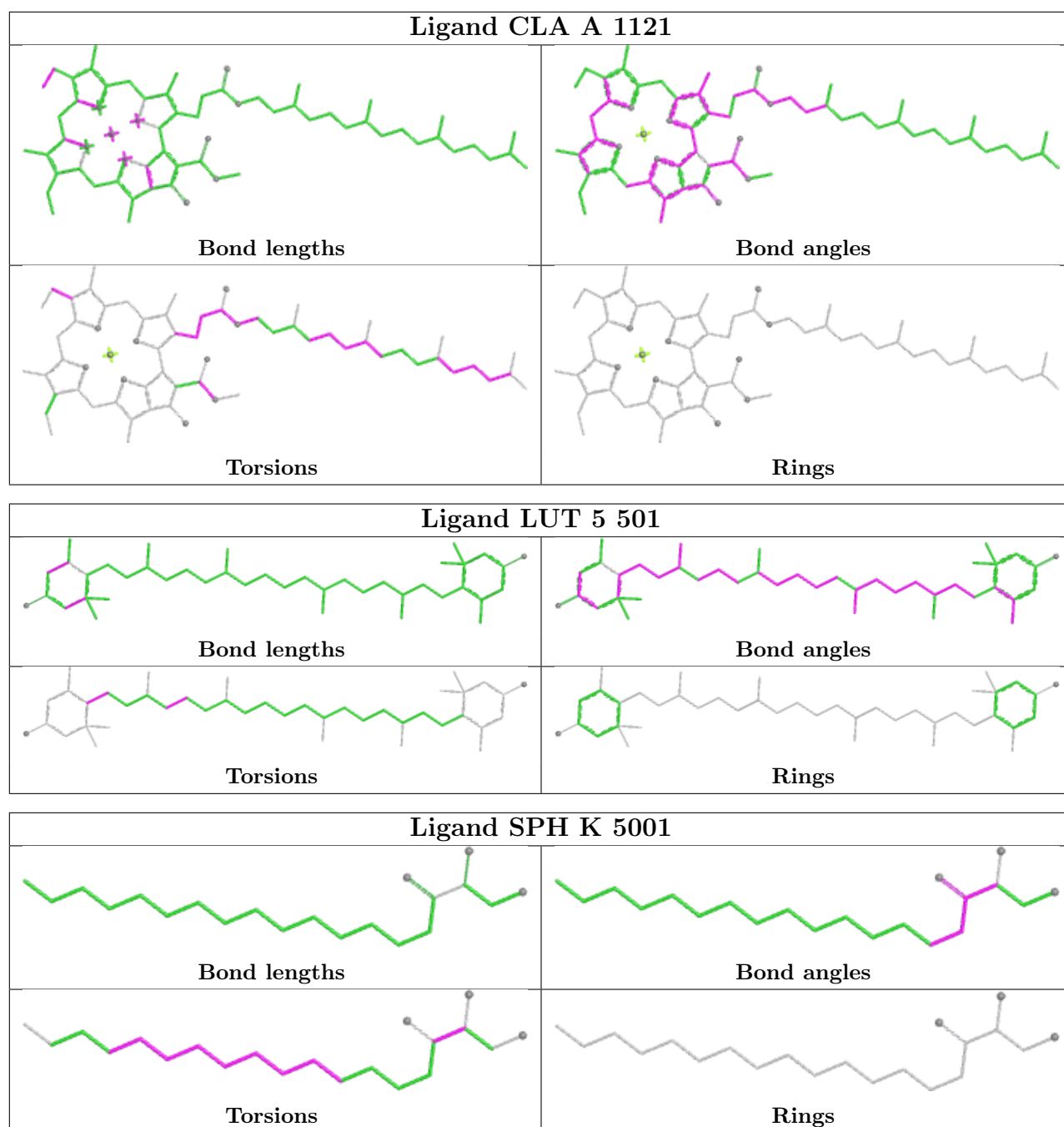




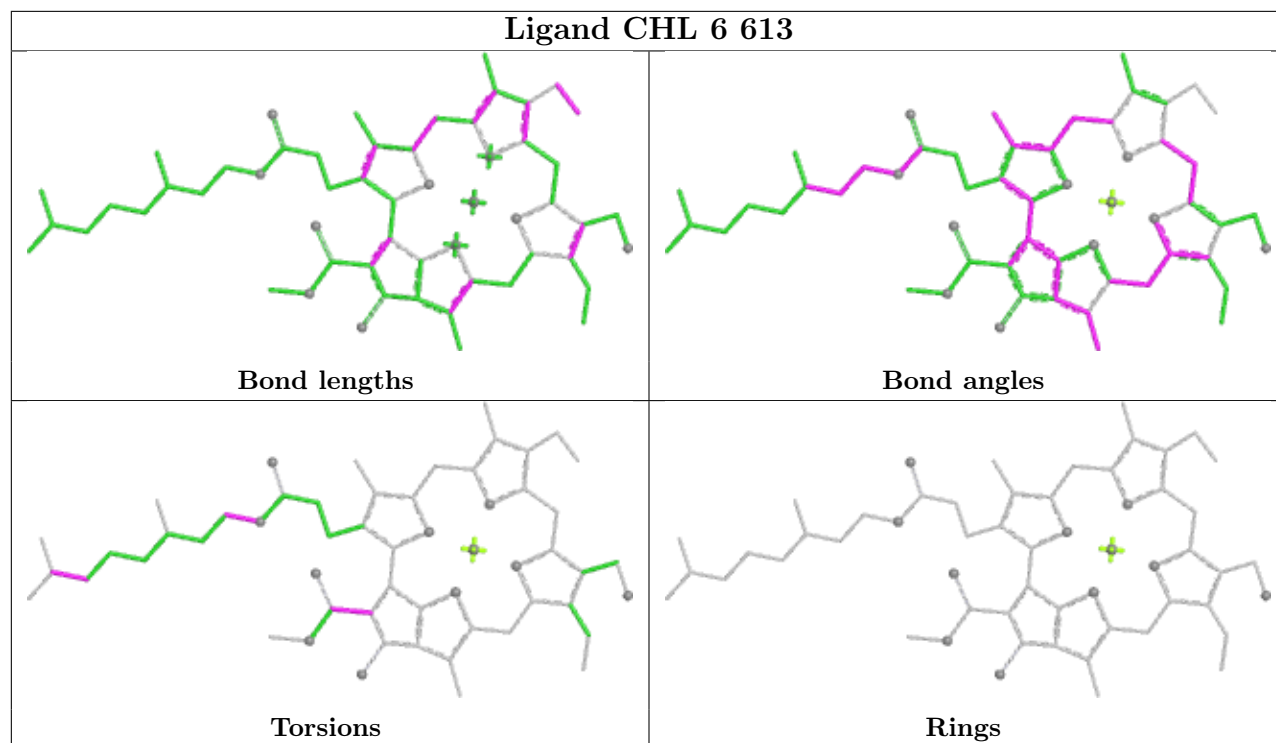
## Ligand CLA 7 611



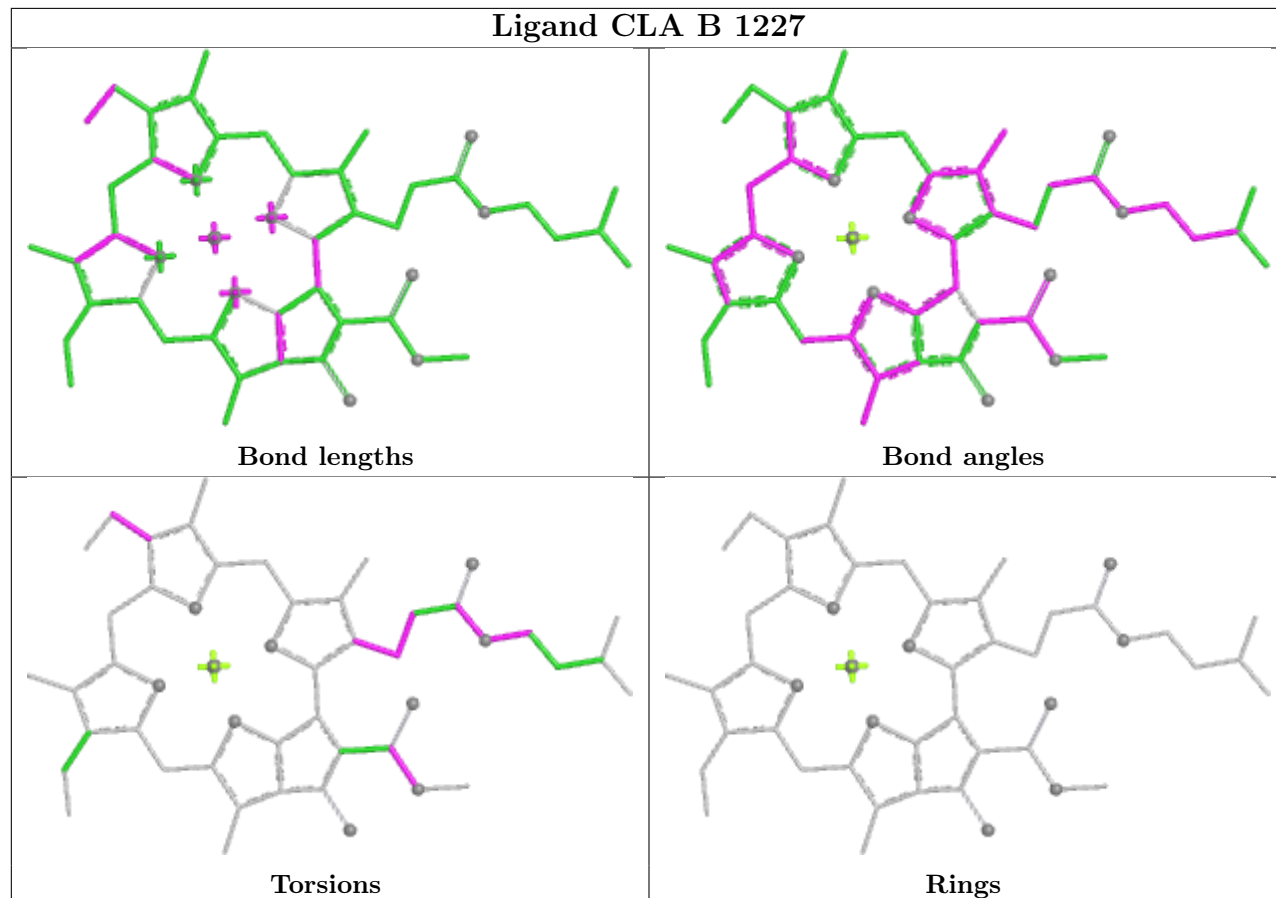


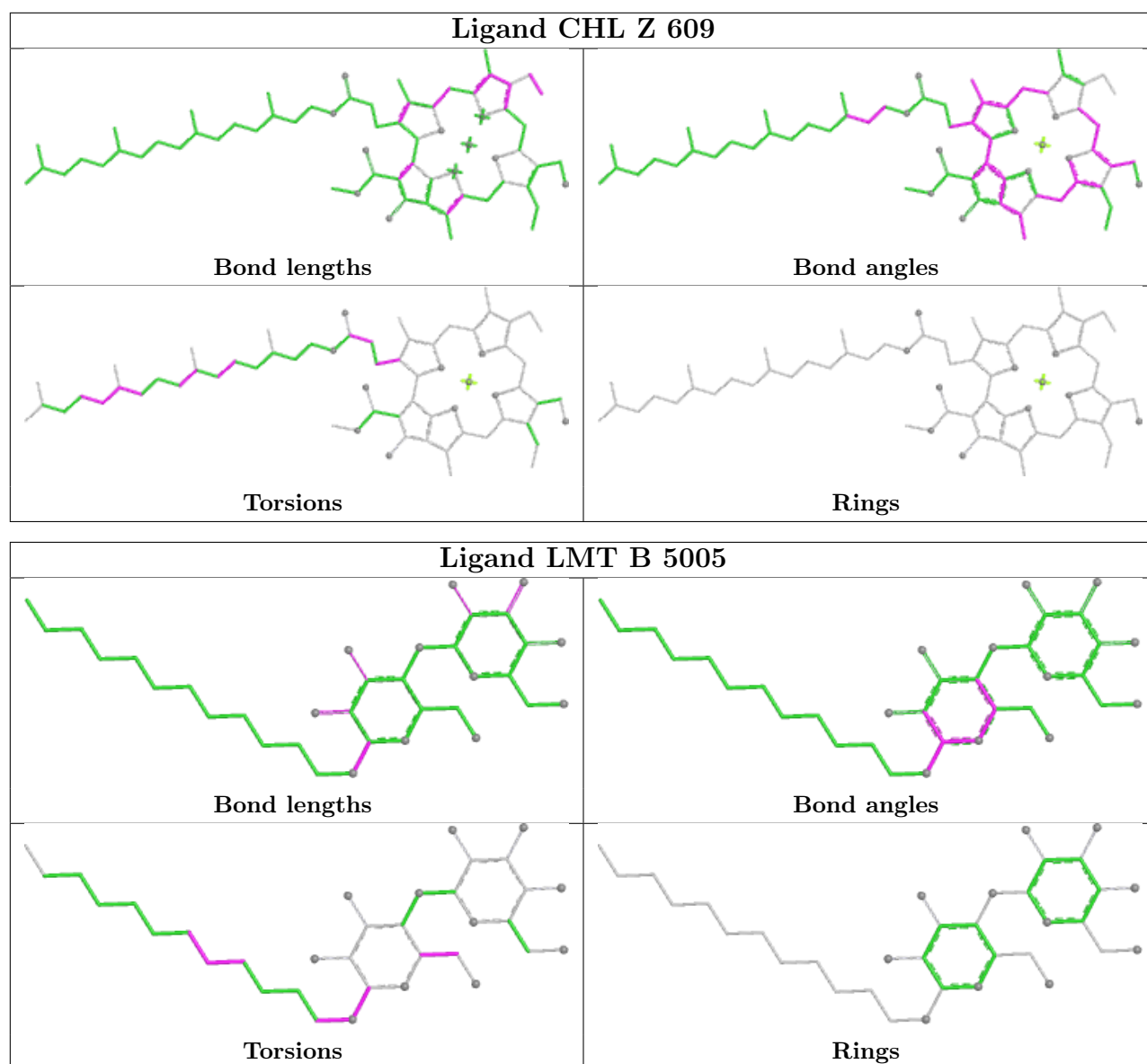


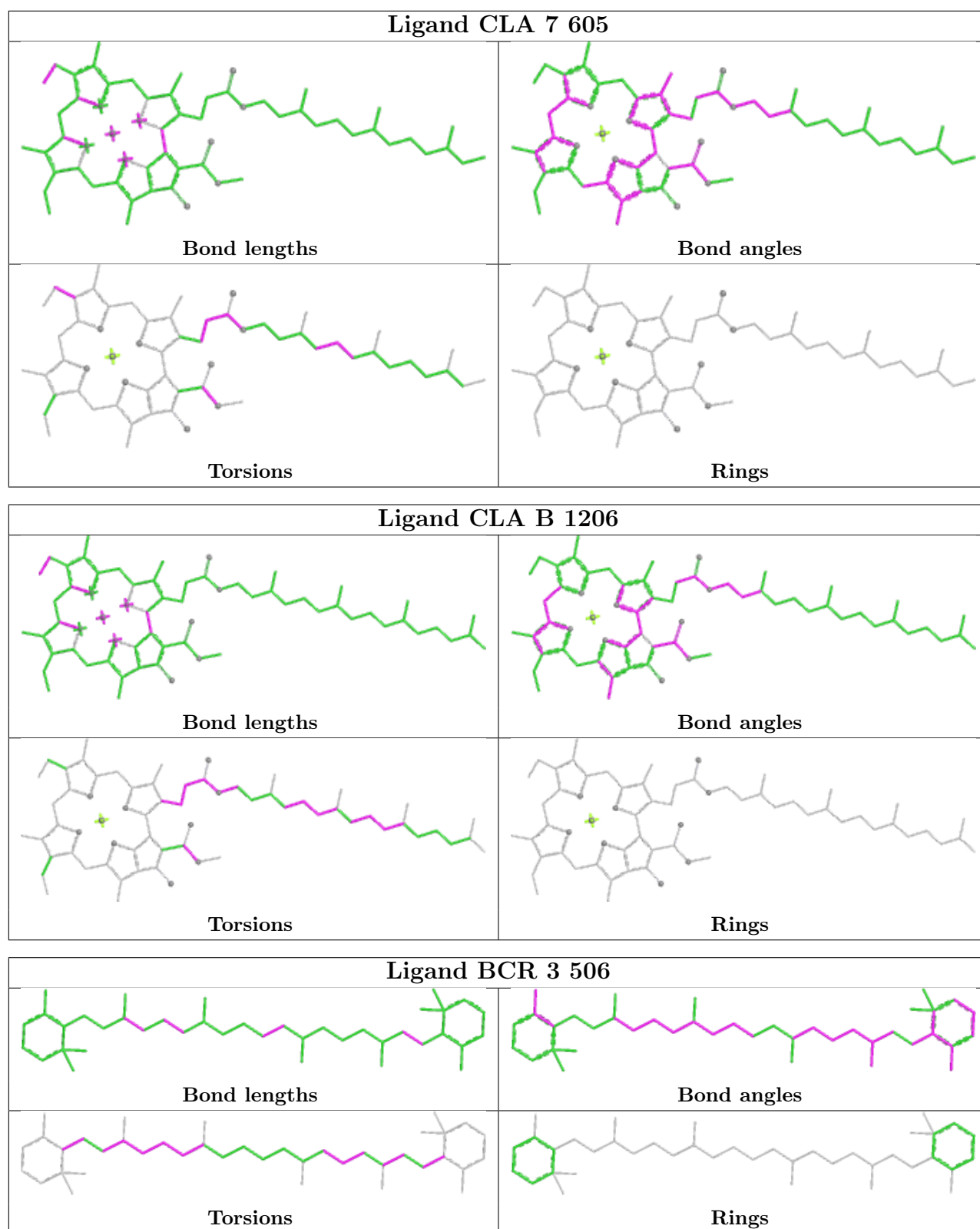
## Ligand CHL 6 613

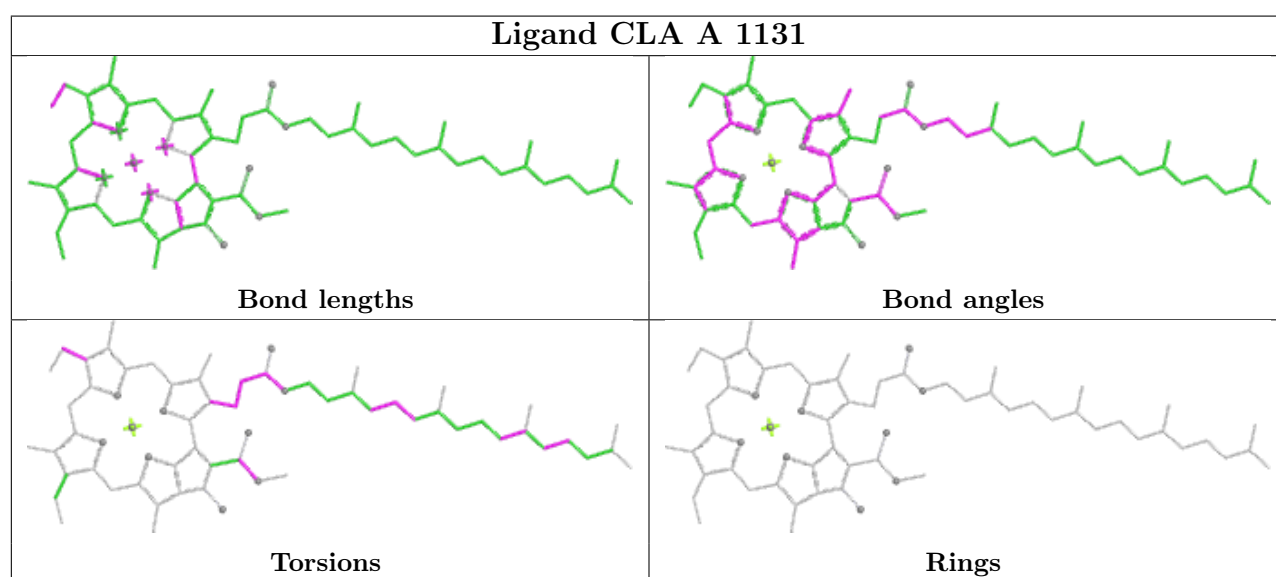
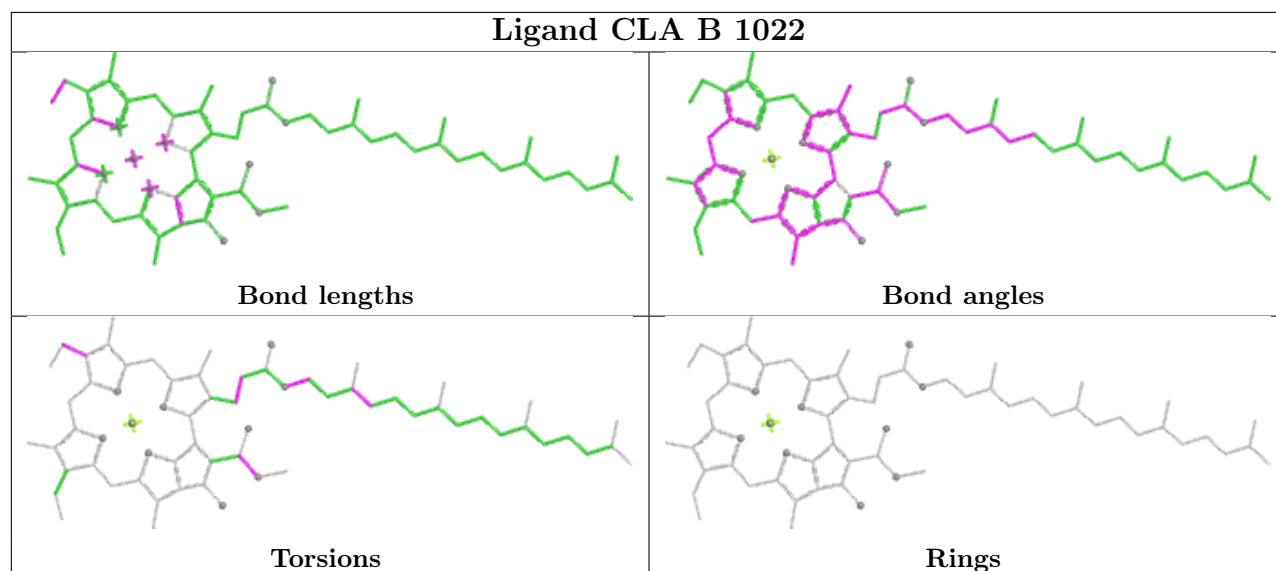
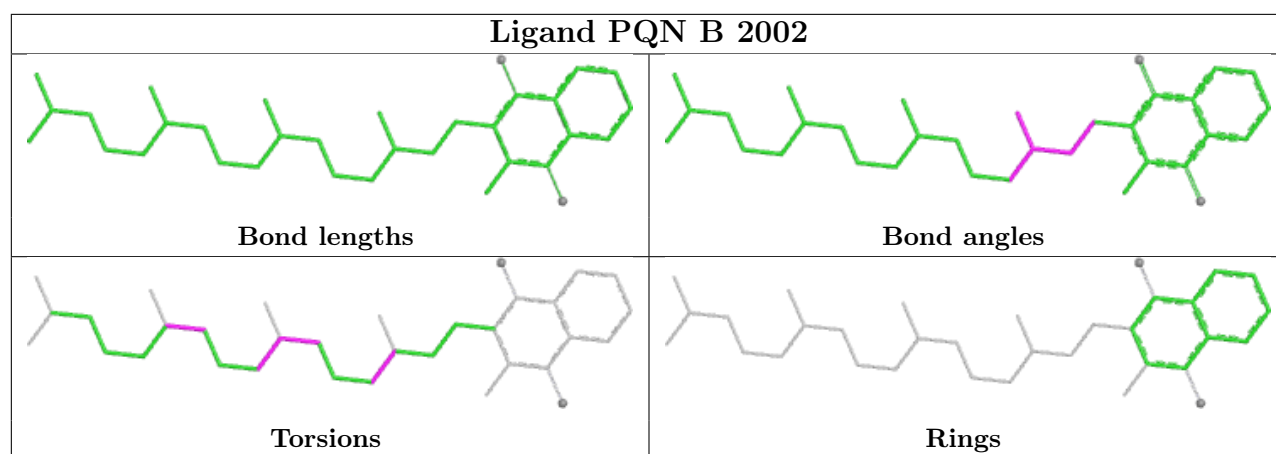


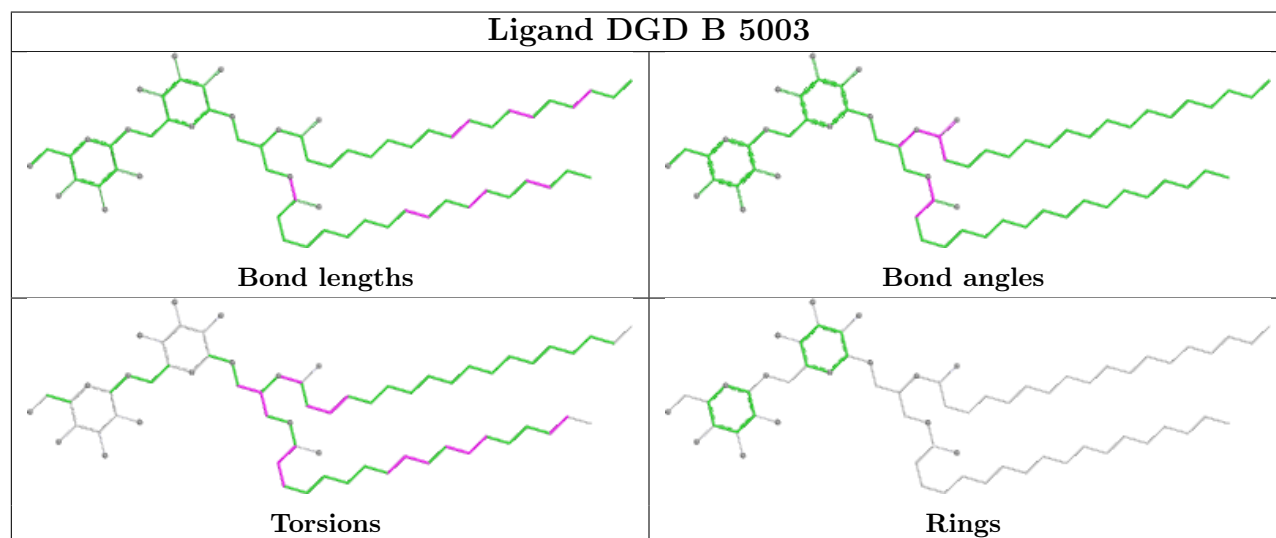
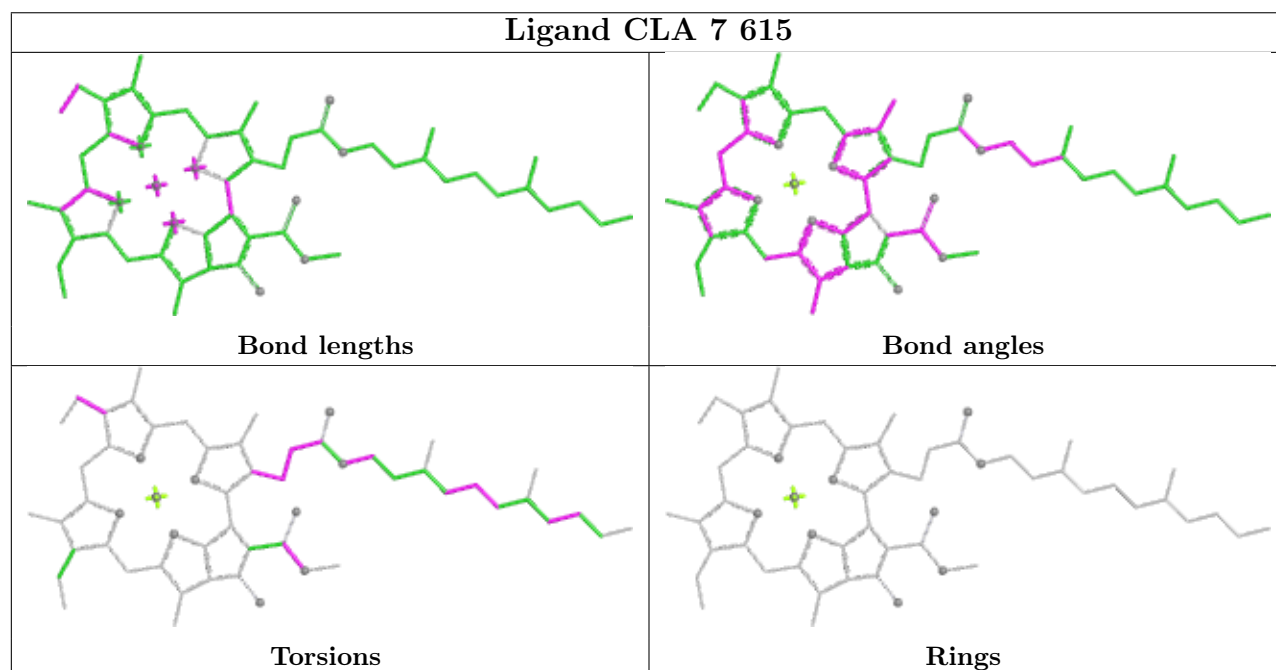
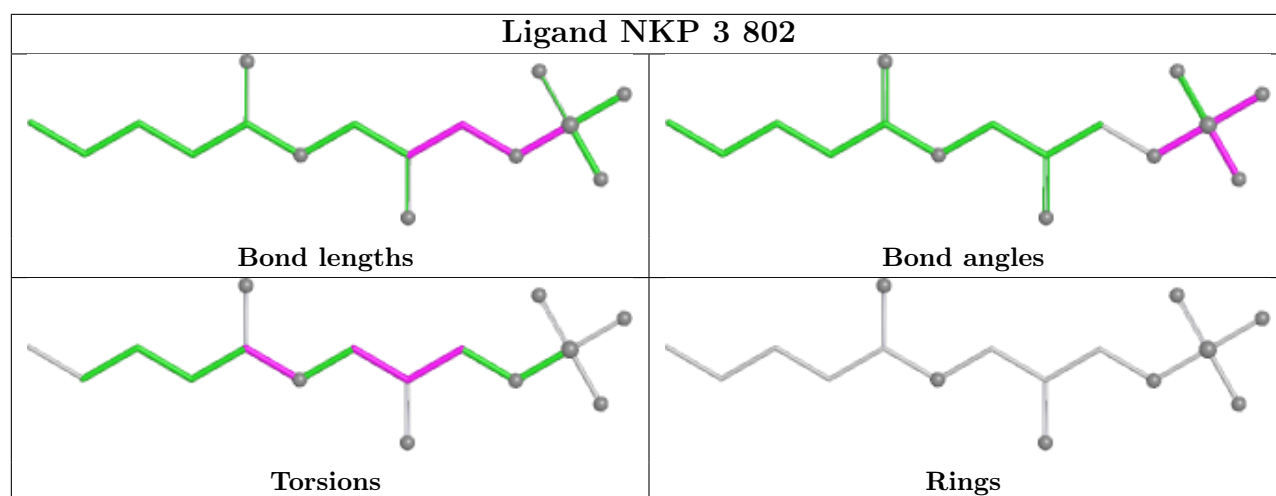
## Ligand CLA B 1227

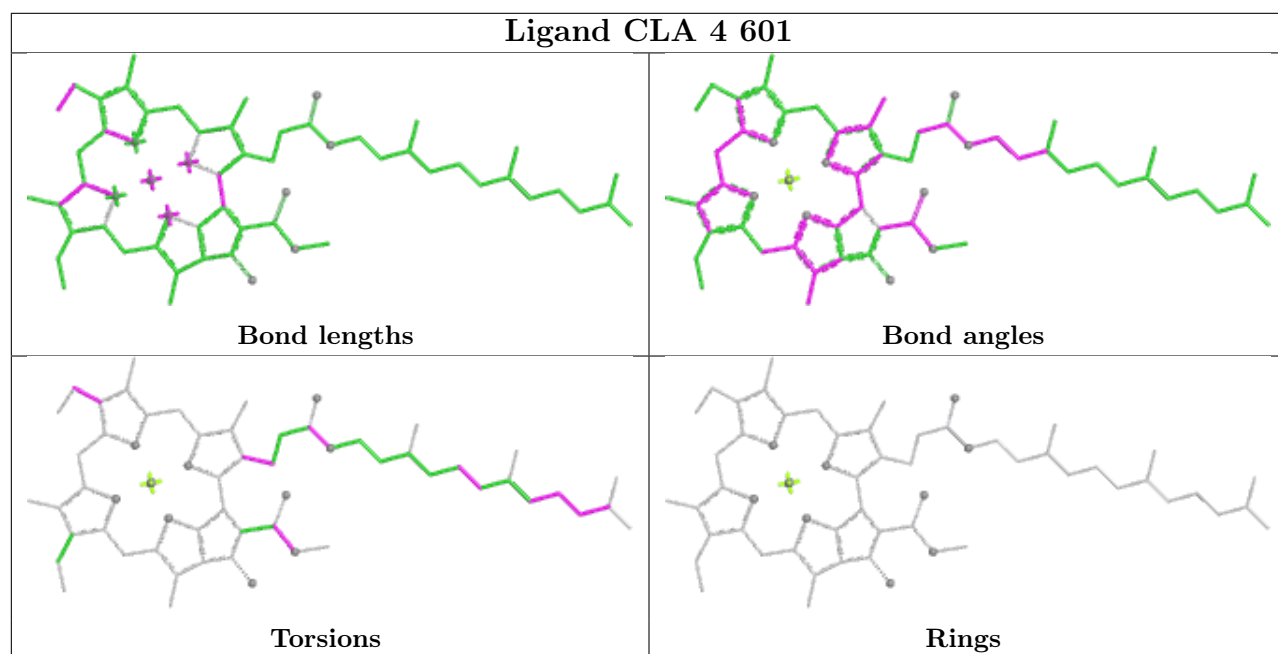
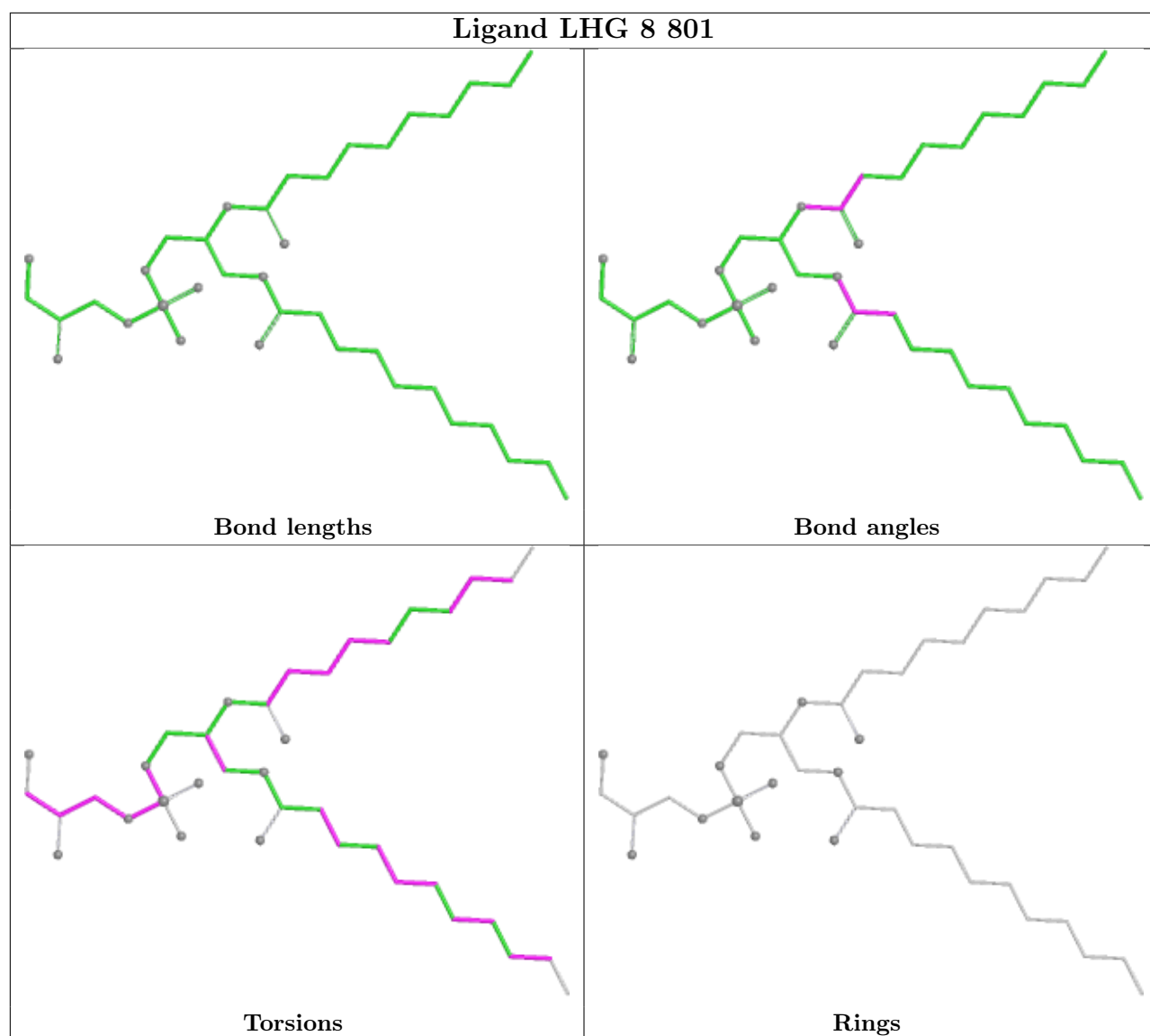


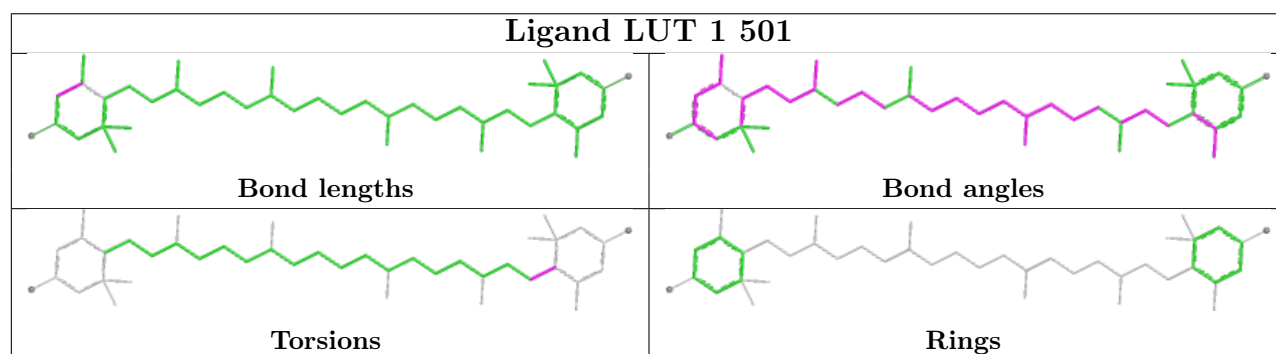
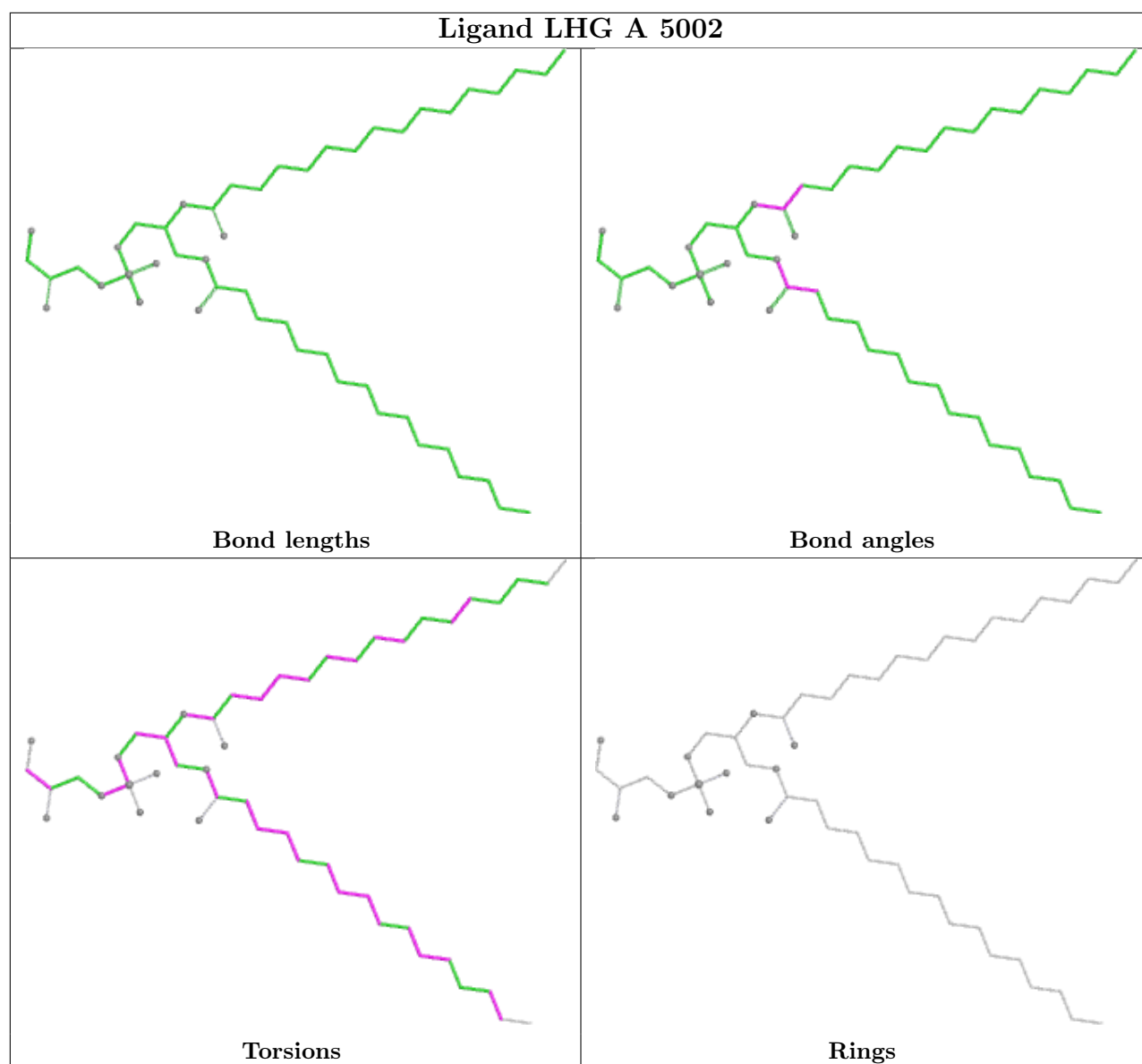


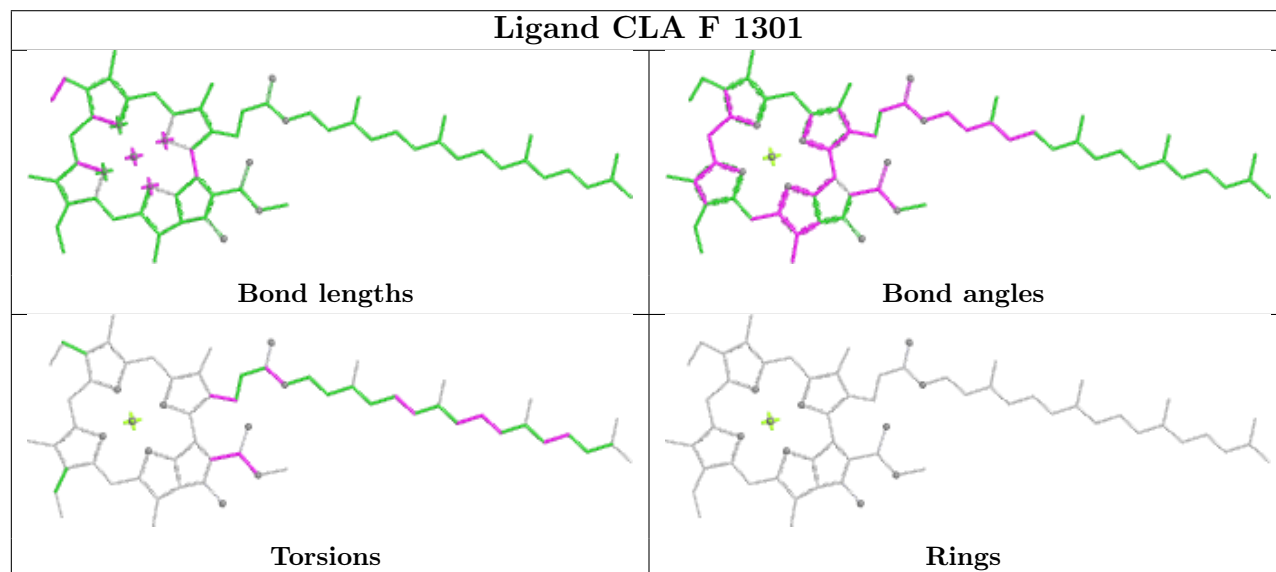
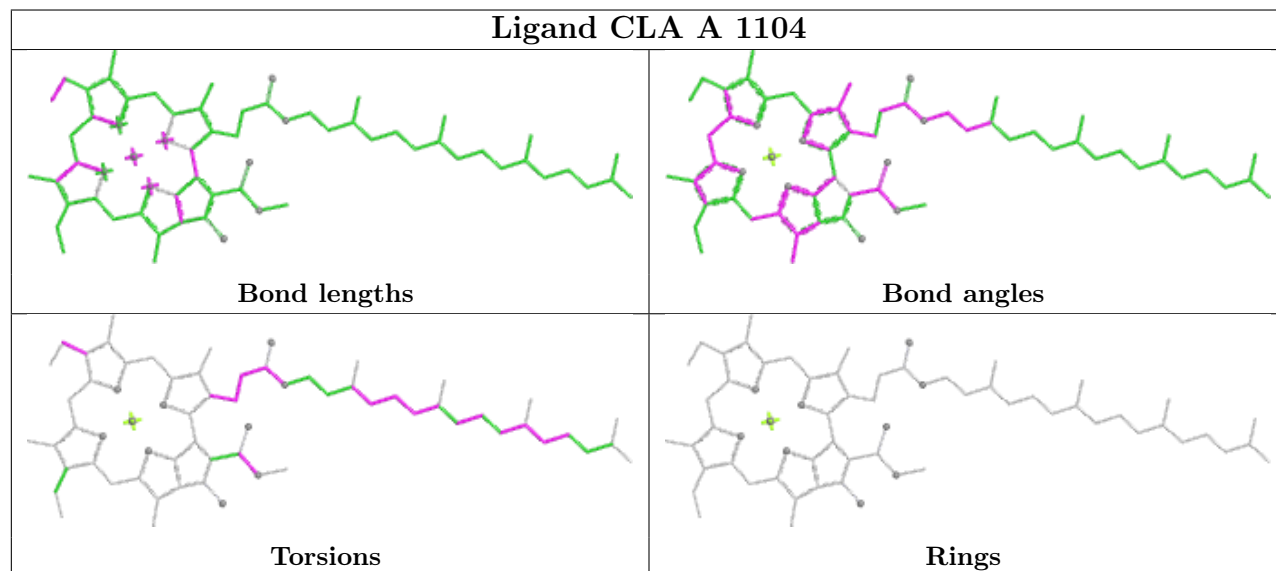
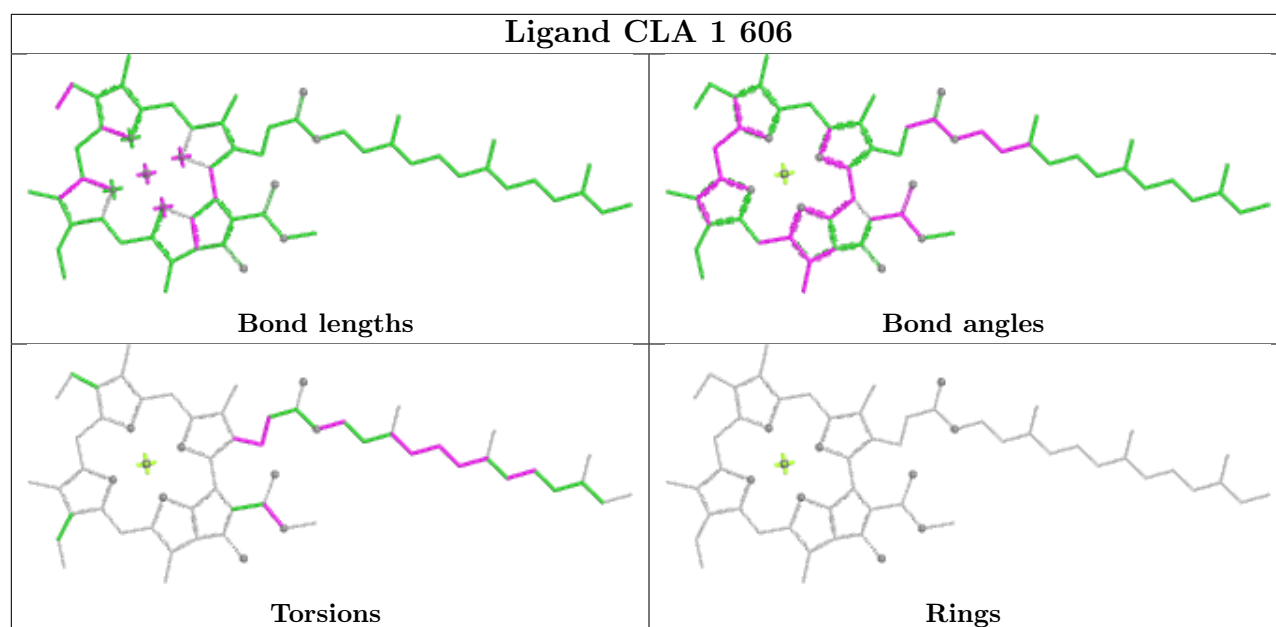




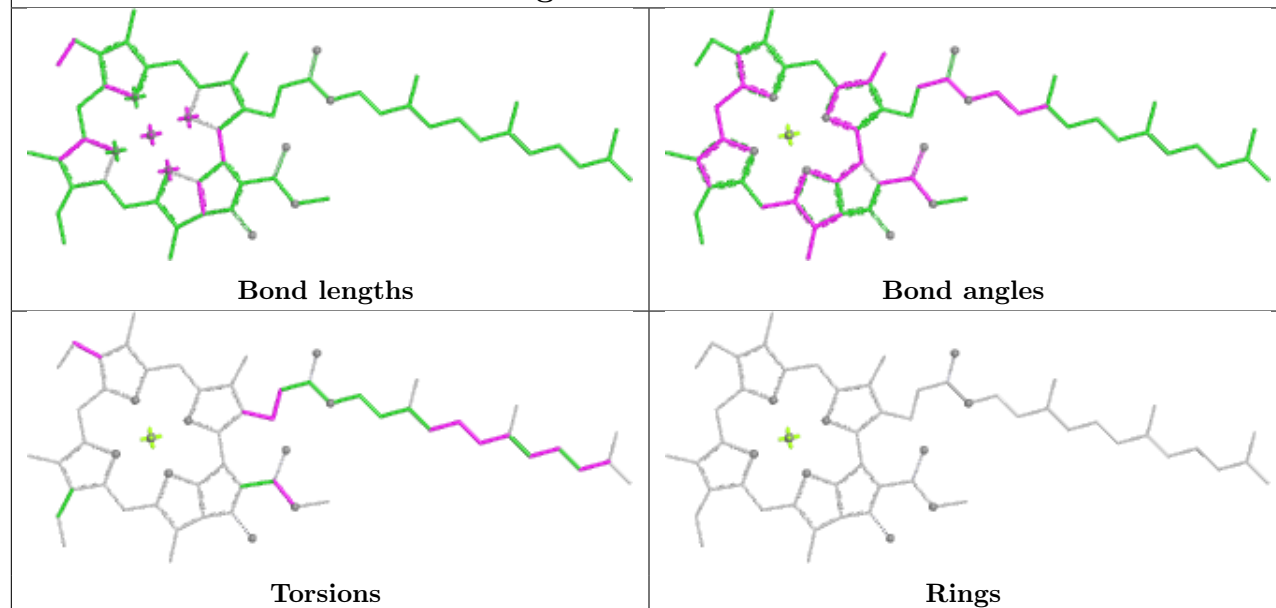




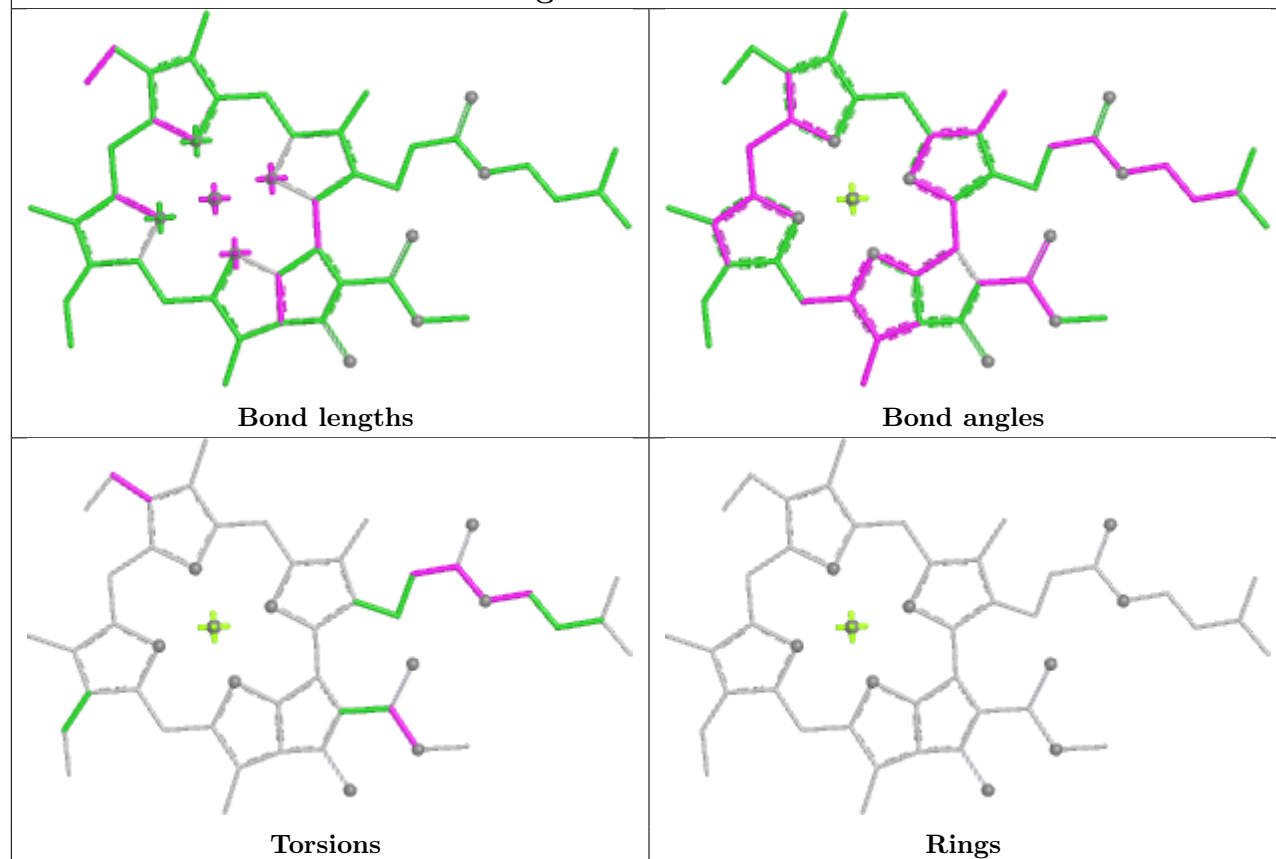


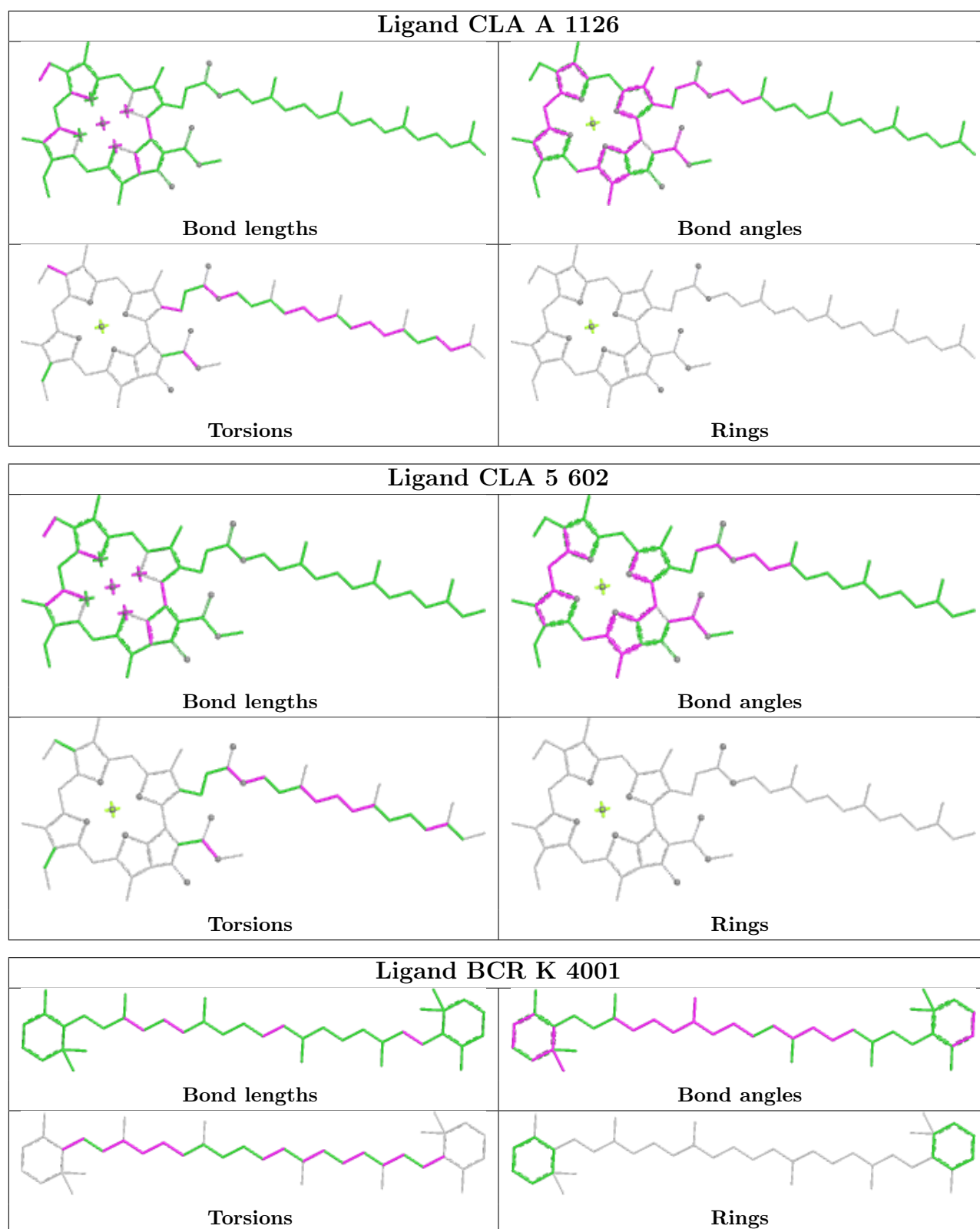


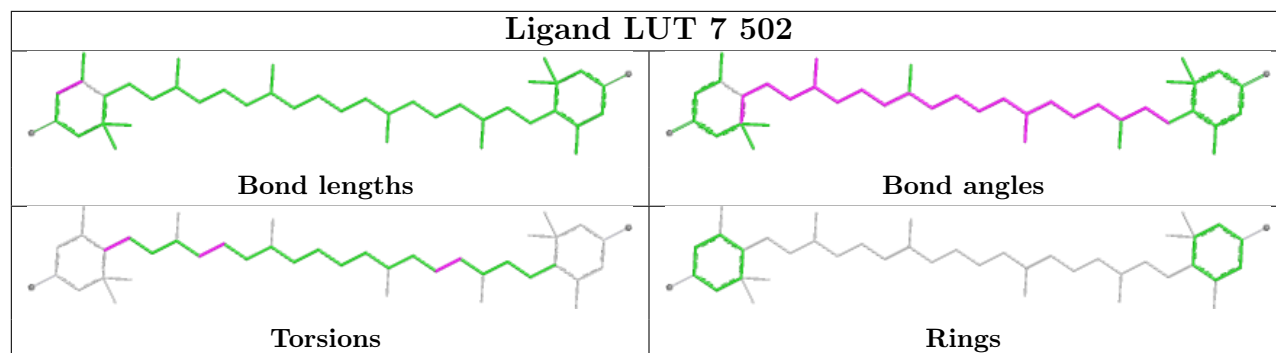
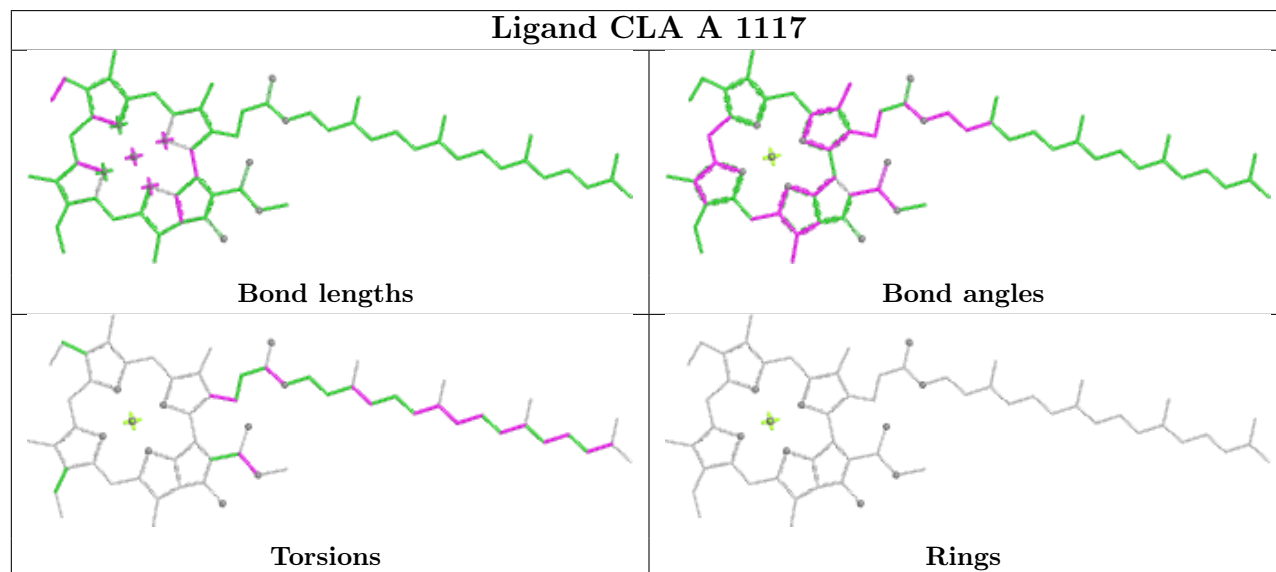
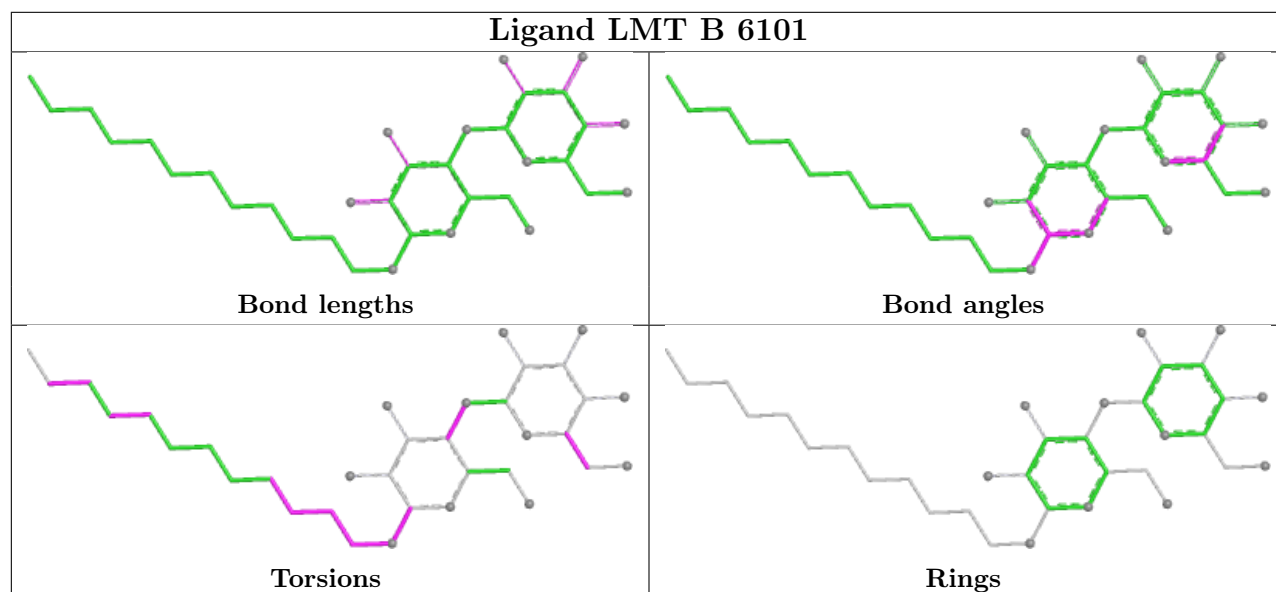
## Ligand CLA 3 612

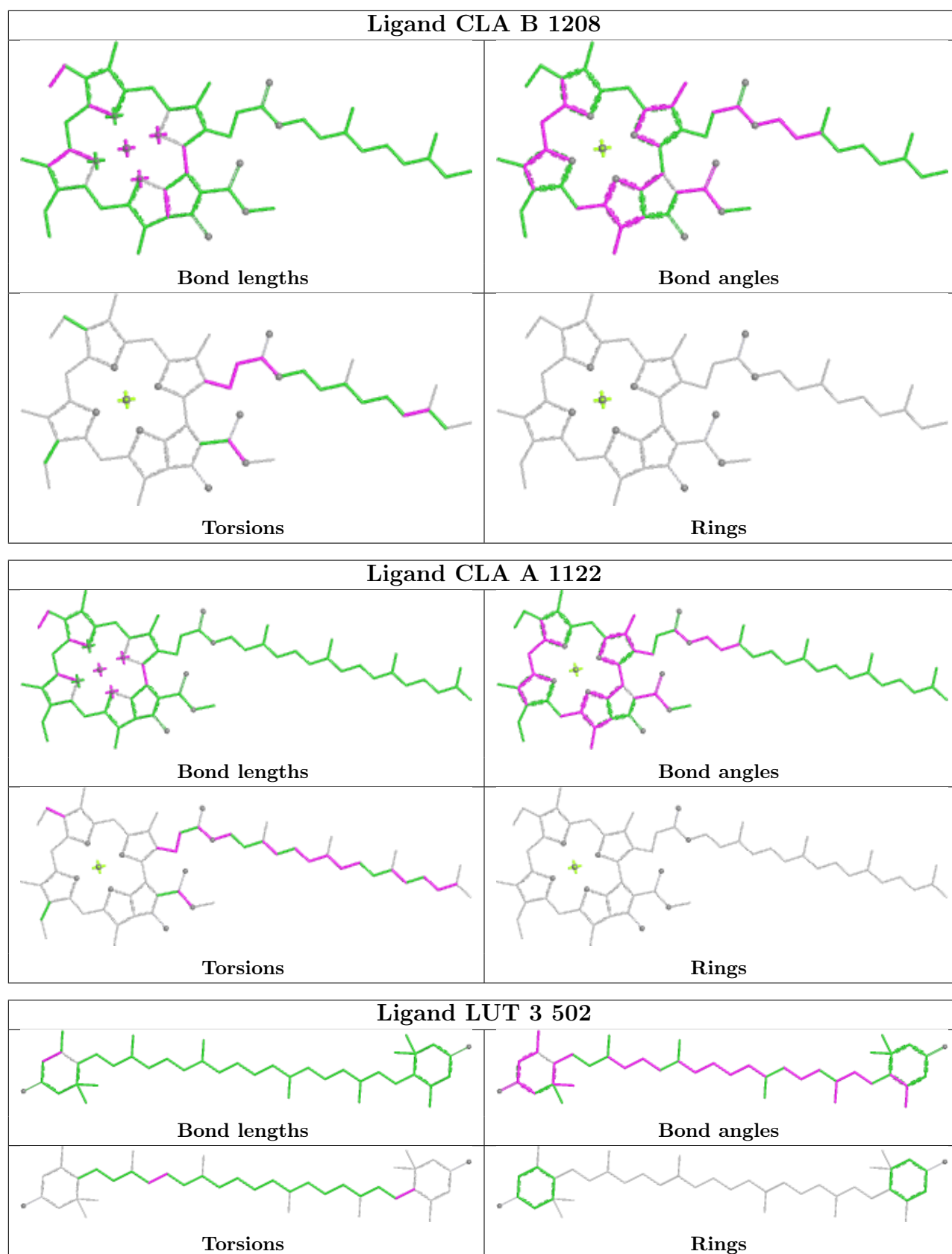


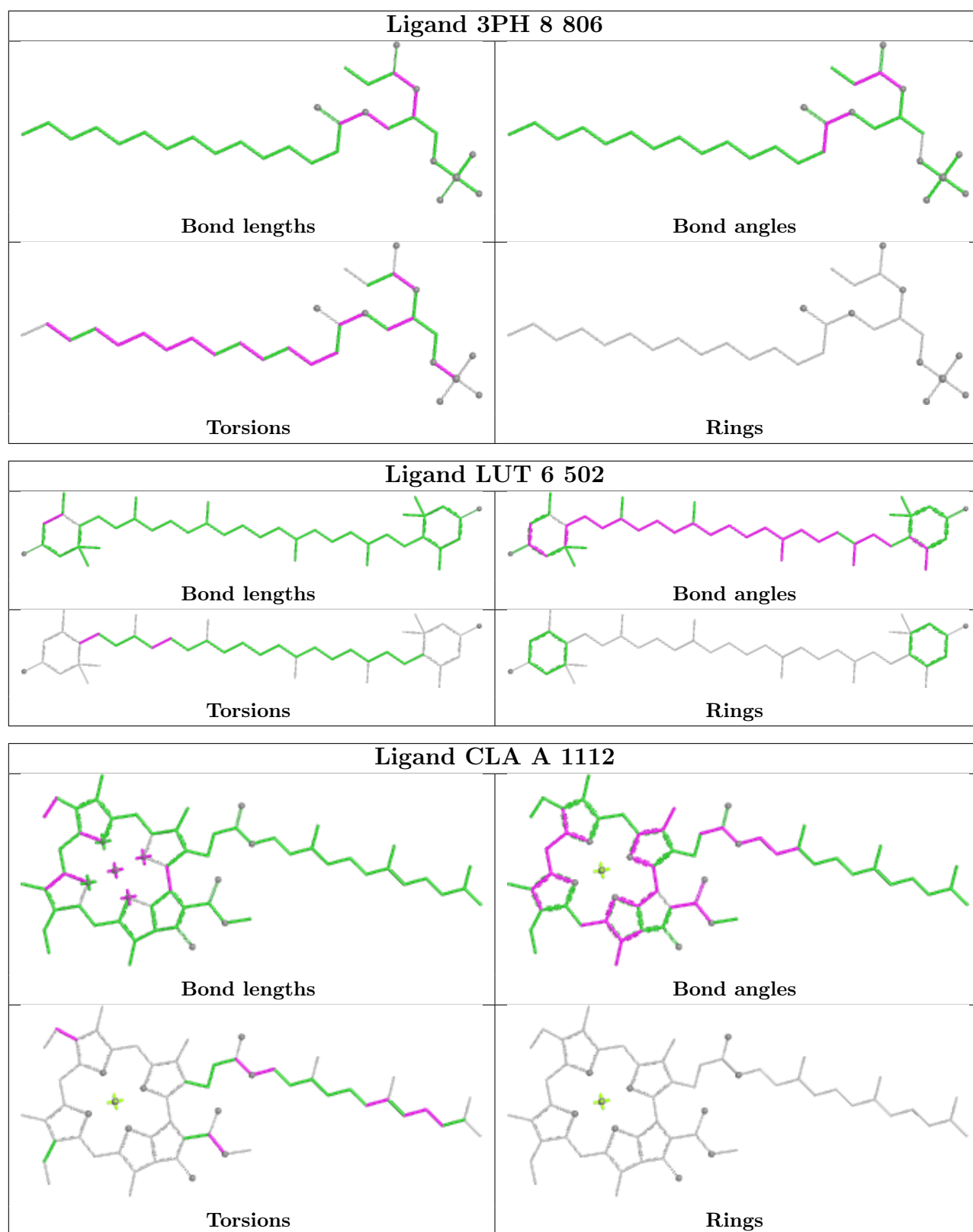
## Ligand CLA 8 611



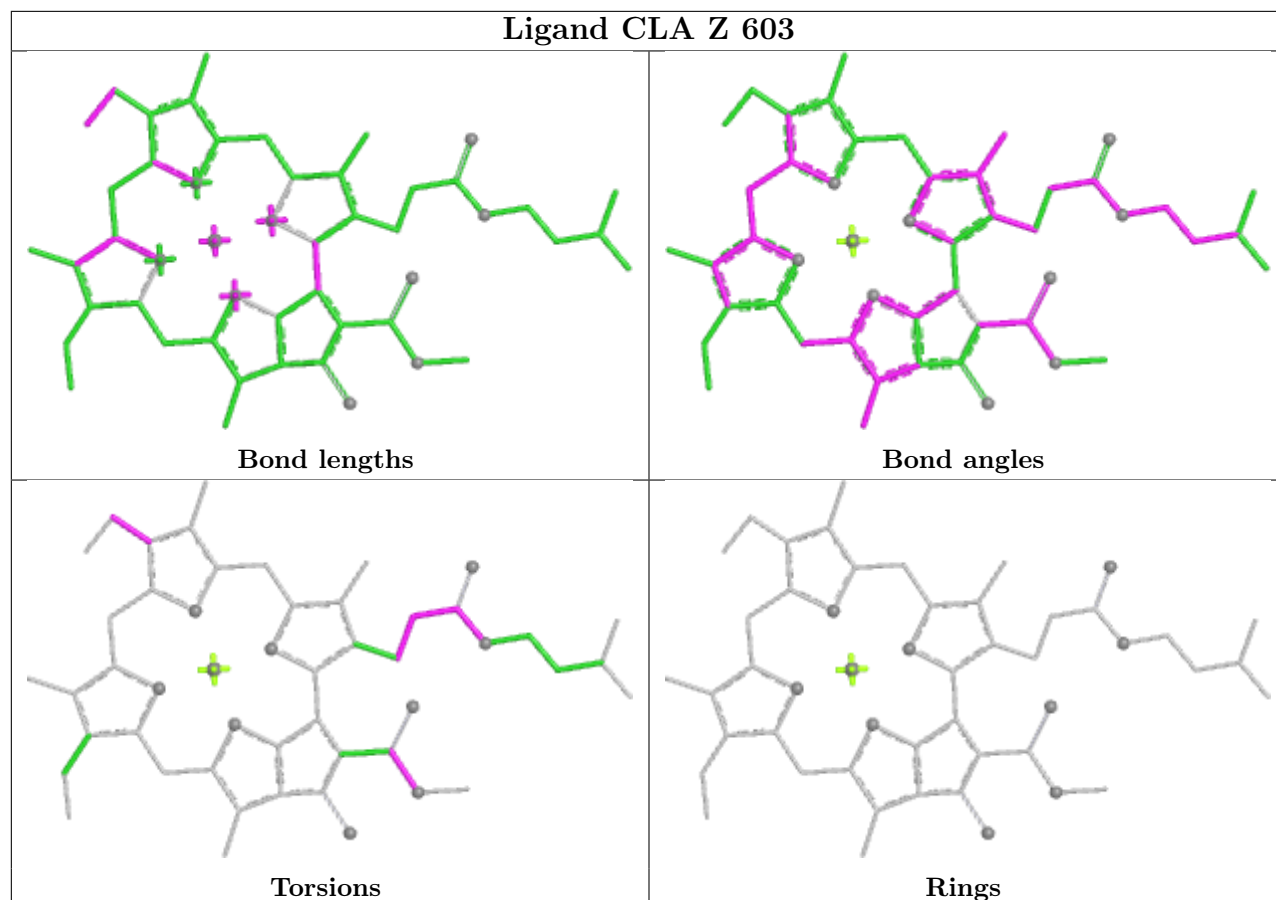


**Ligand LUT 7 502****Ligand CLA A 1117****Ligand LMT B 6101**

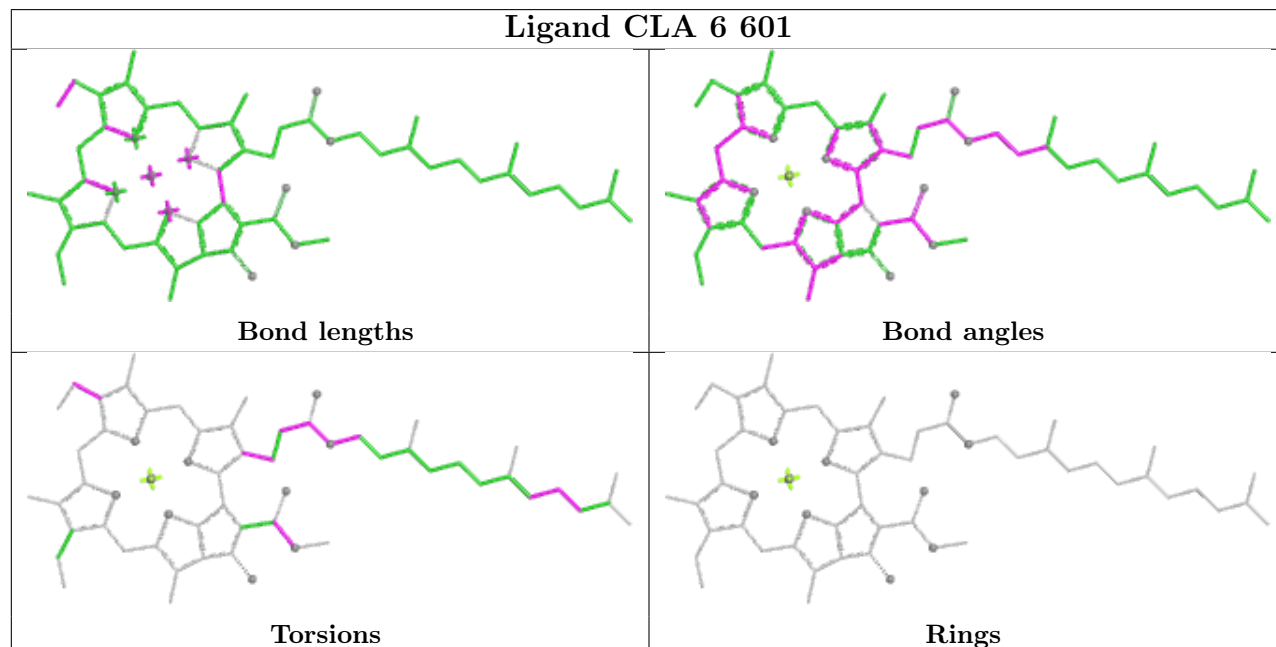


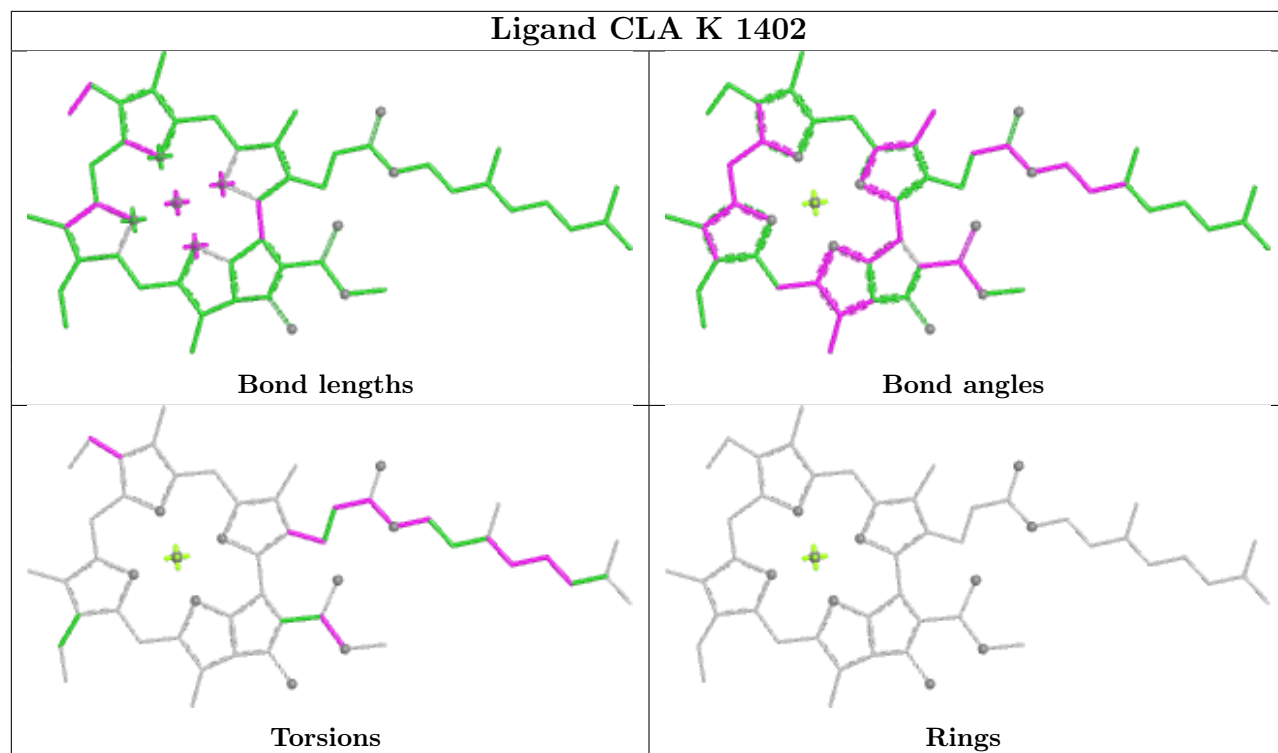


## Ligand CLA Z 603

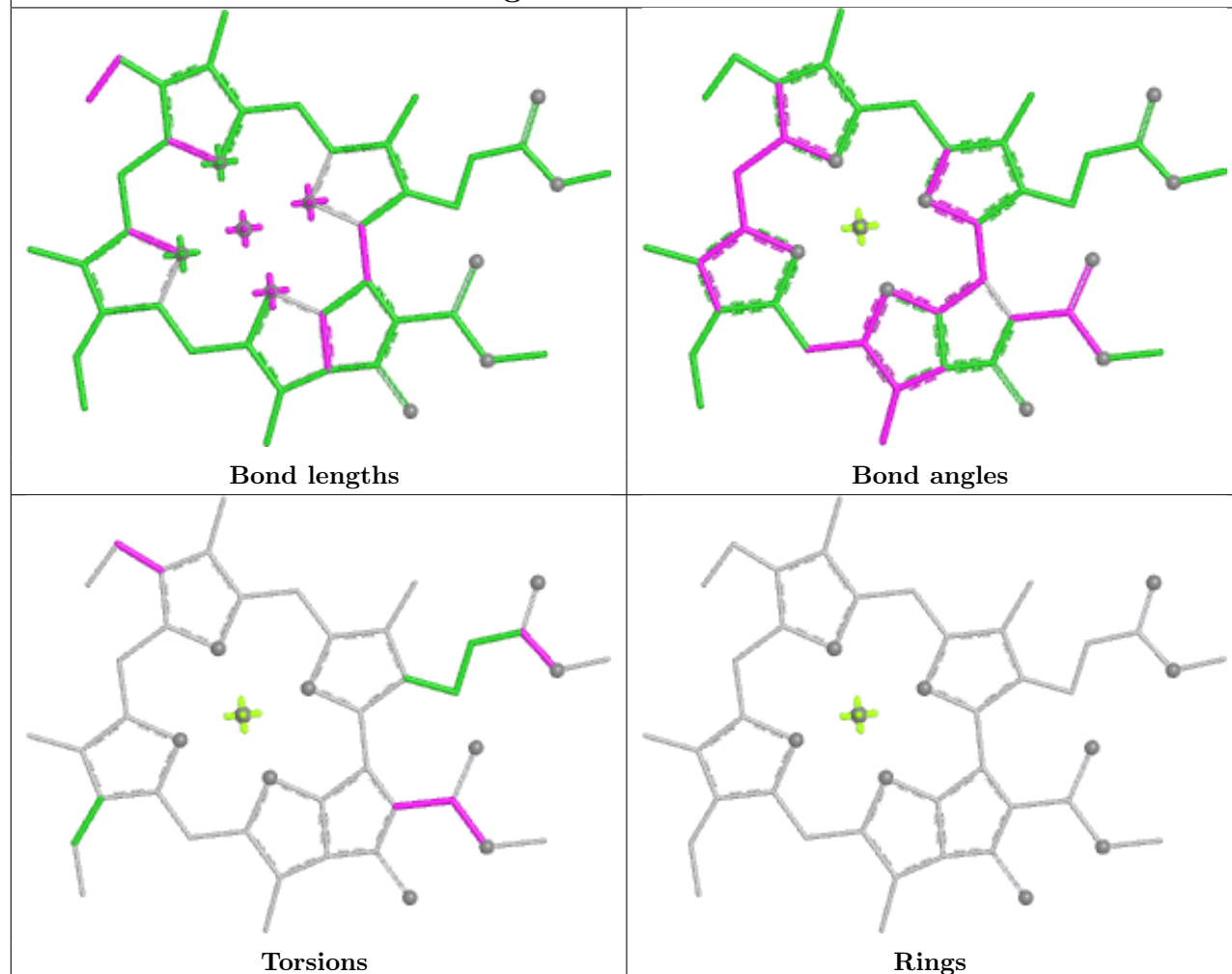


## Ligand CLA 6 601

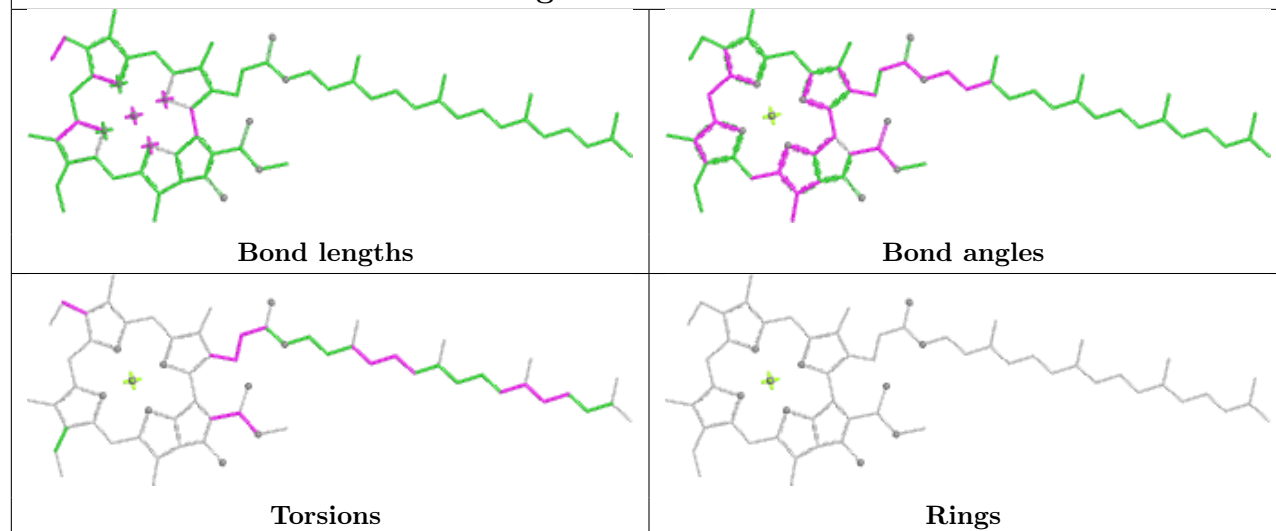


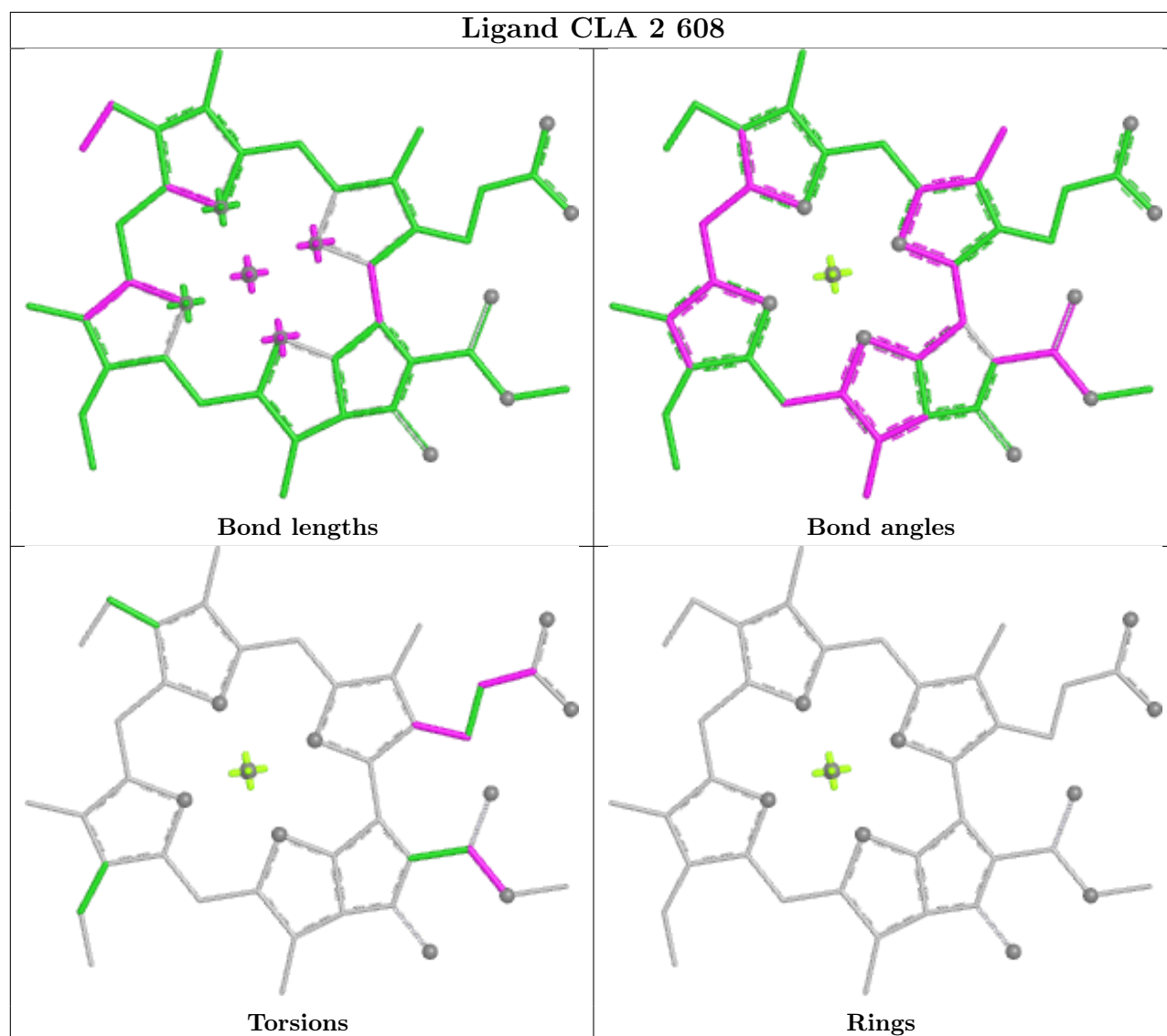
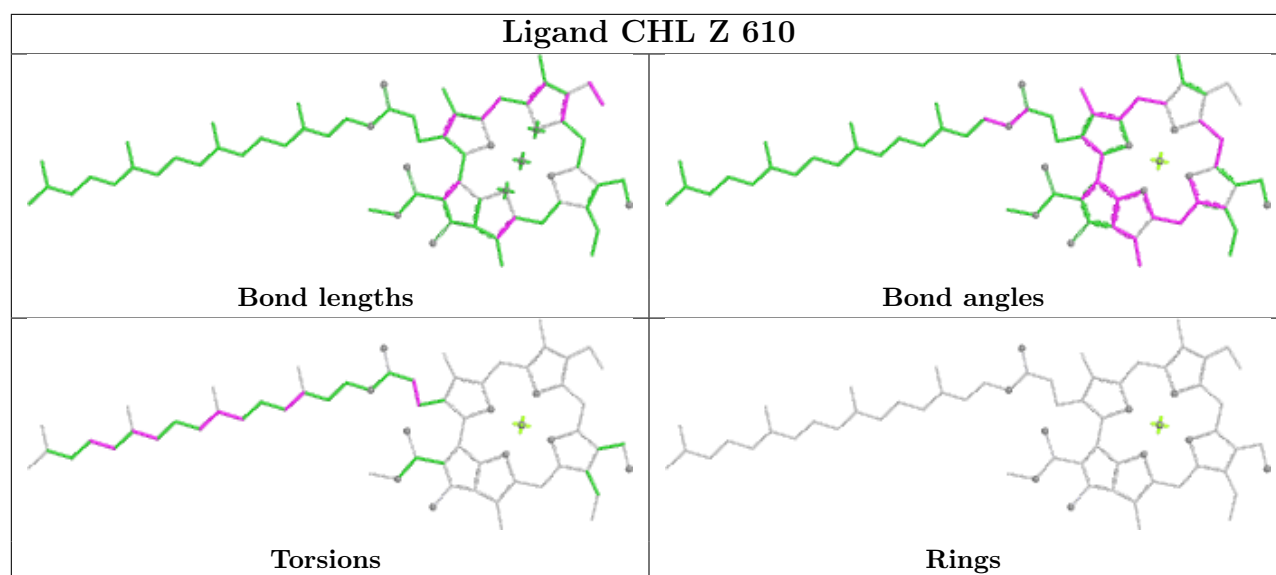


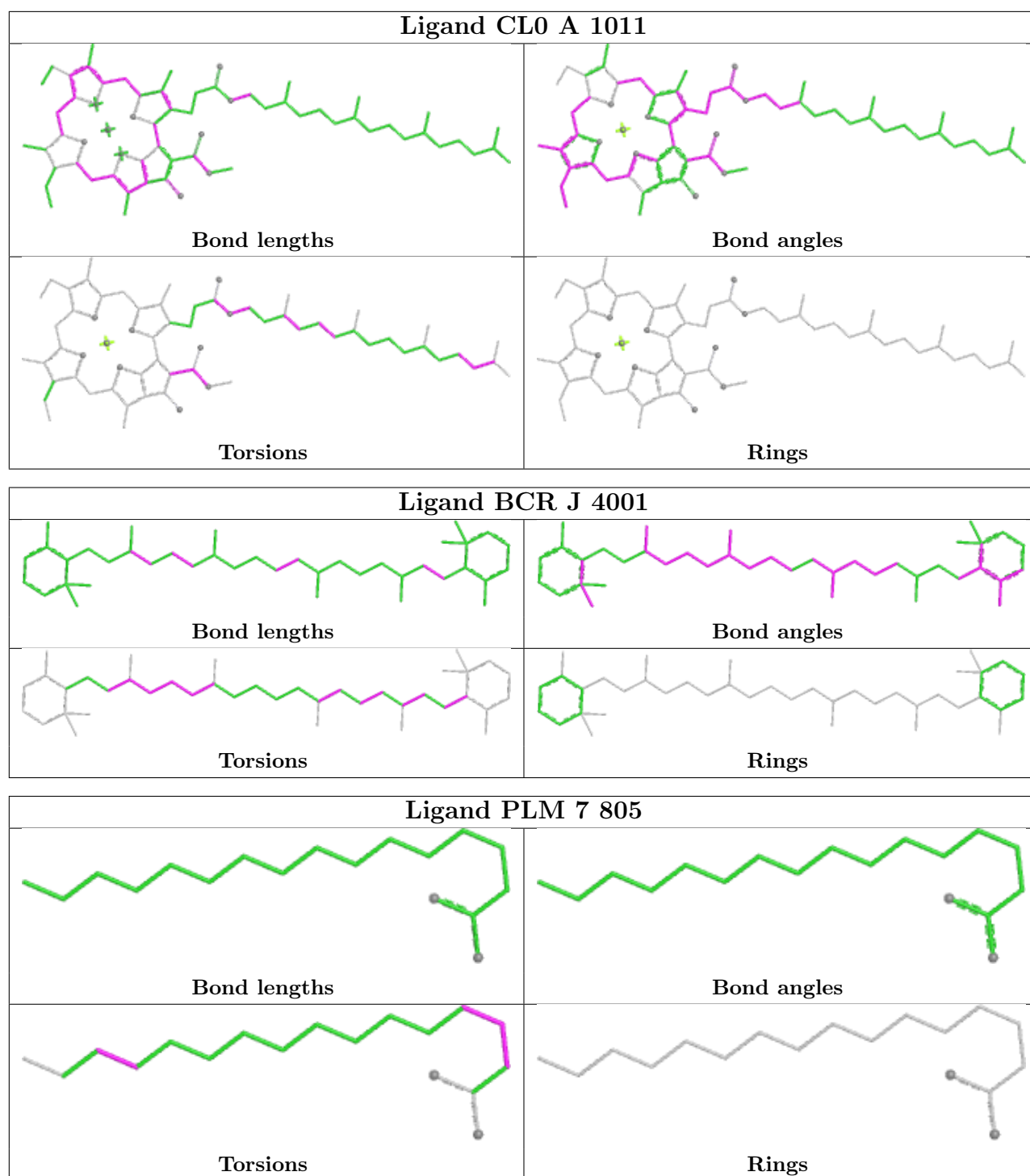
## Ligand CLA G 1602



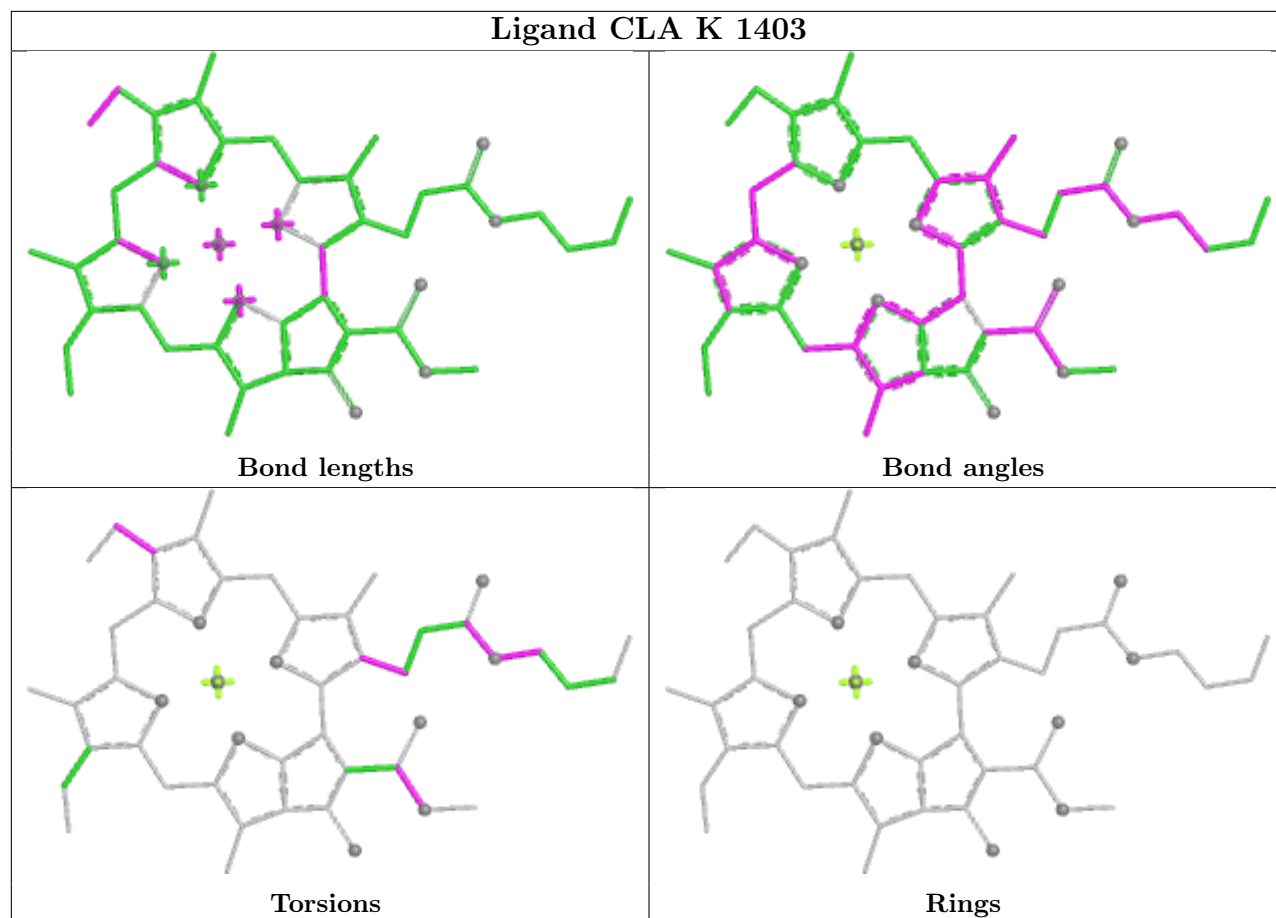
## Ligand CLA 7 609



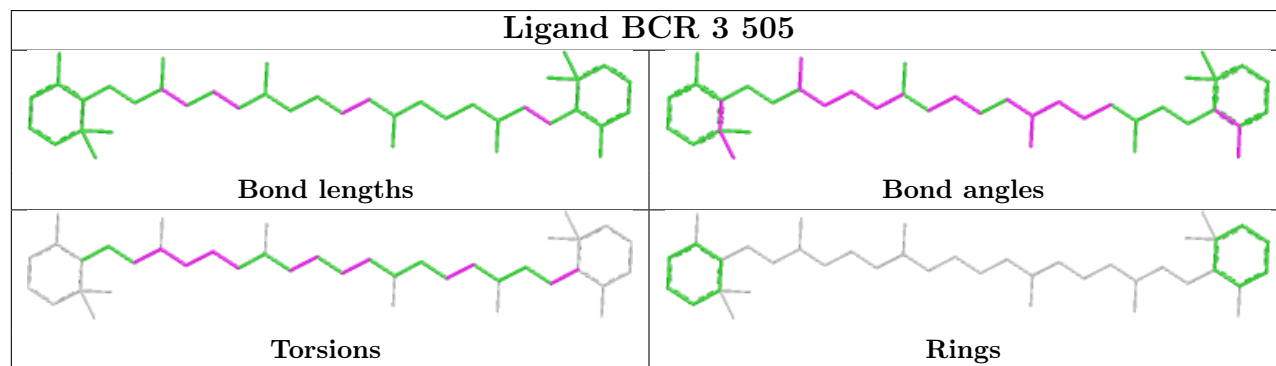


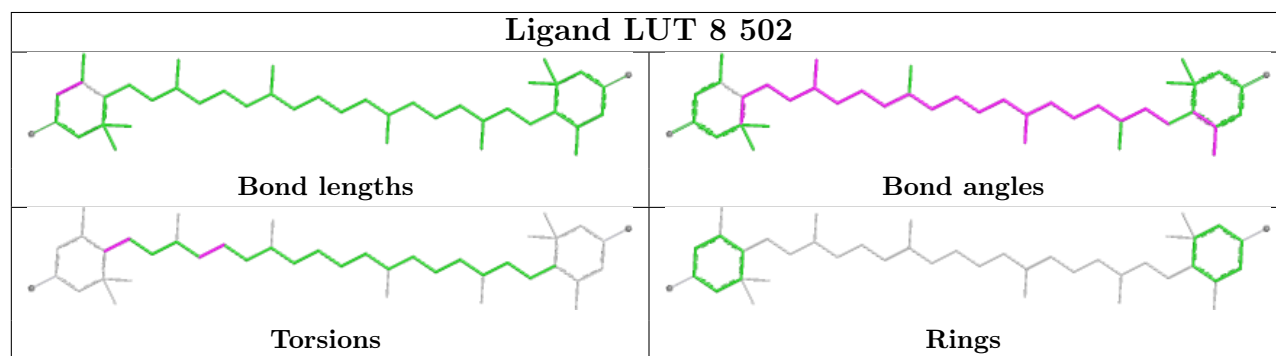
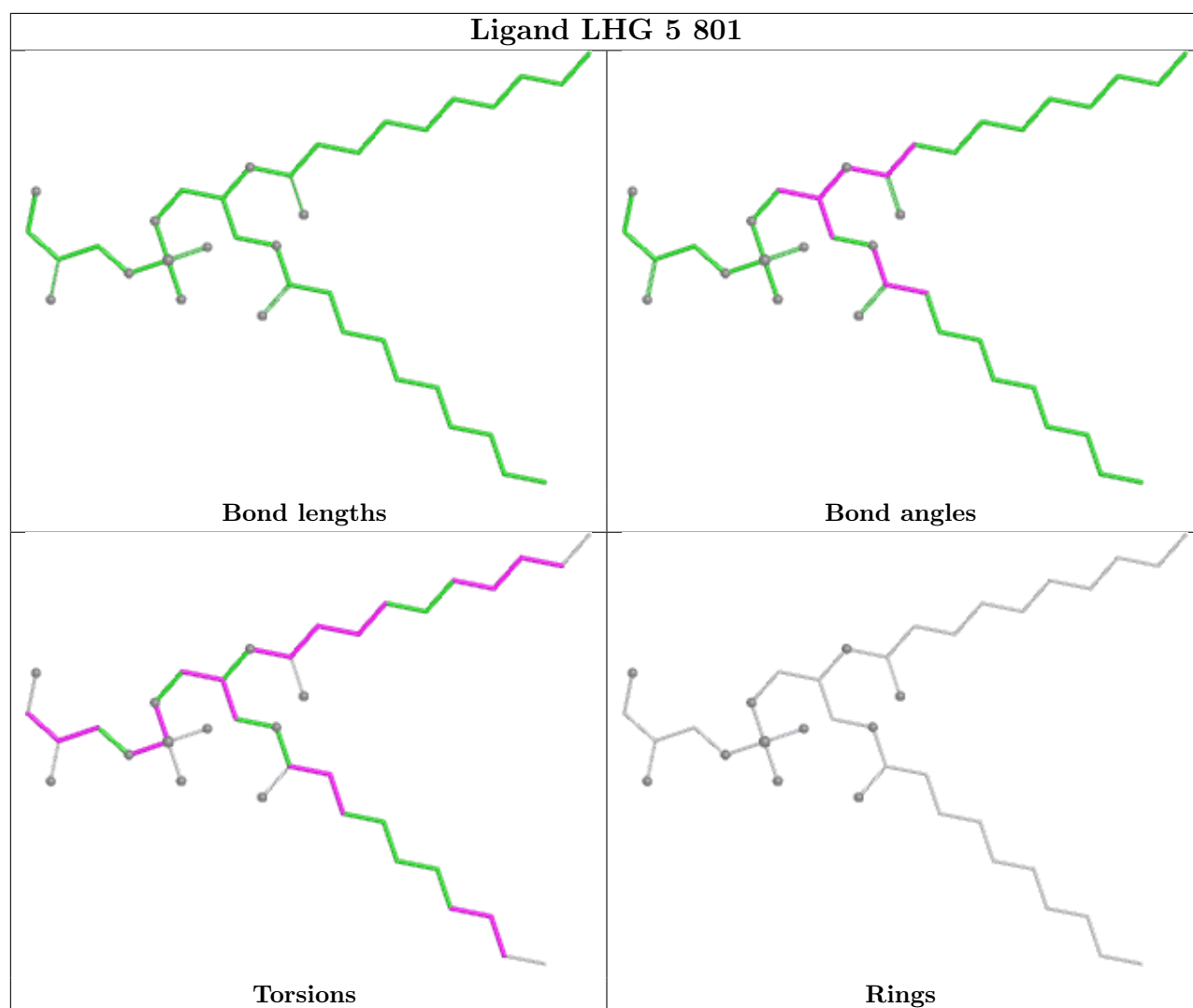


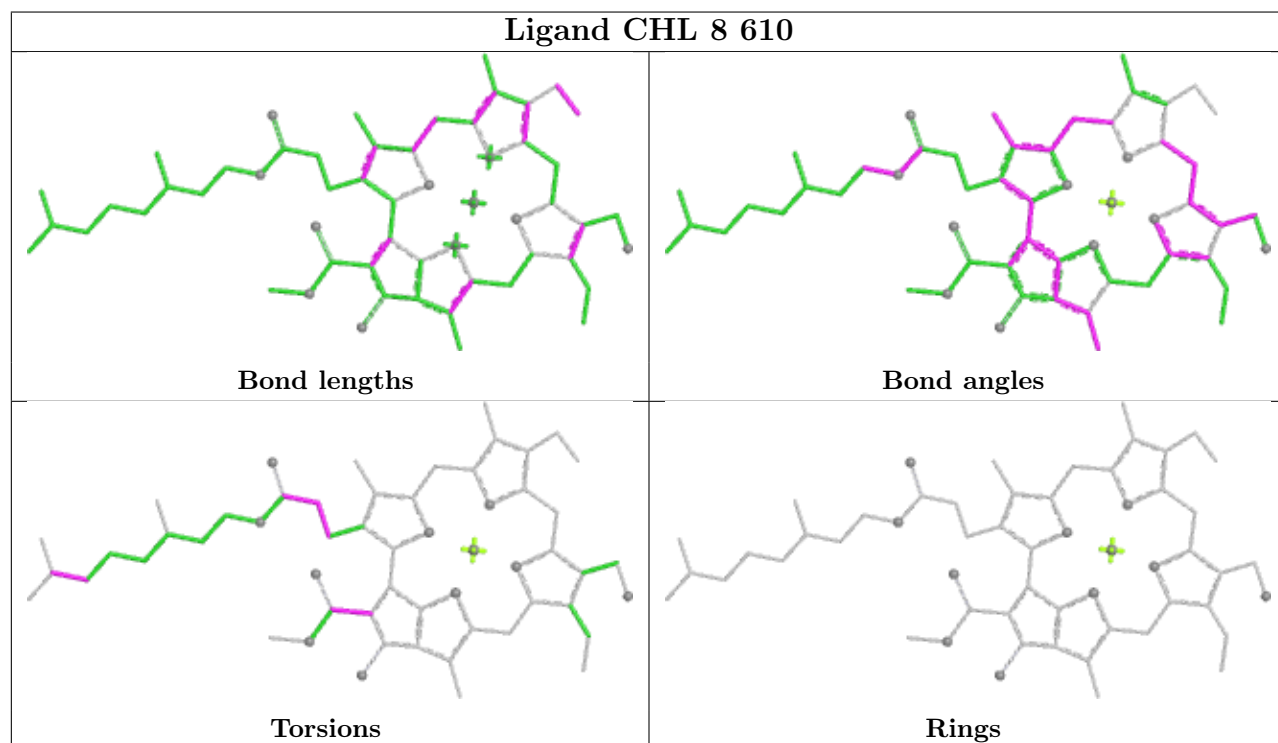
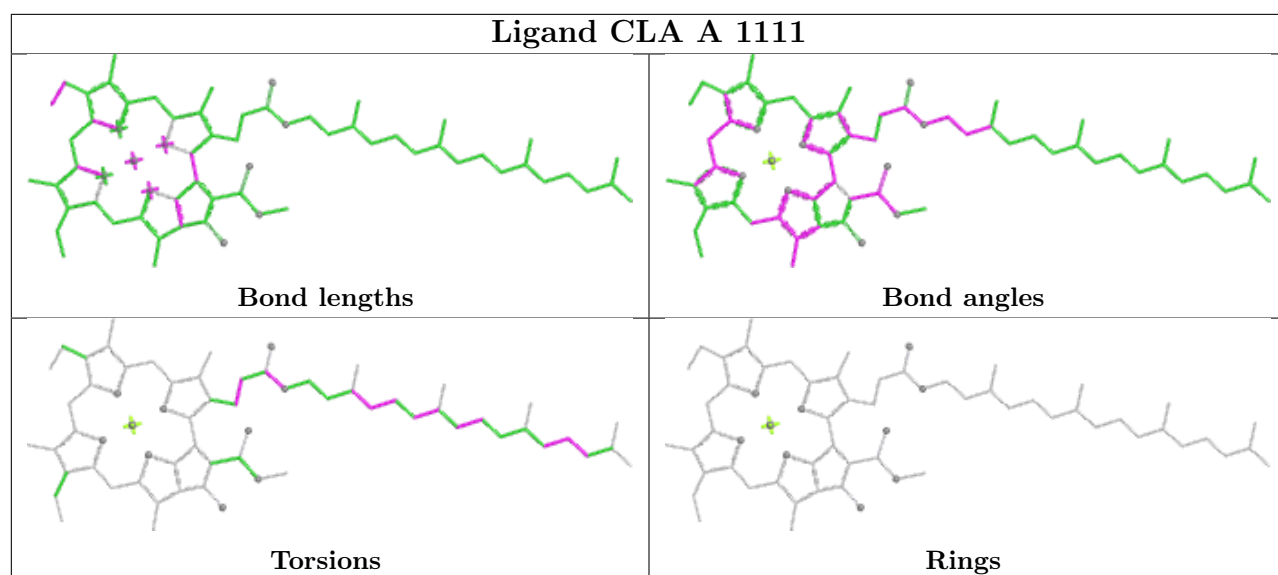
## Ligand CLA K 1403

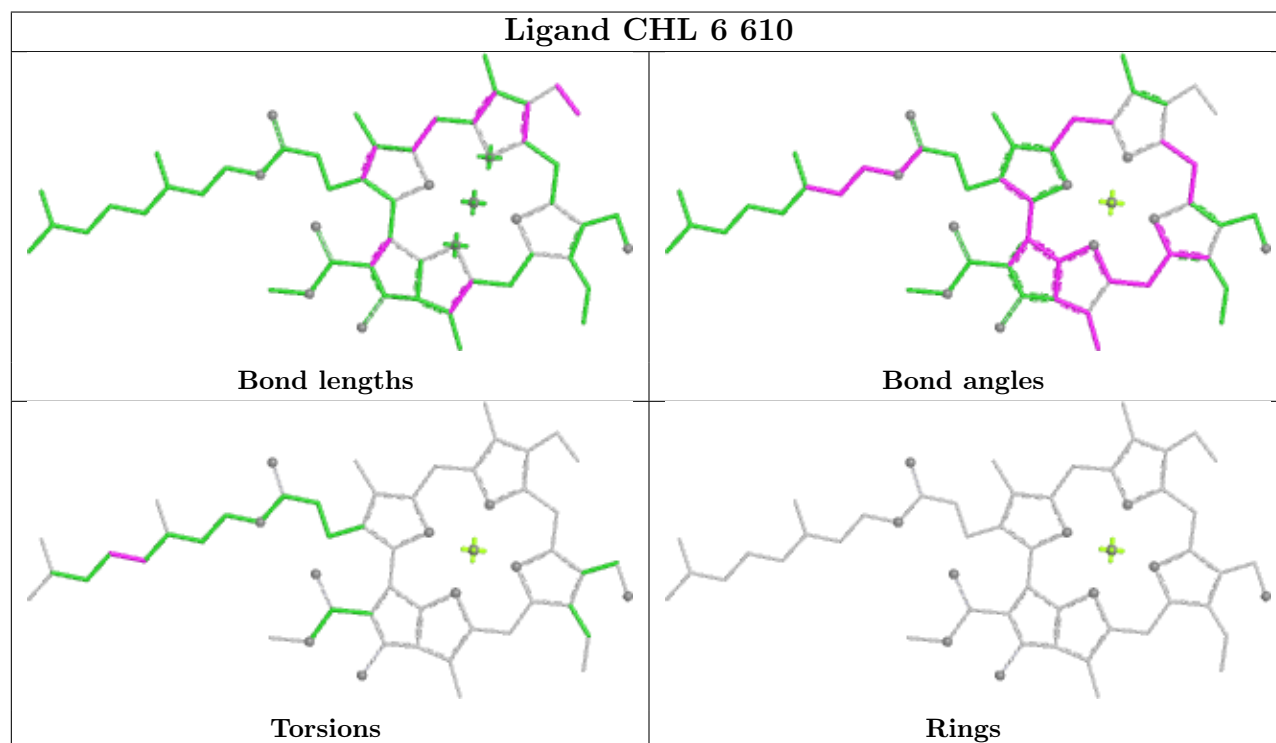
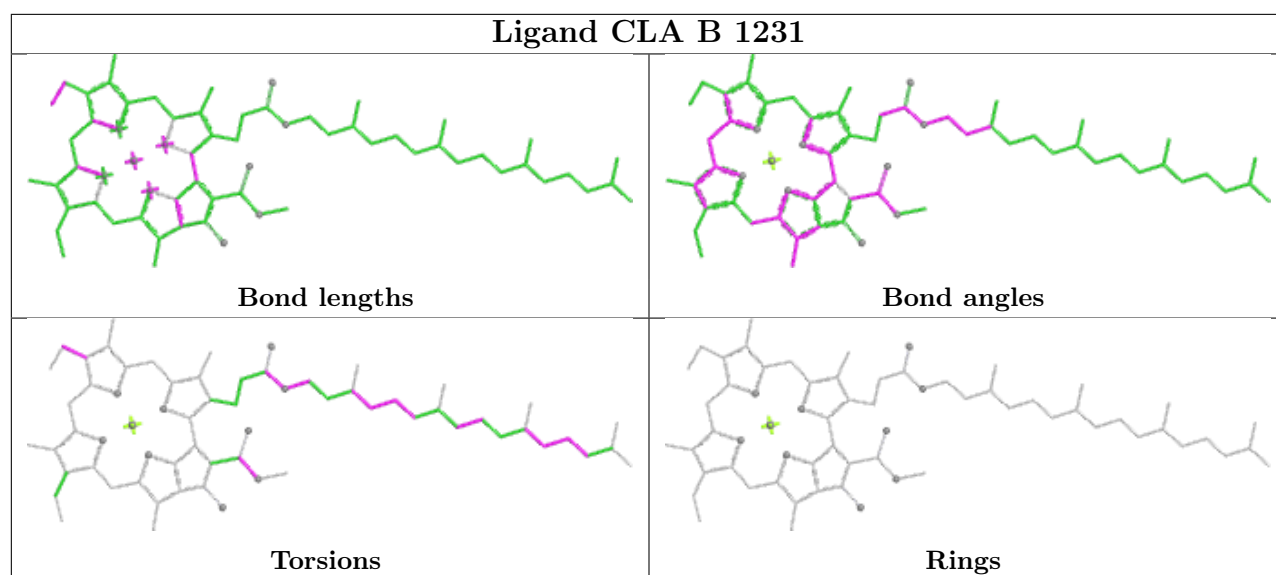


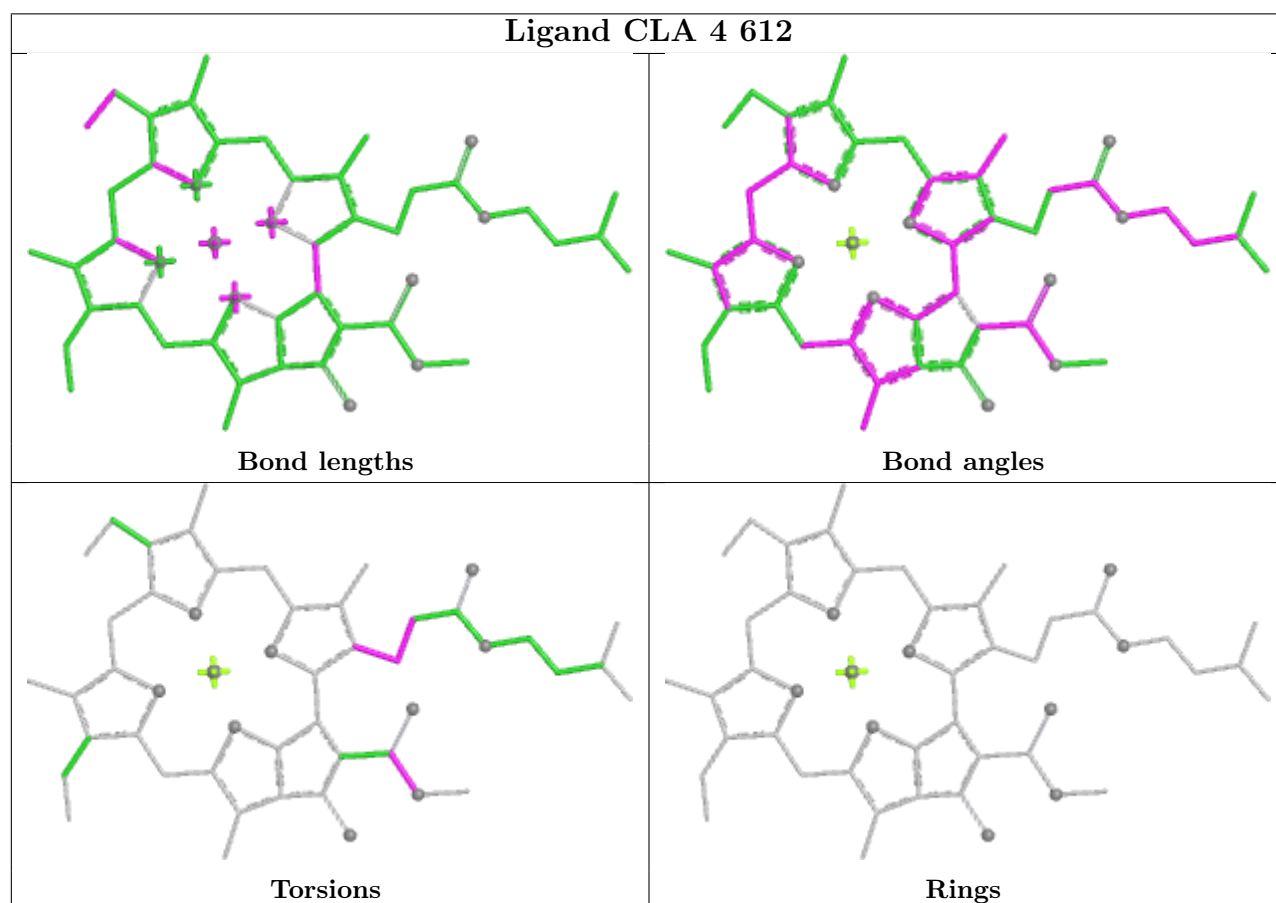
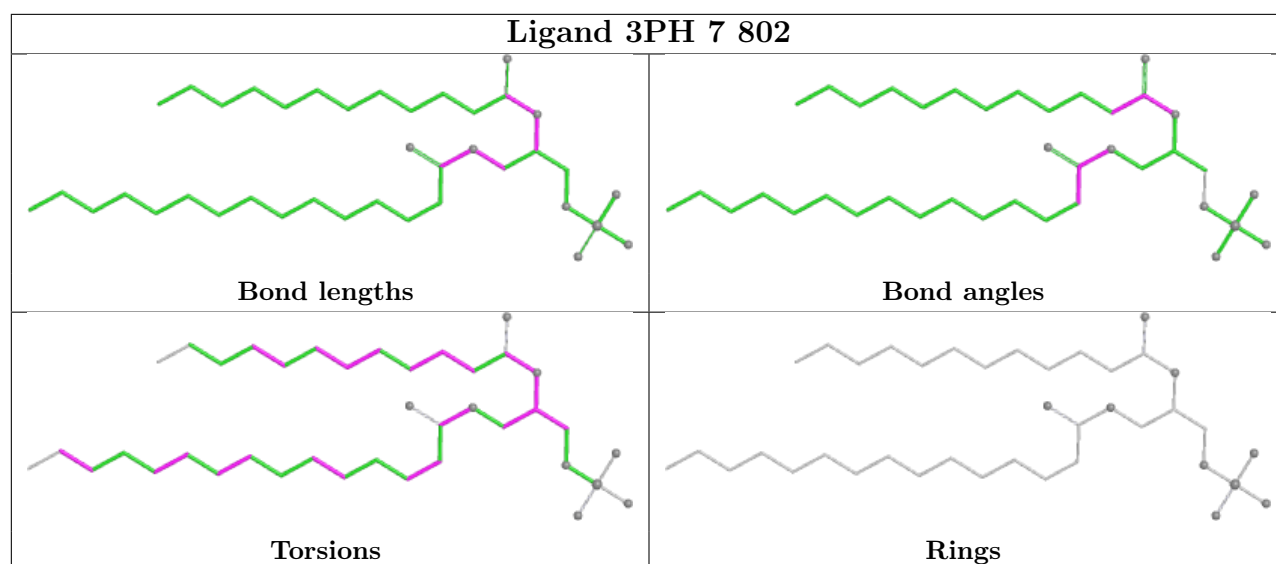
## Ligand BCR 3 505

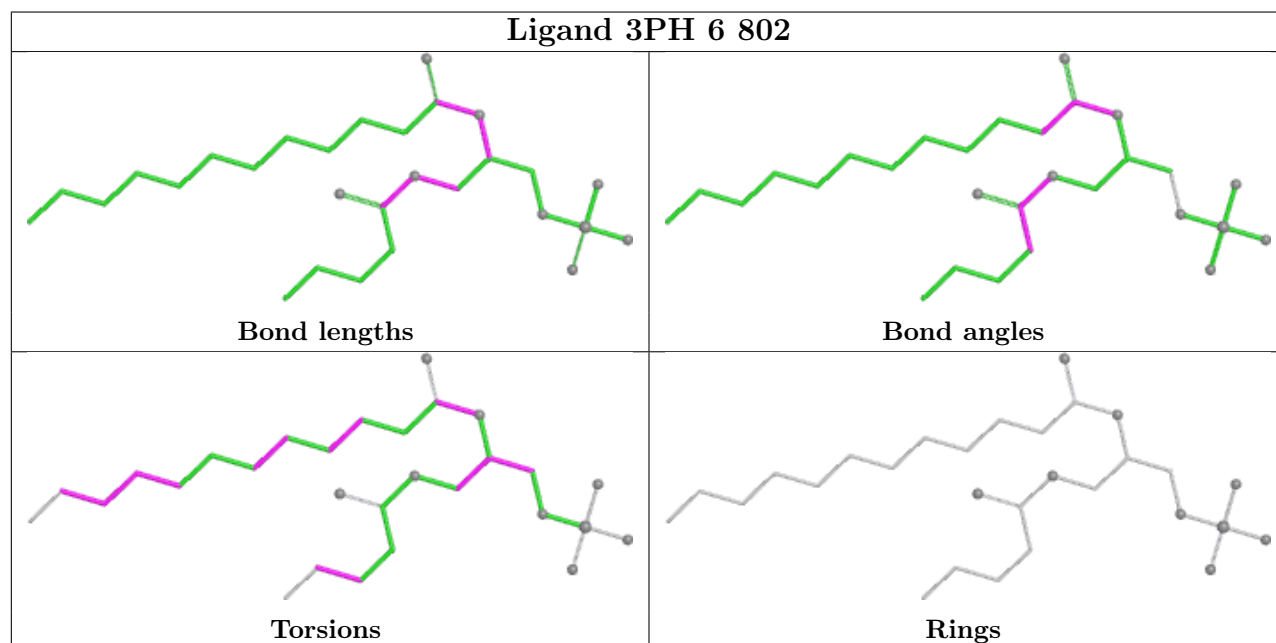
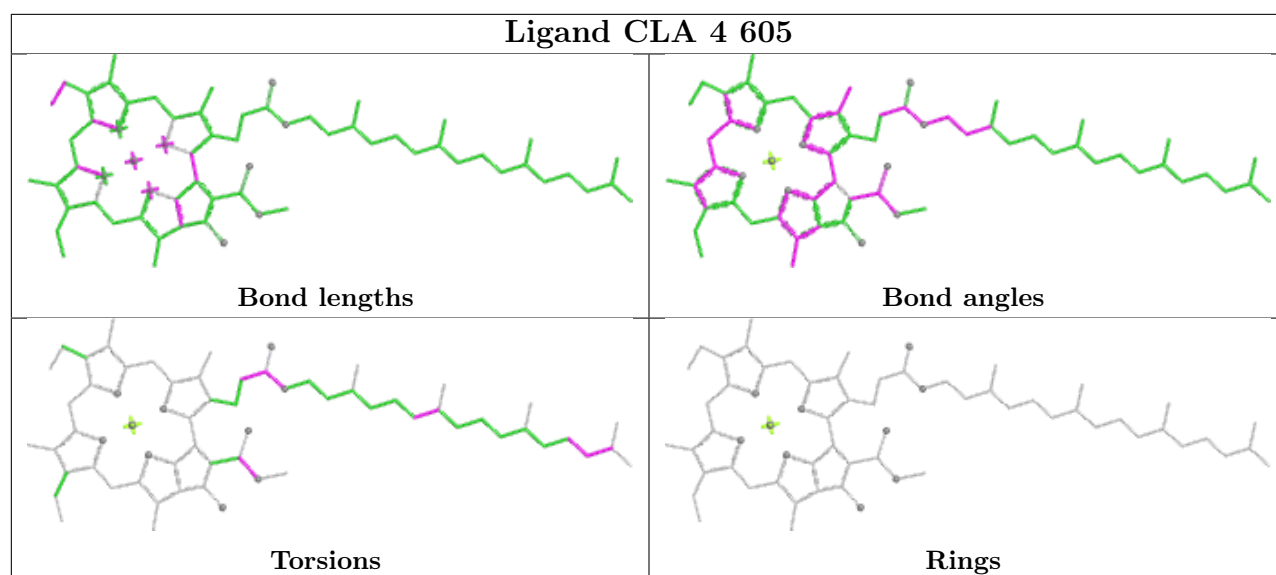


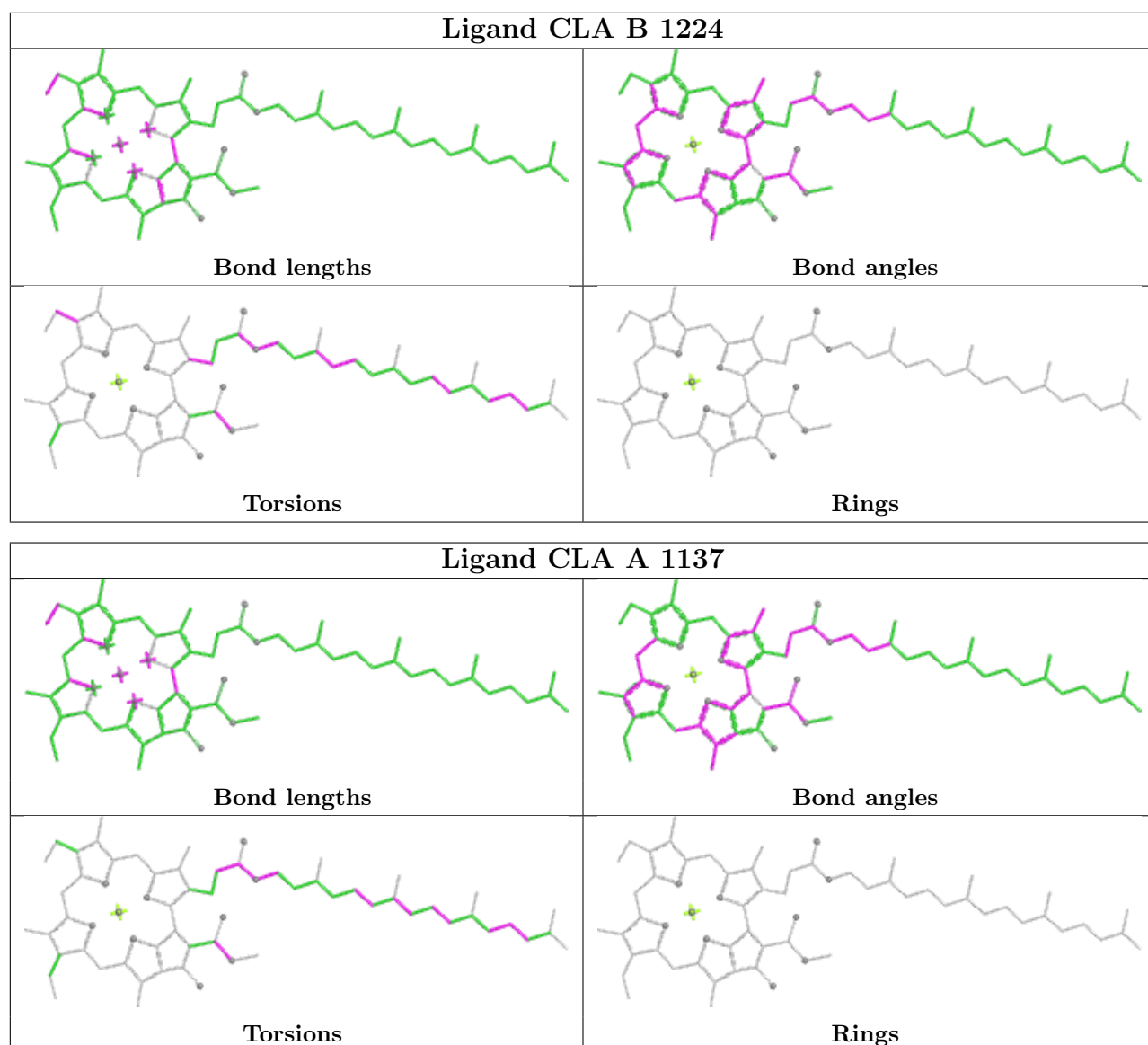




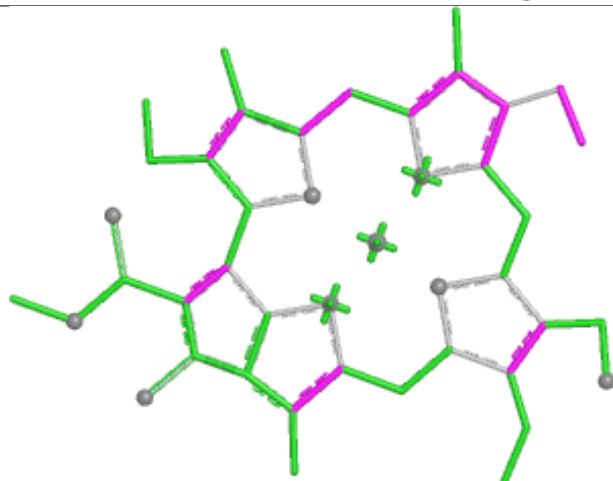




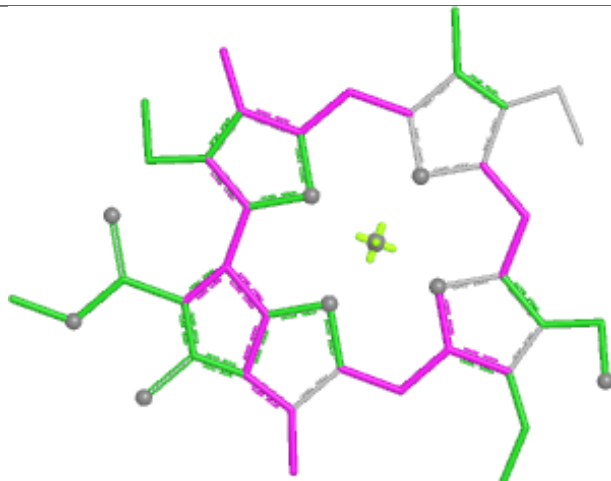




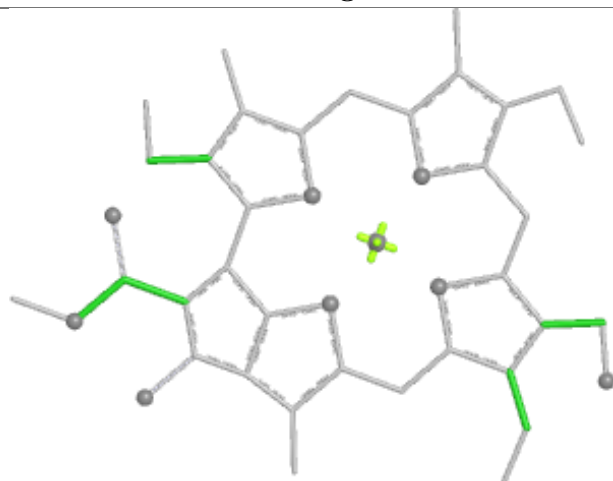
## Ligand CHL 6 617



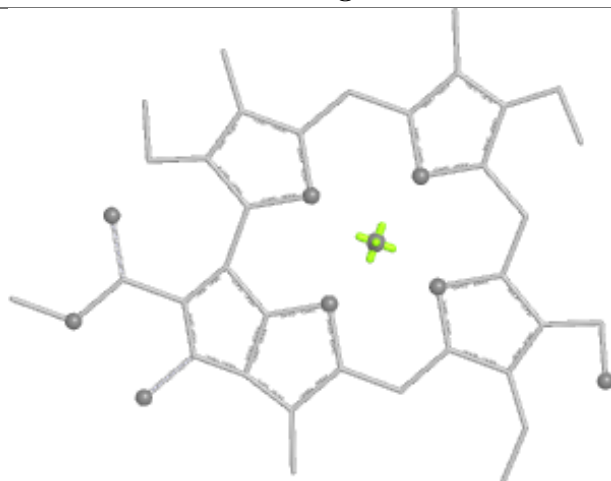
Bond lengths



Bond angles

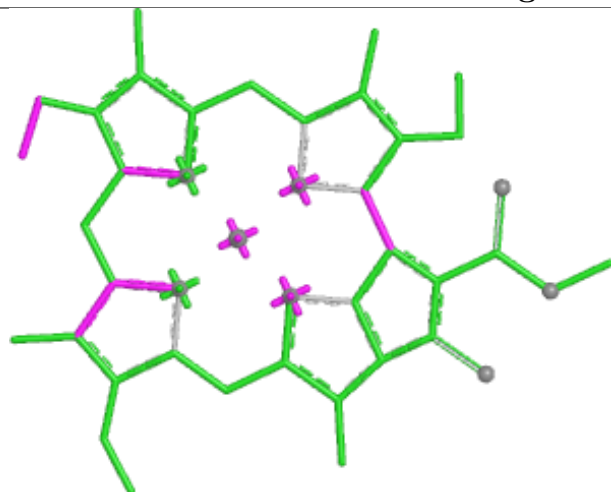


Torsions



Rings

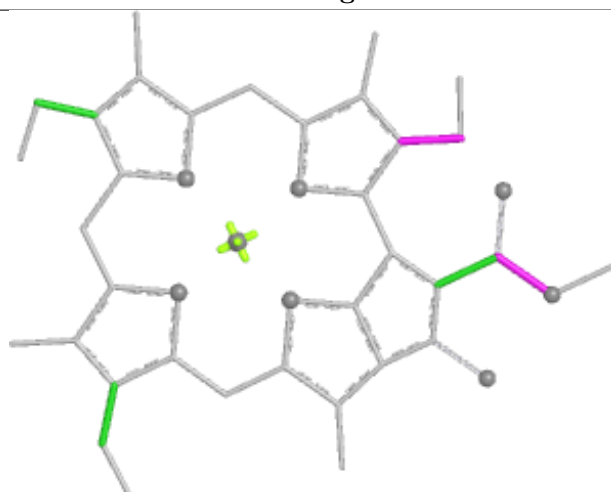
## Ligand CLA 7 613



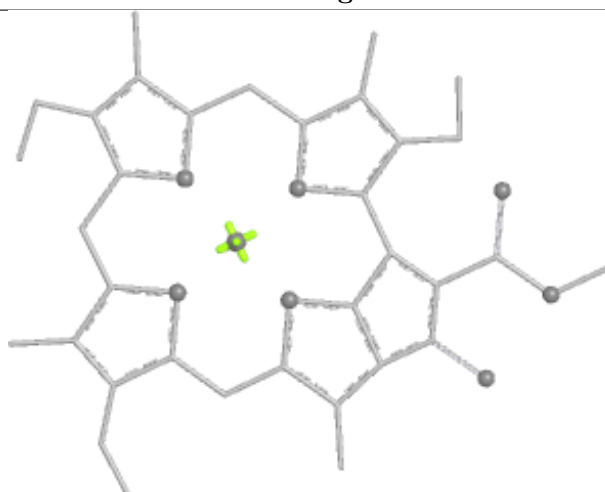
Bond lengths



Bond angles

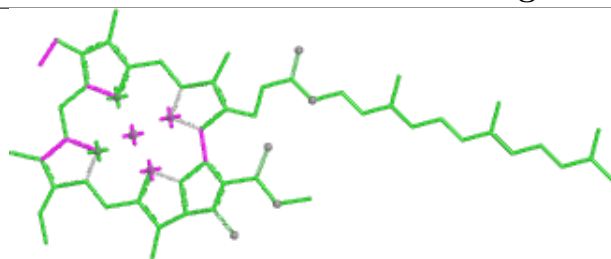


Torsions

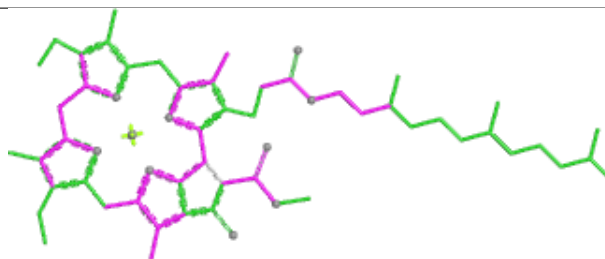


Rings

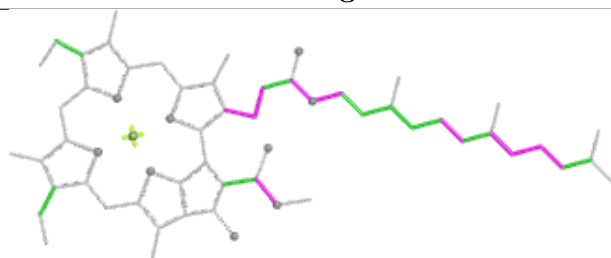
## Ligand CLA 8 606



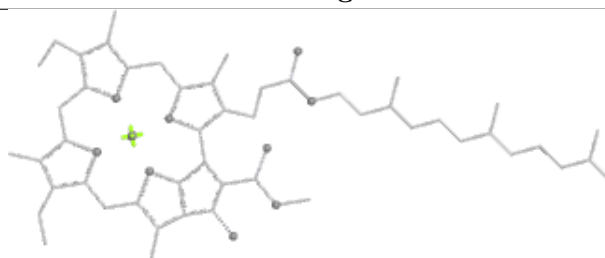
Bond lengths



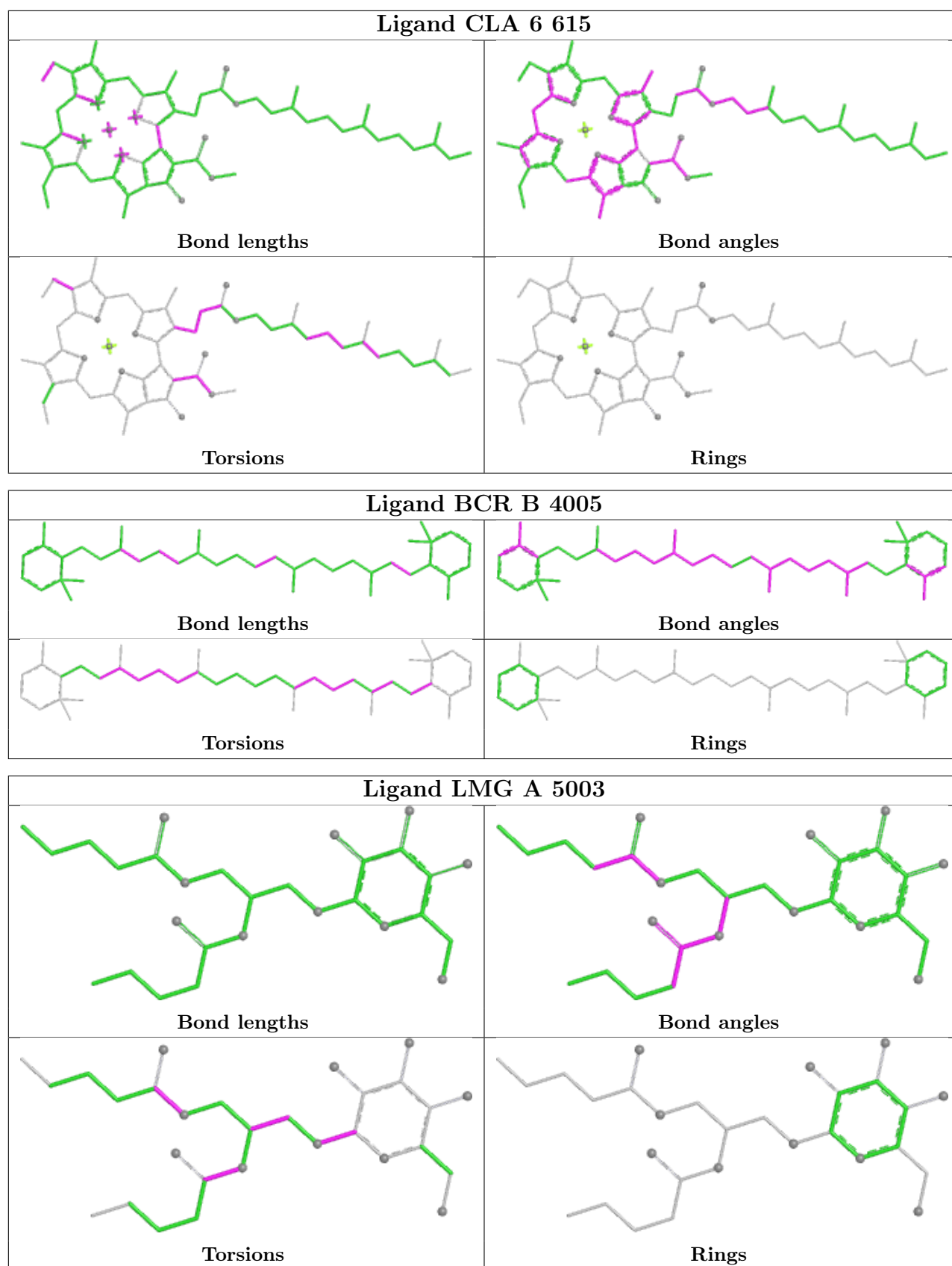
Bond angles

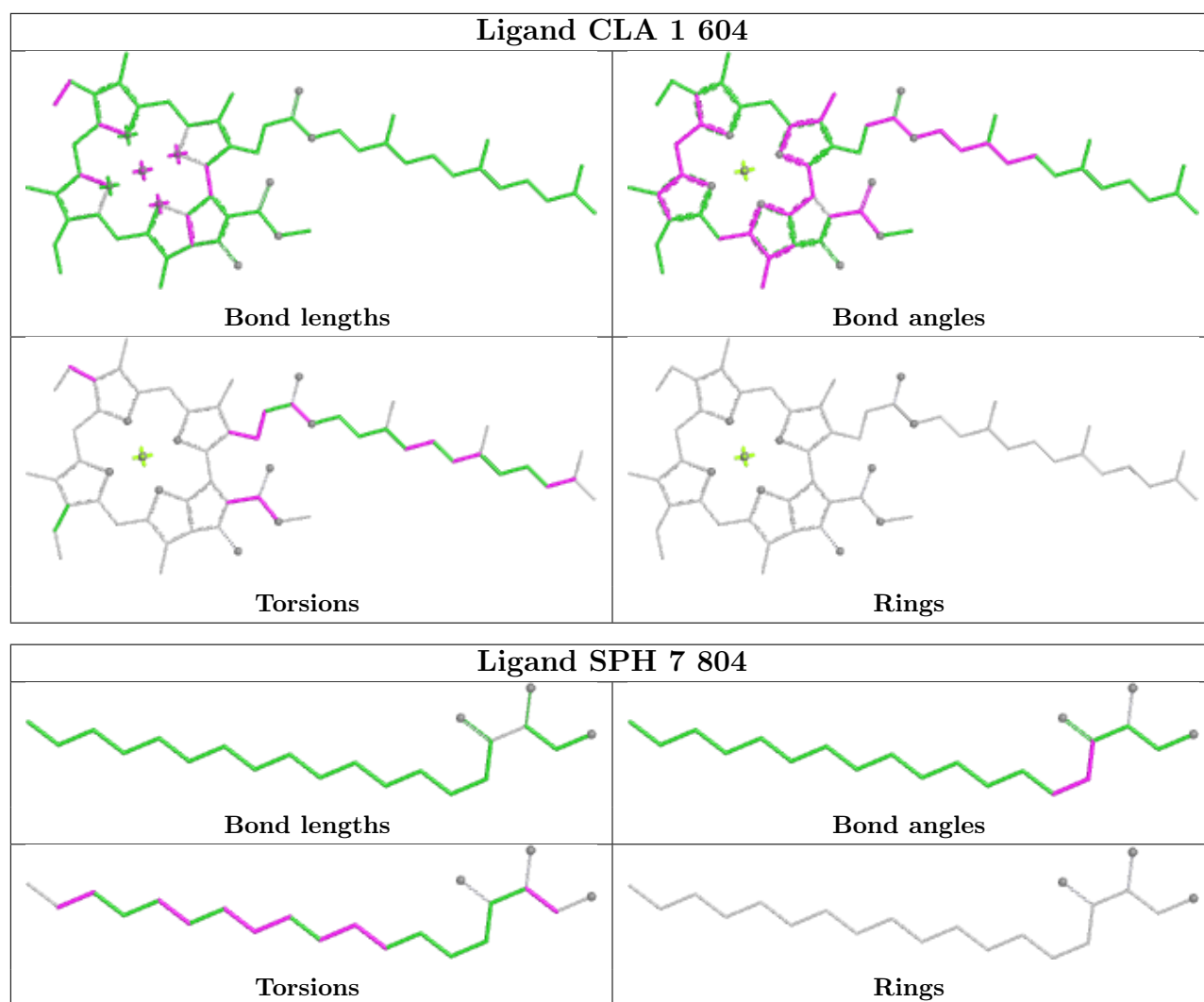


Torsions

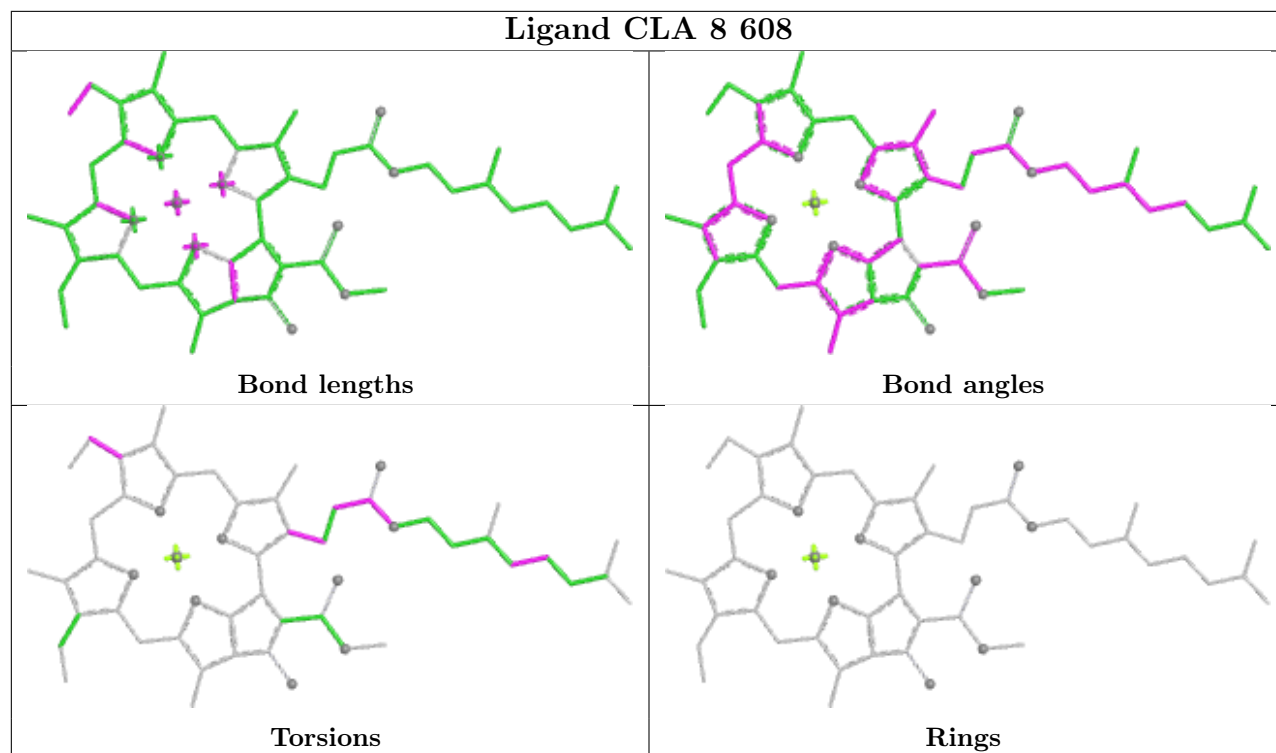


Rings

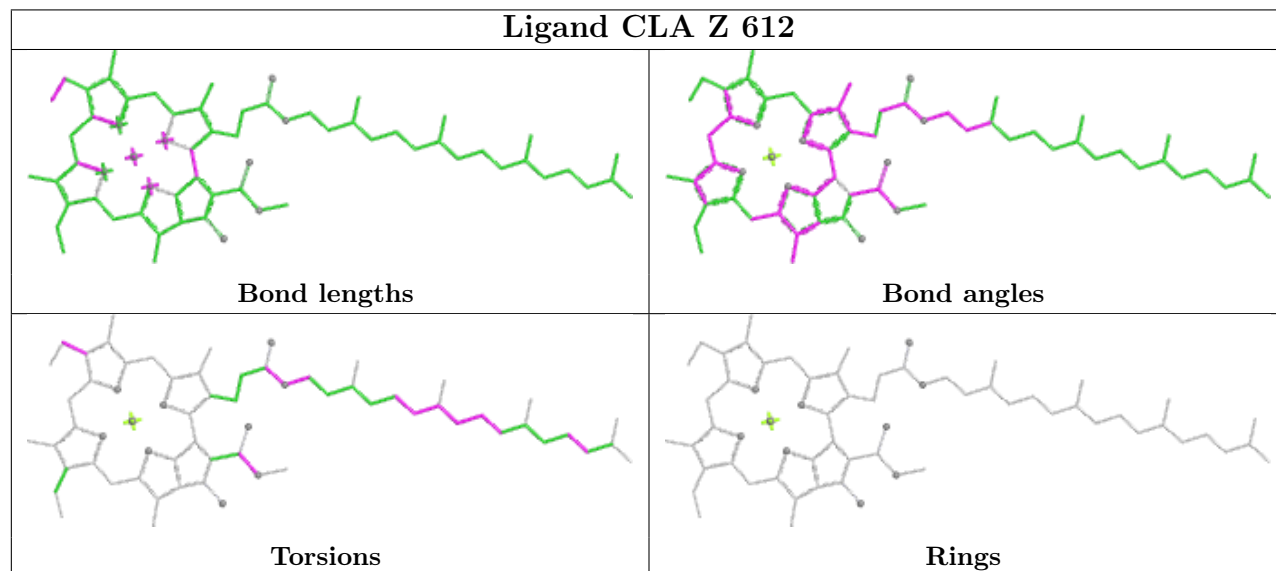


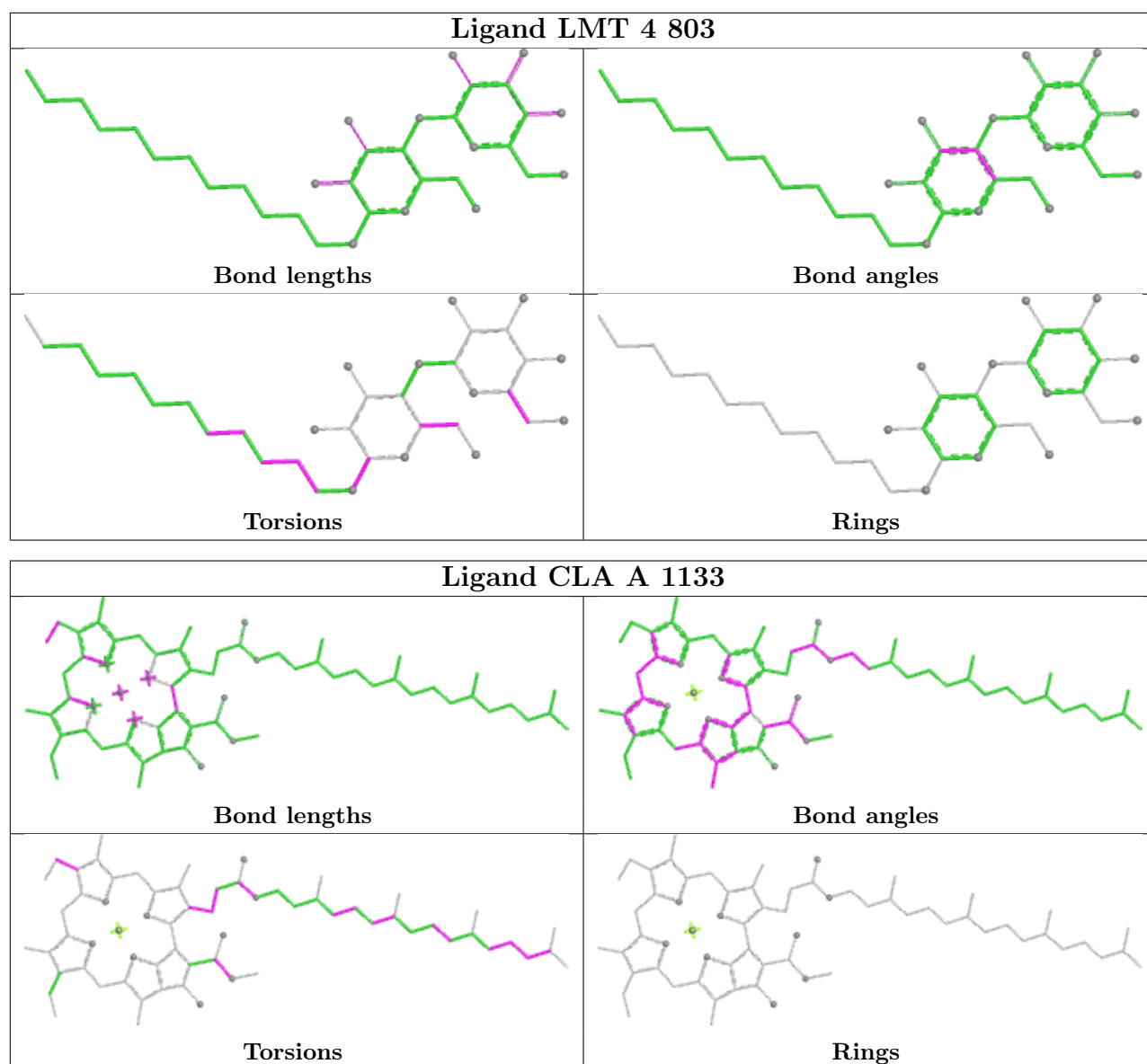


## Ligand CLA 8 608

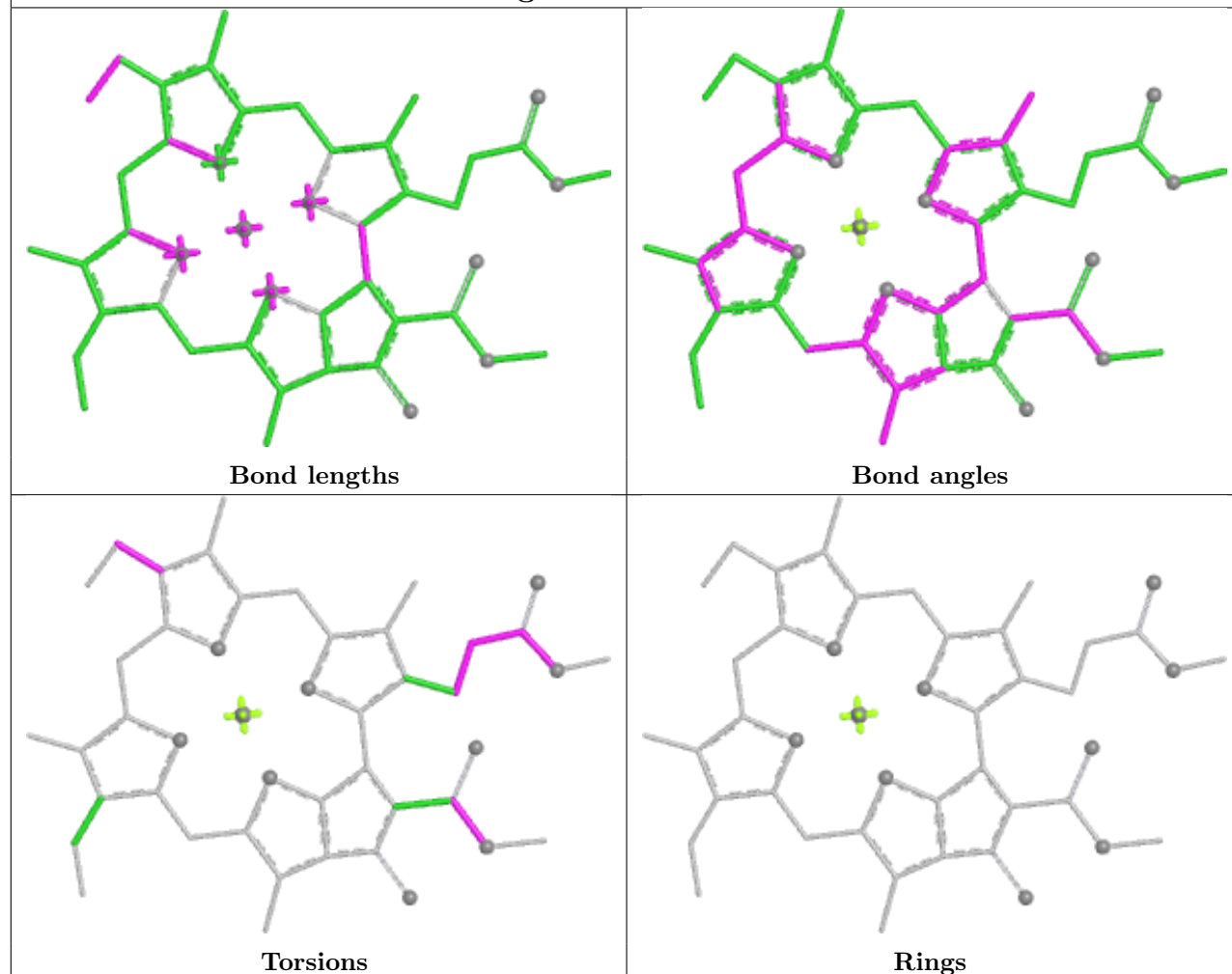


## Ligand CLA Z 612

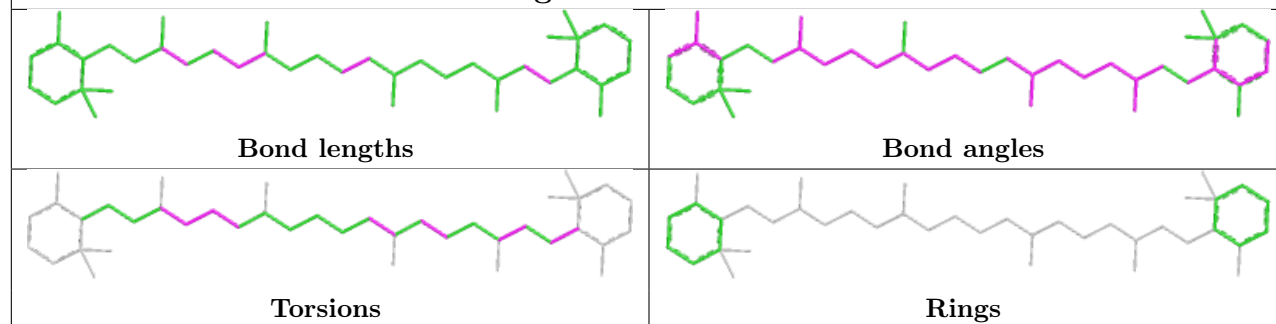


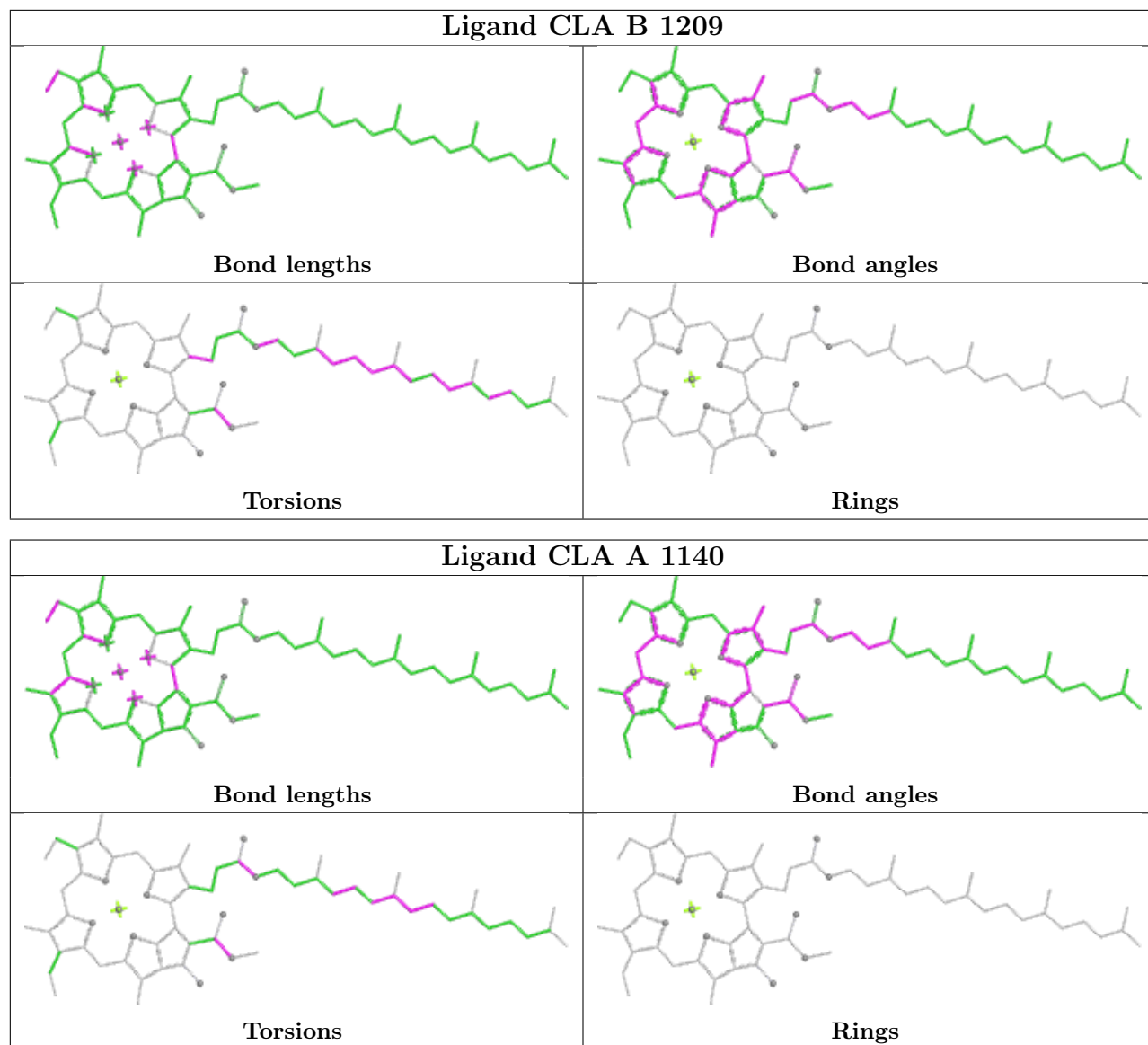


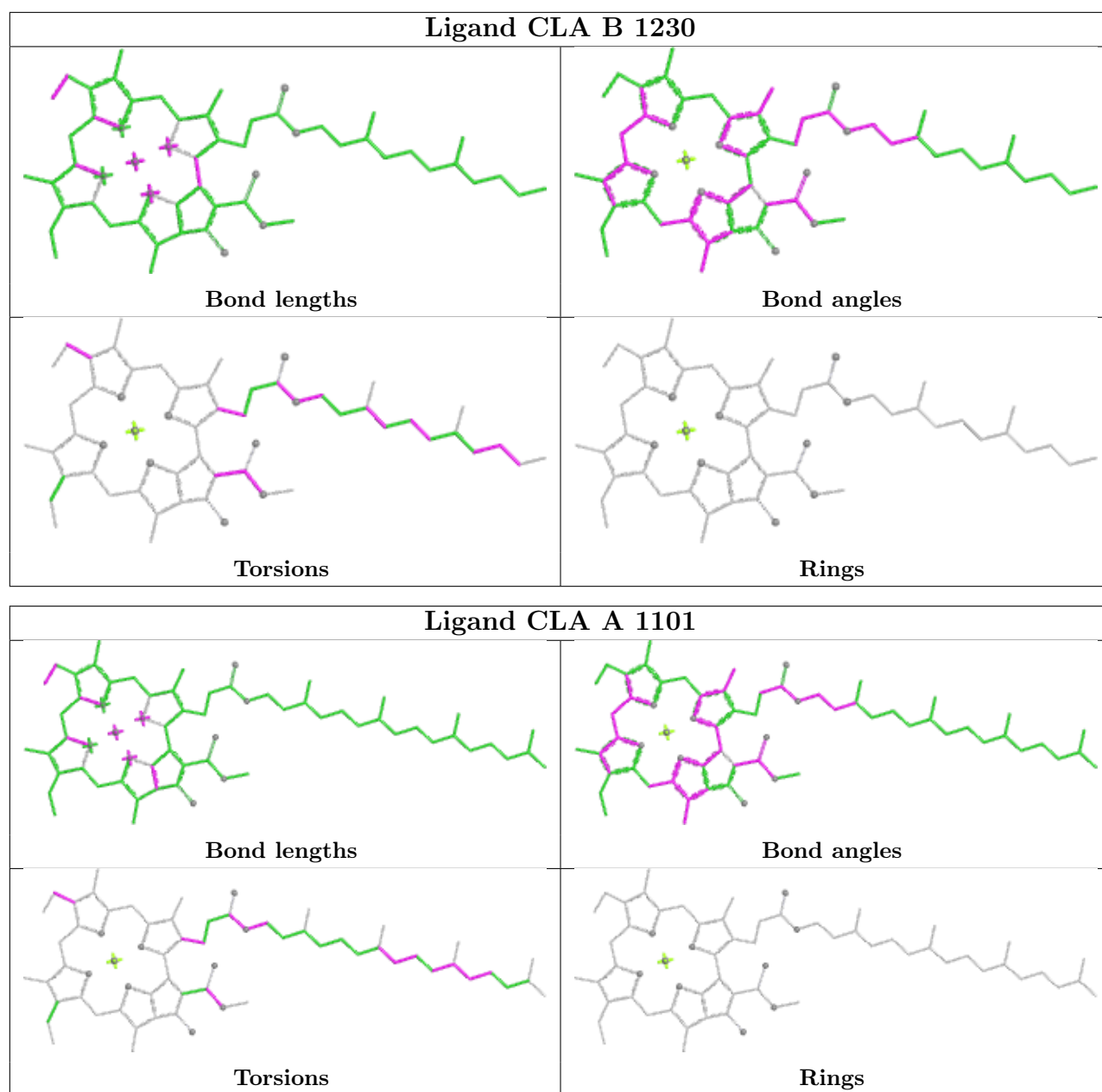
## Ligand CLA 2 607

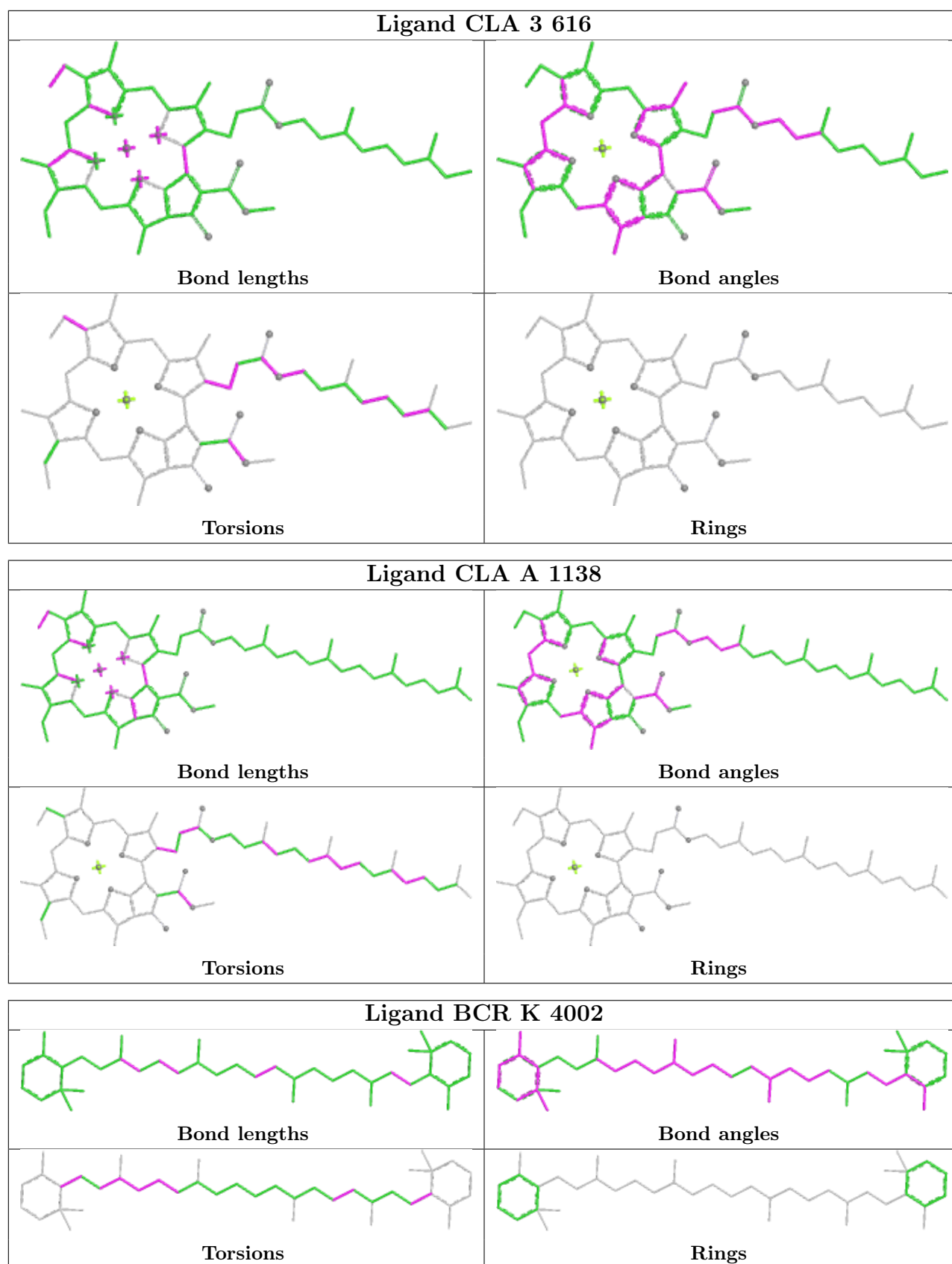


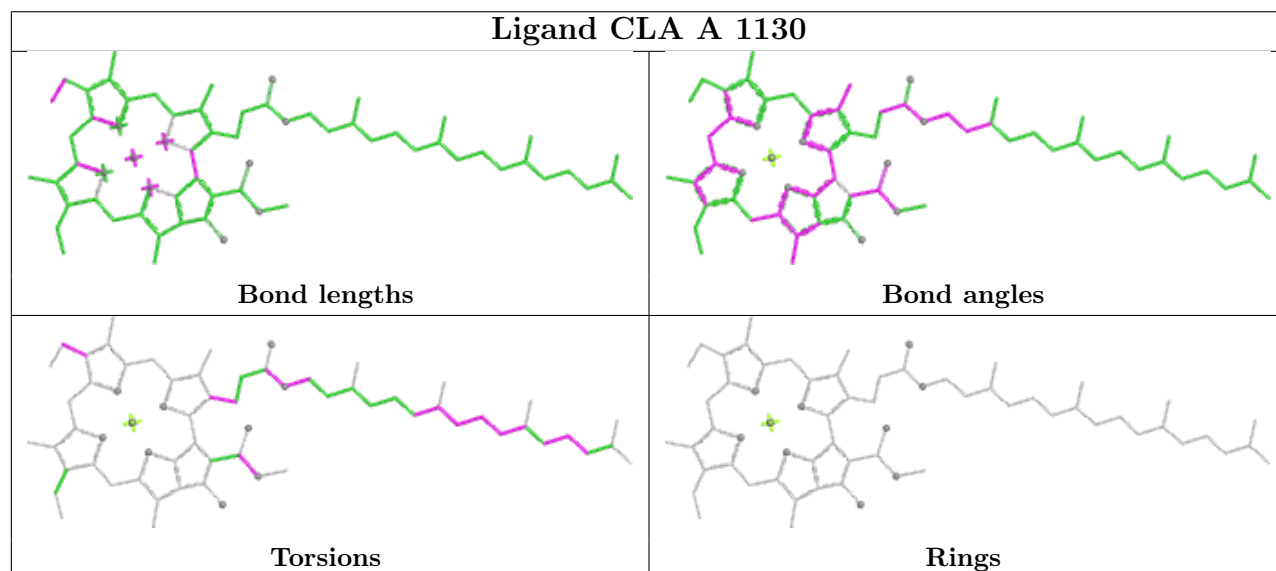
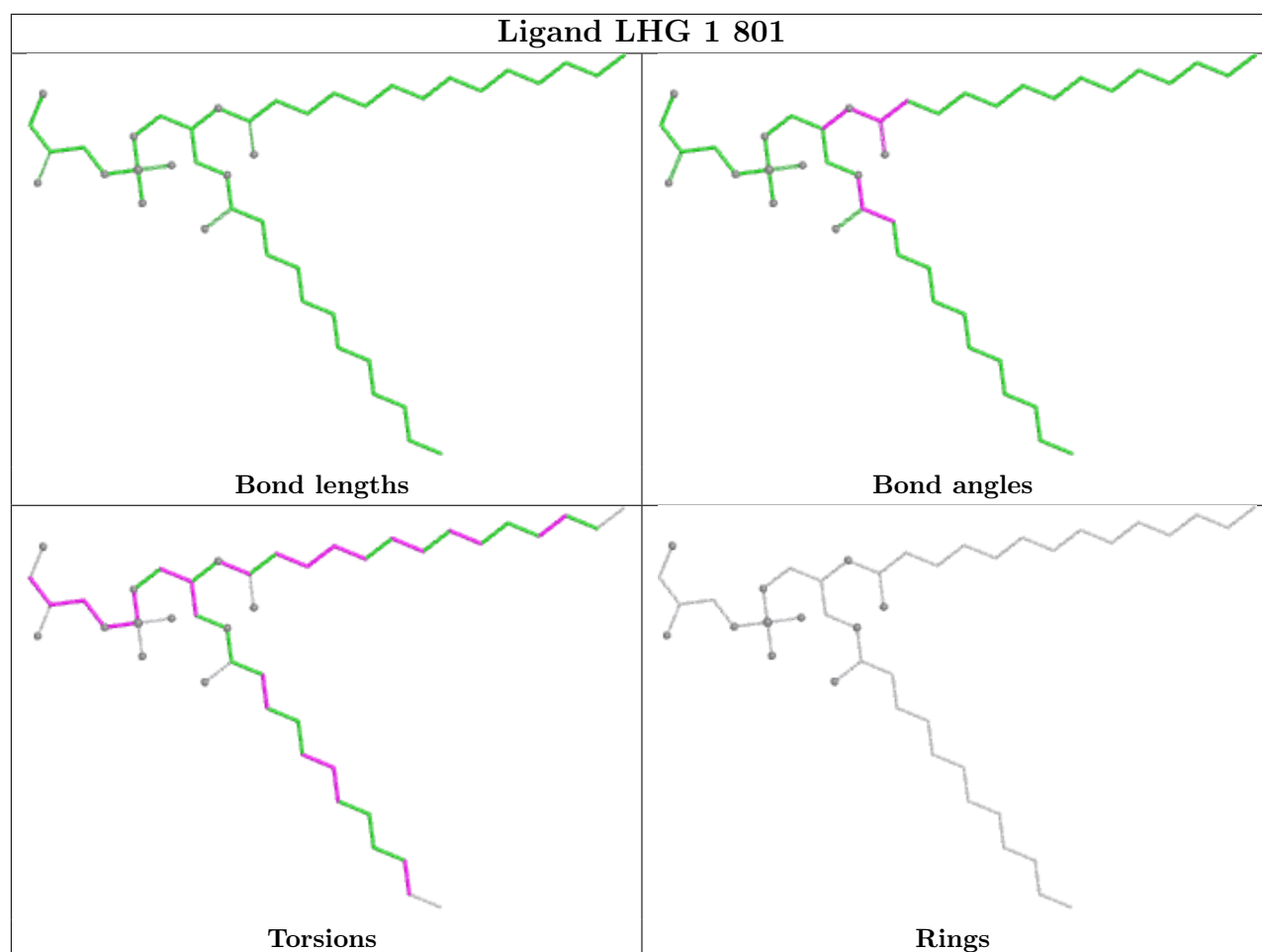
## Ligand BCR 5 504

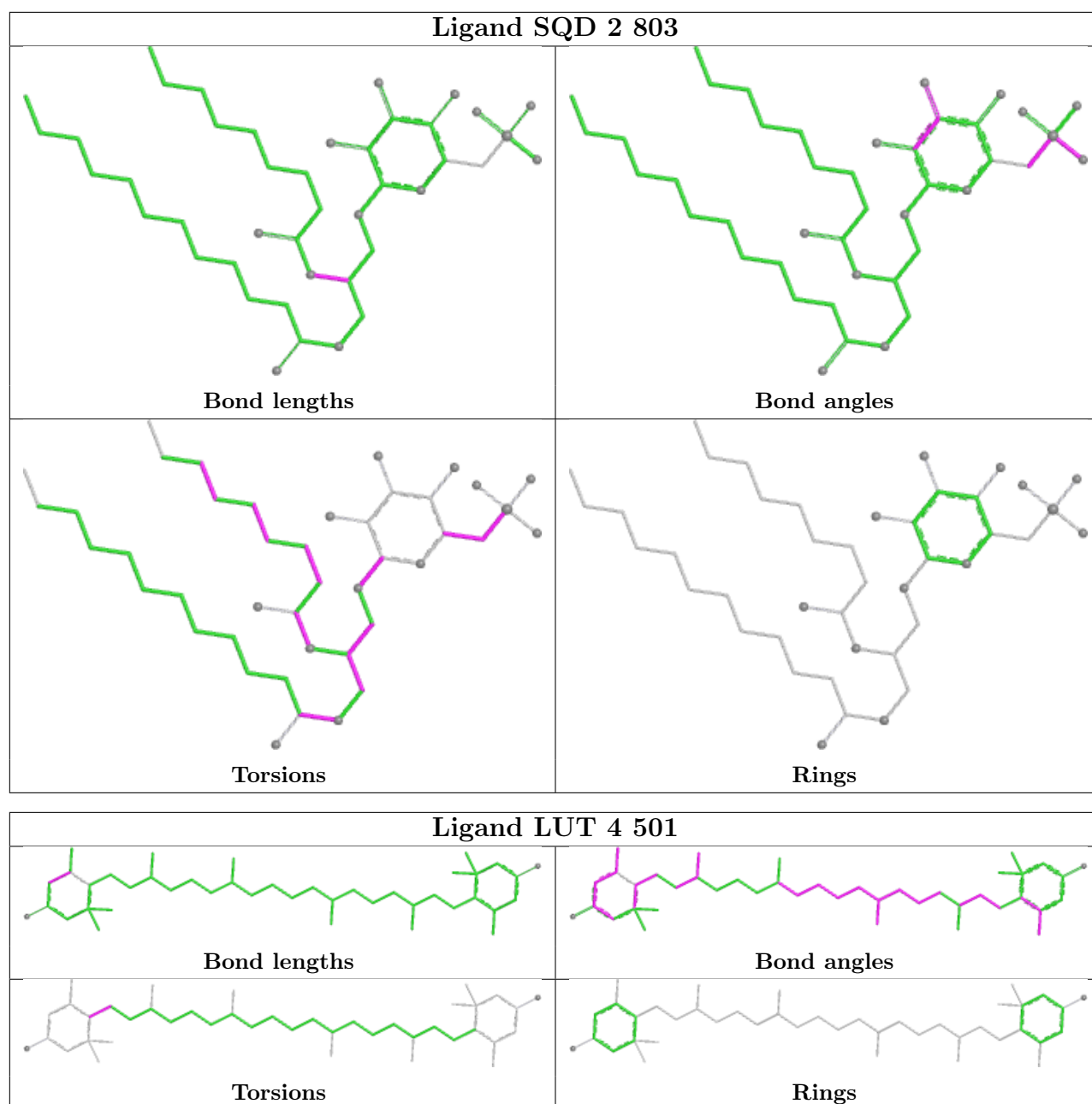




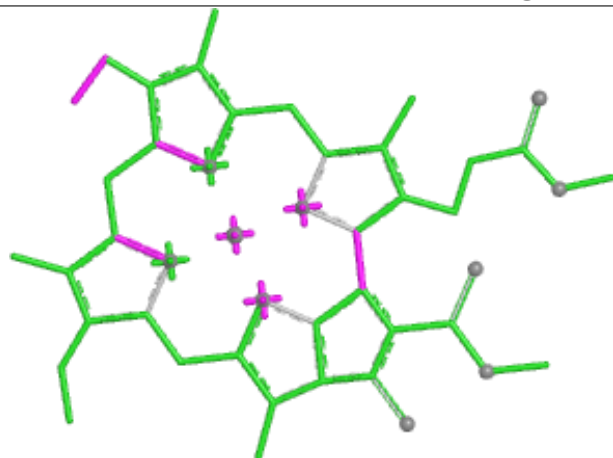




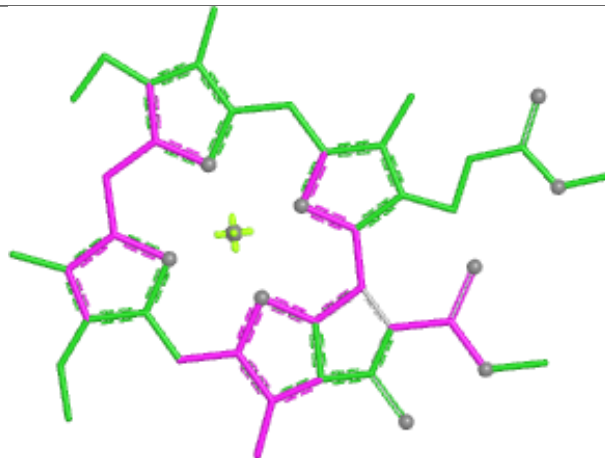




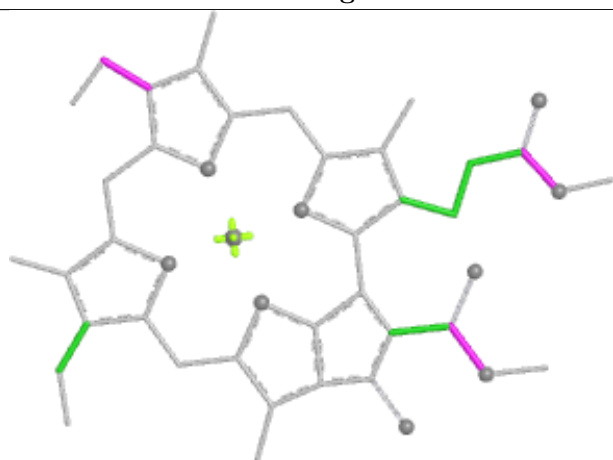
## Ligand CLA 3 602



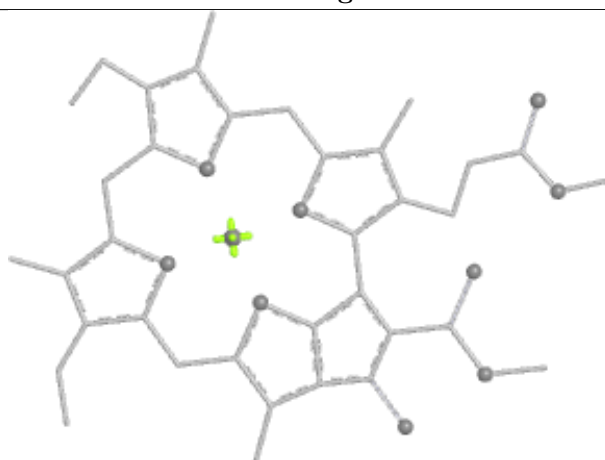
Bond lengths



Bond angles

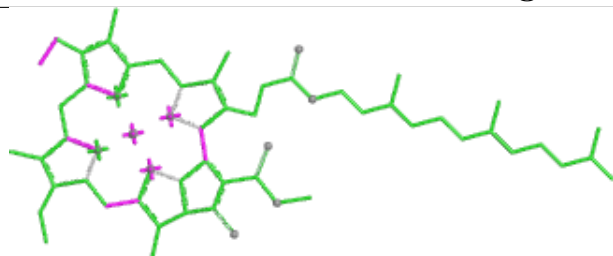


Torsions

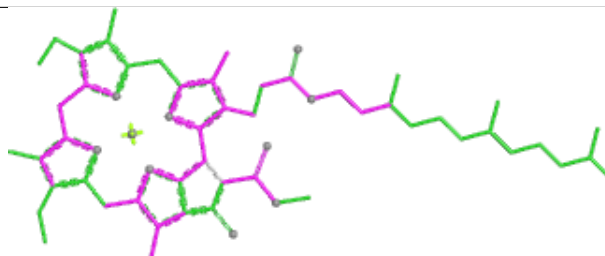


Rings

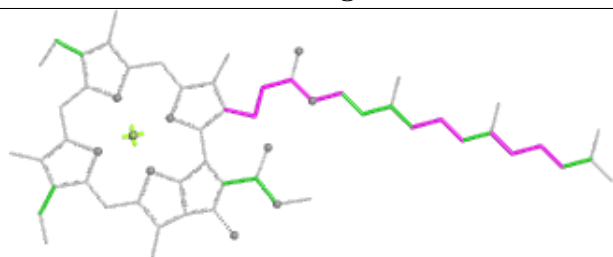
## Ligand CLA 3 610



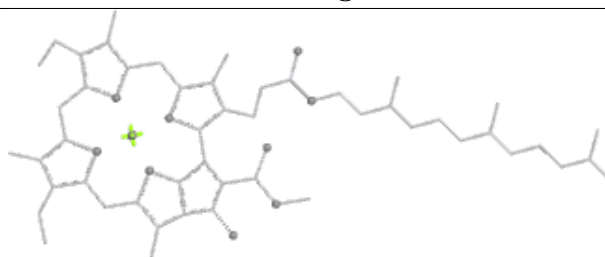
Bond lengths



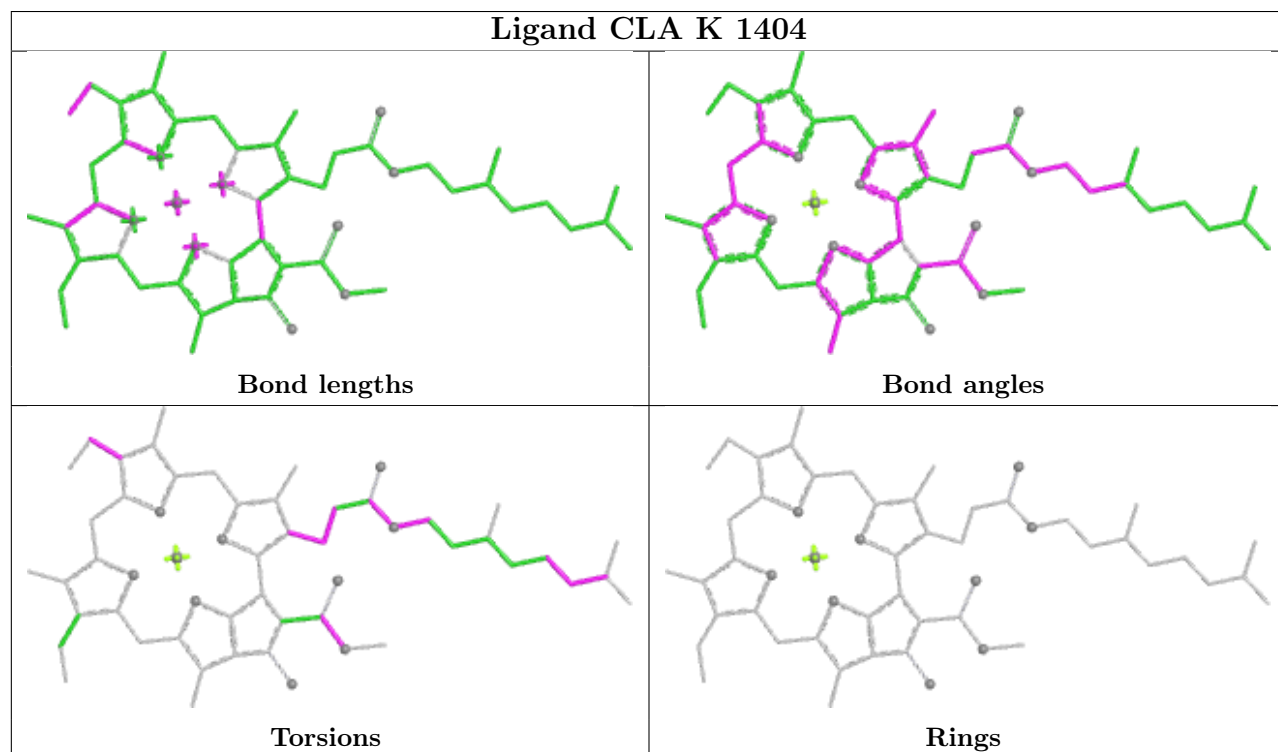
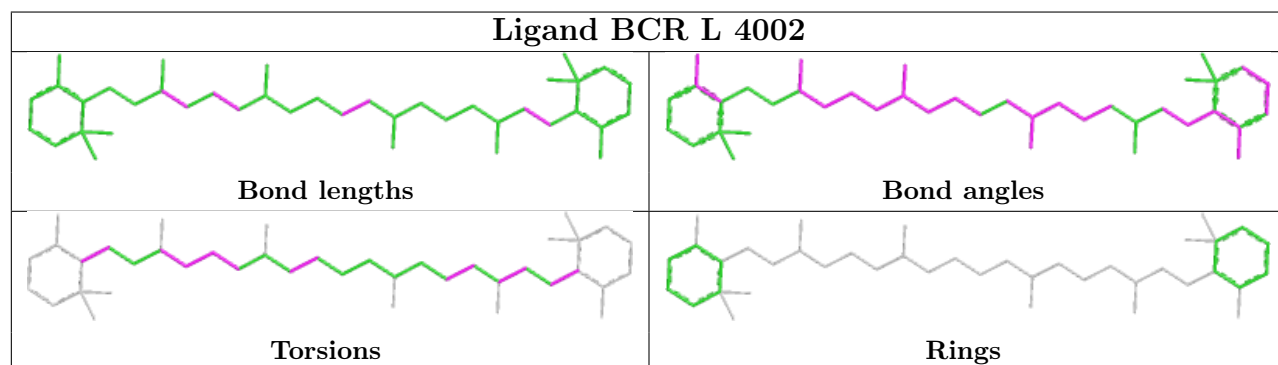
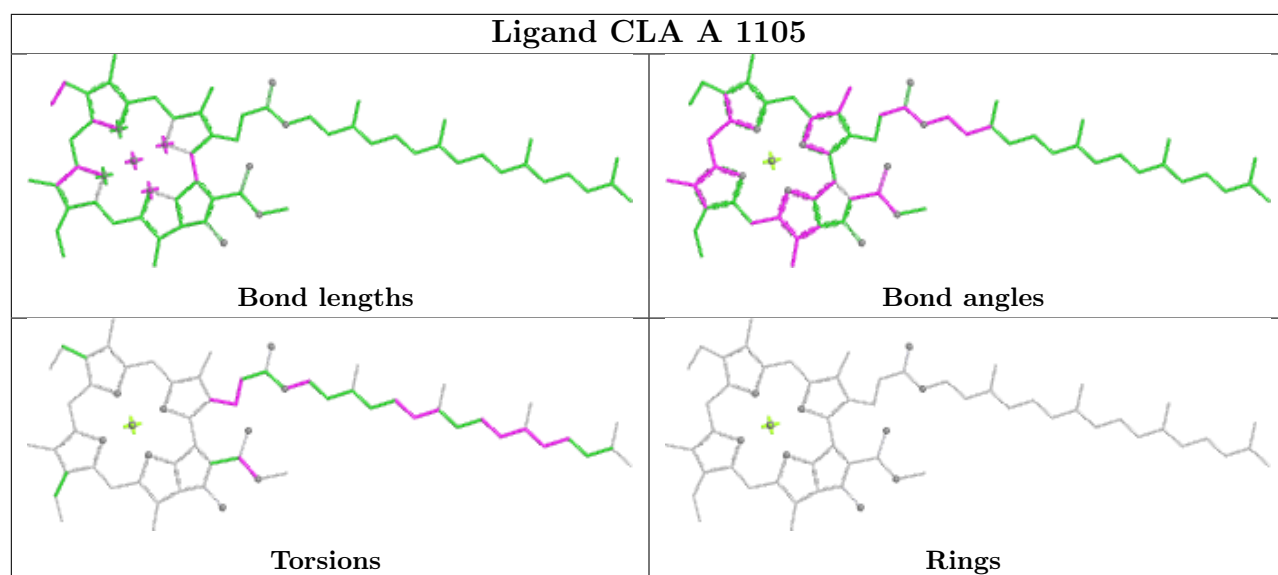
Bond angles



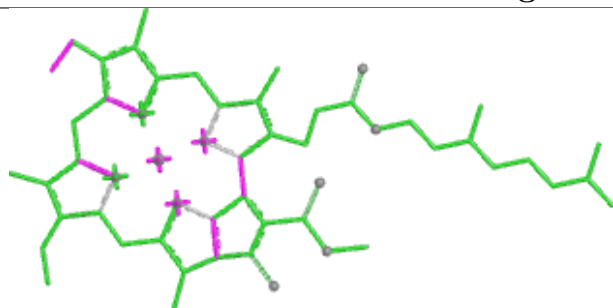
Torsions



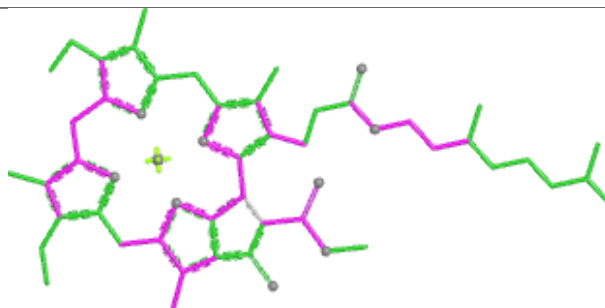
Rings



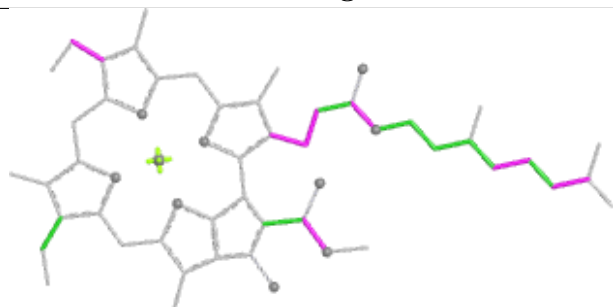
## Ligand CLA 6 608



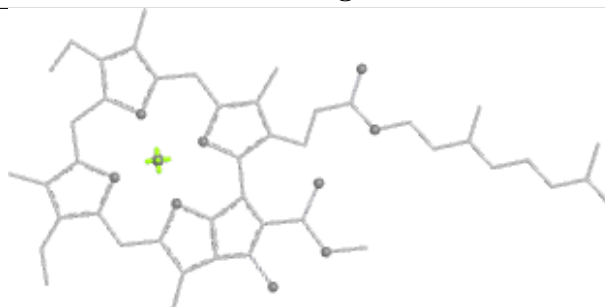
Bond lengths



Bond angles

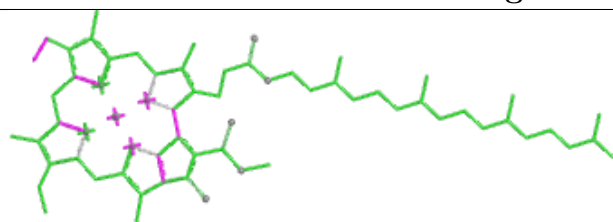


Torsions

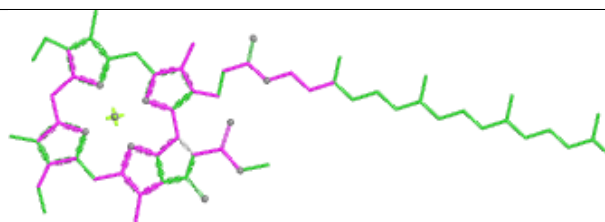


Rings

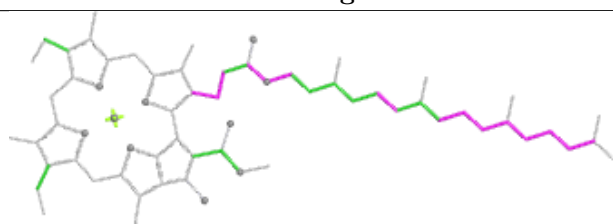
## Ligand CLA B 1210



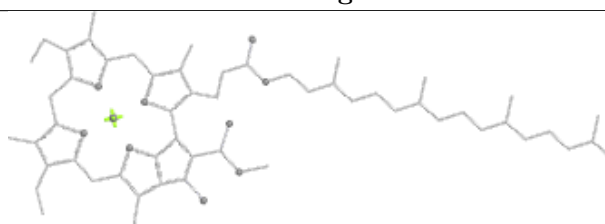
Bond lengths



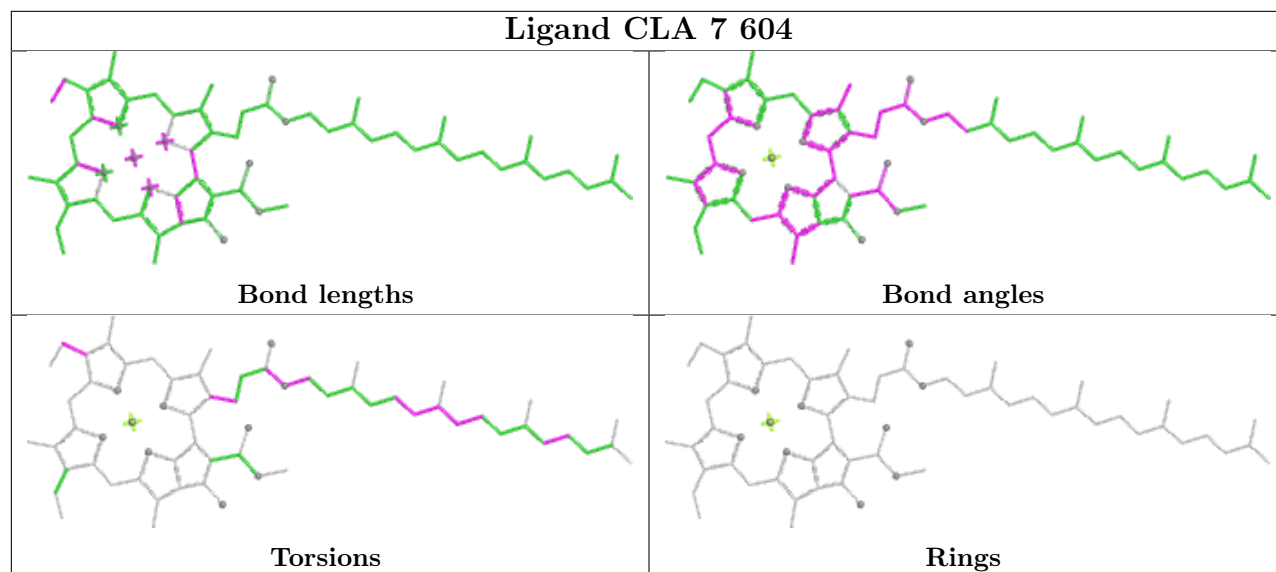
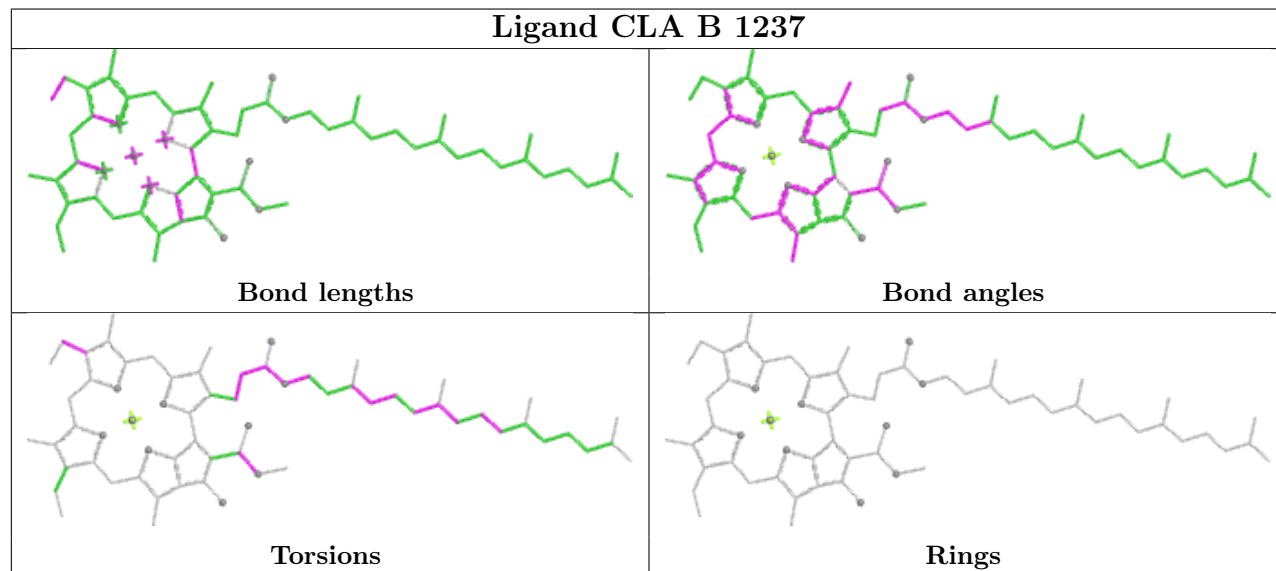
Bond angles

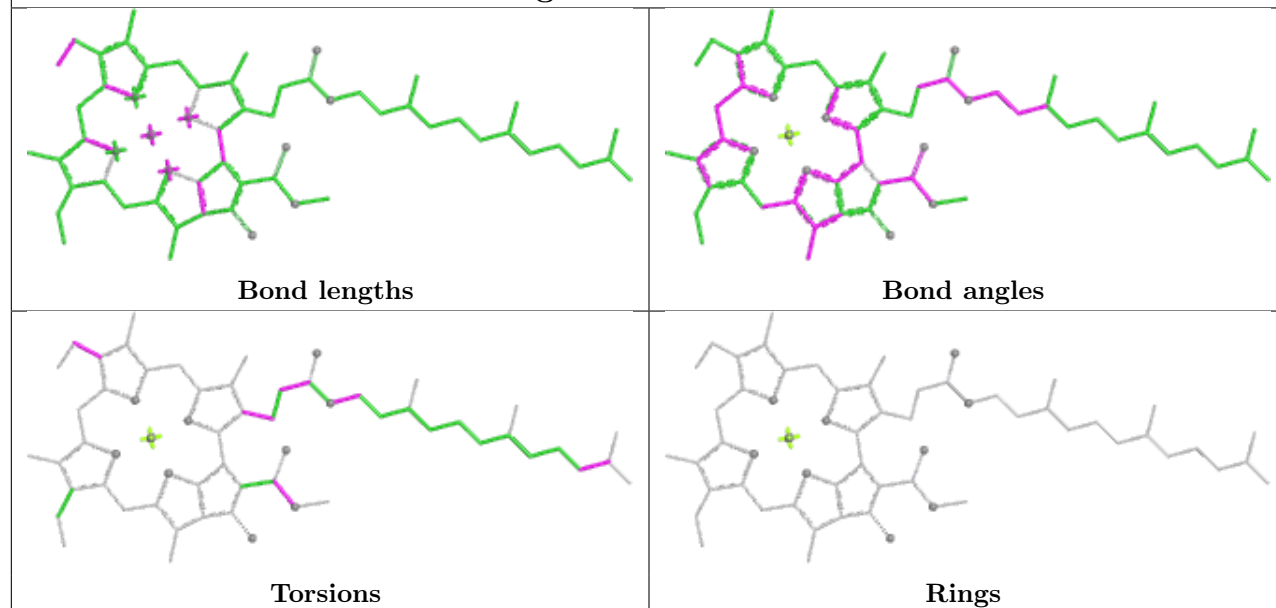
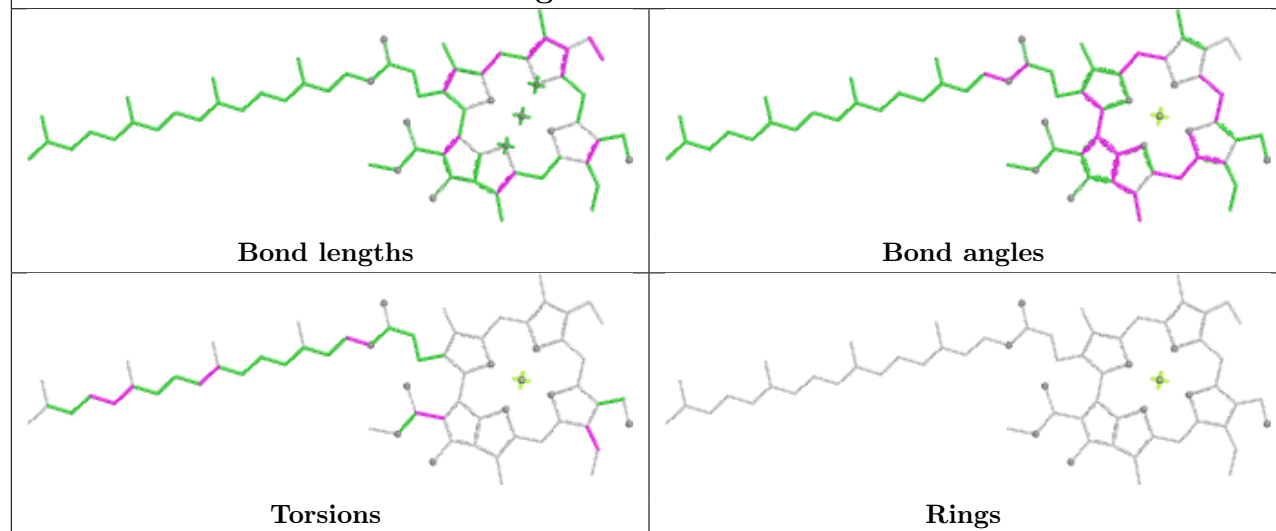


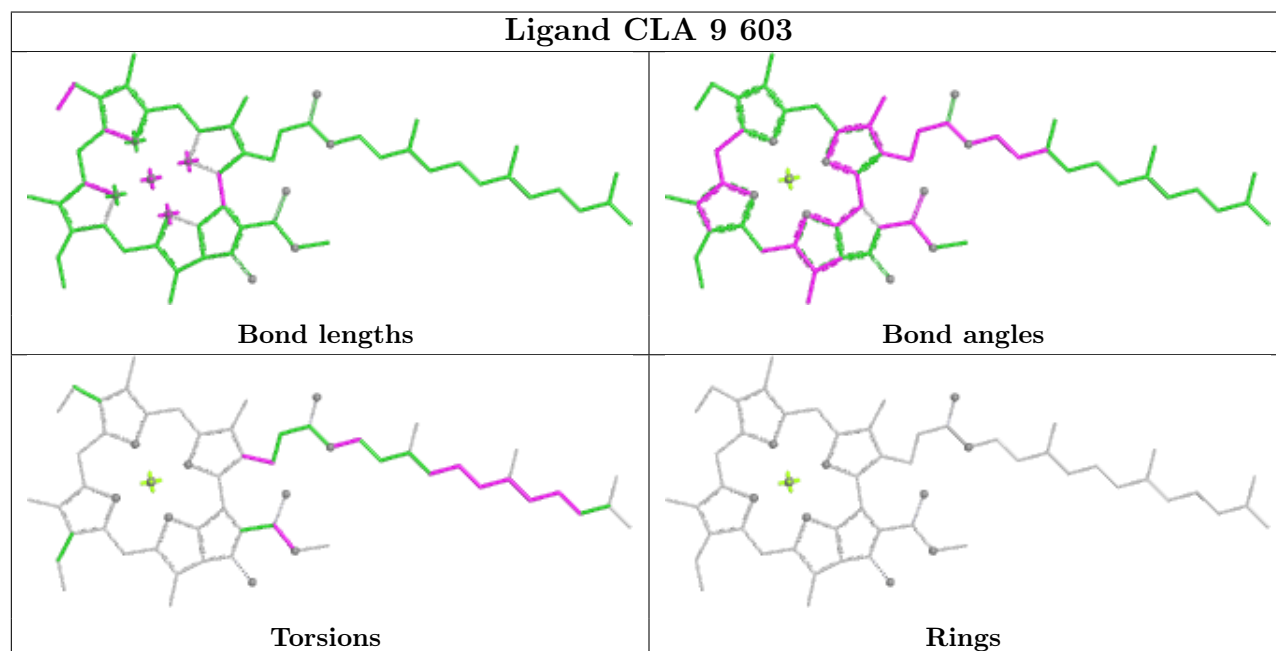
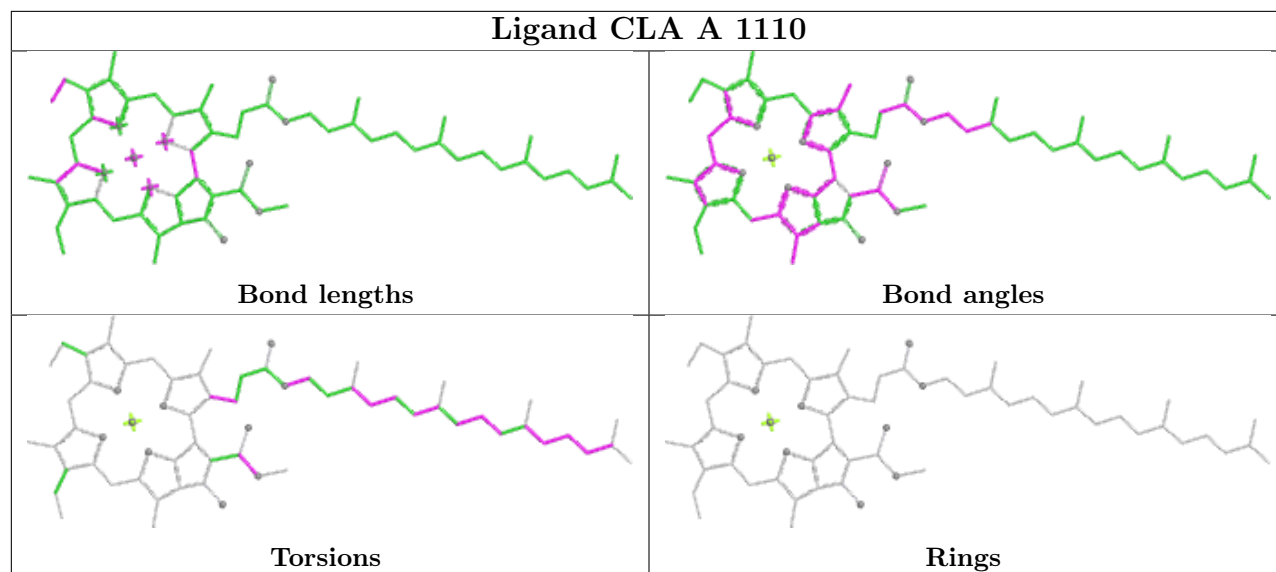
Torsions

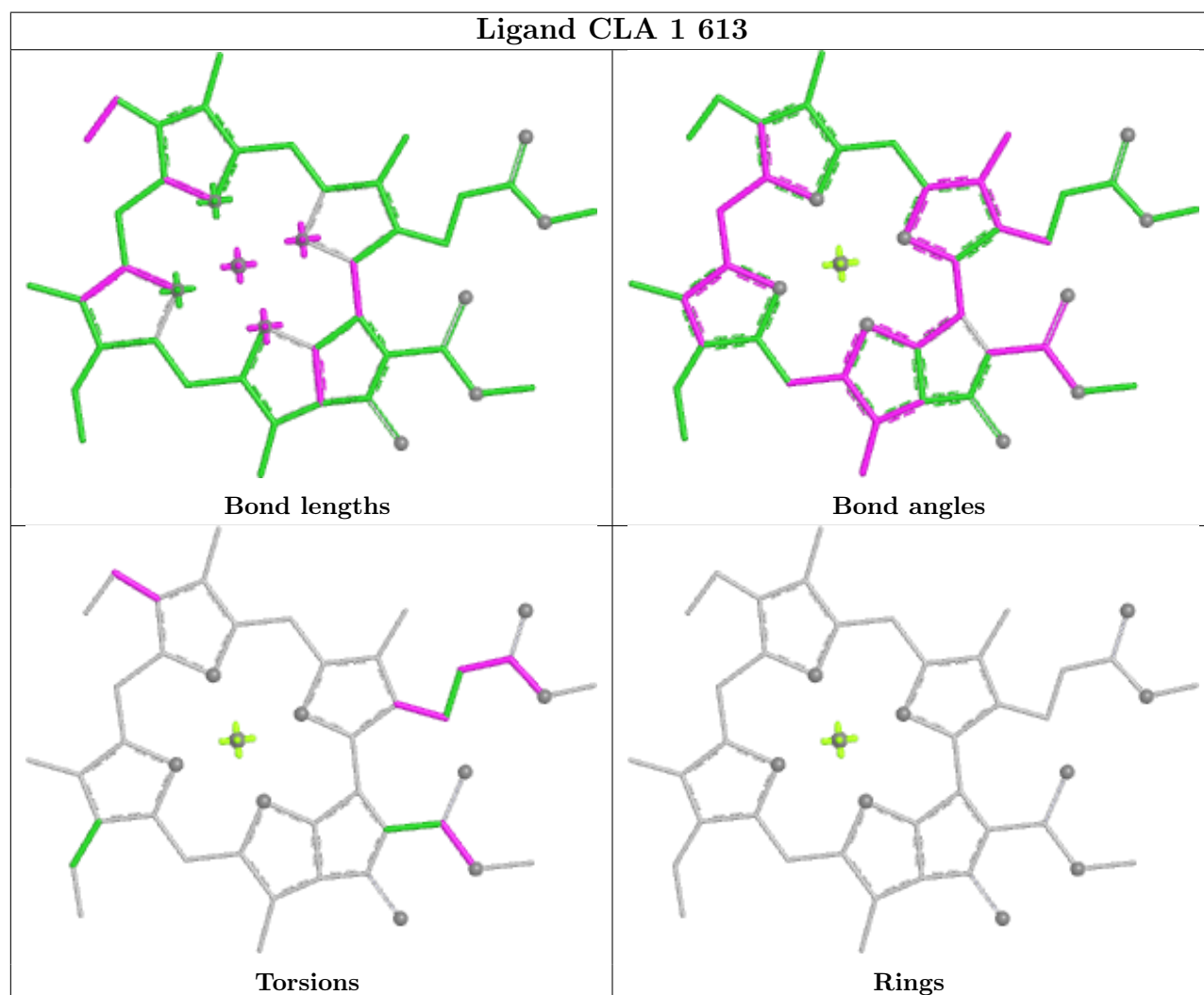
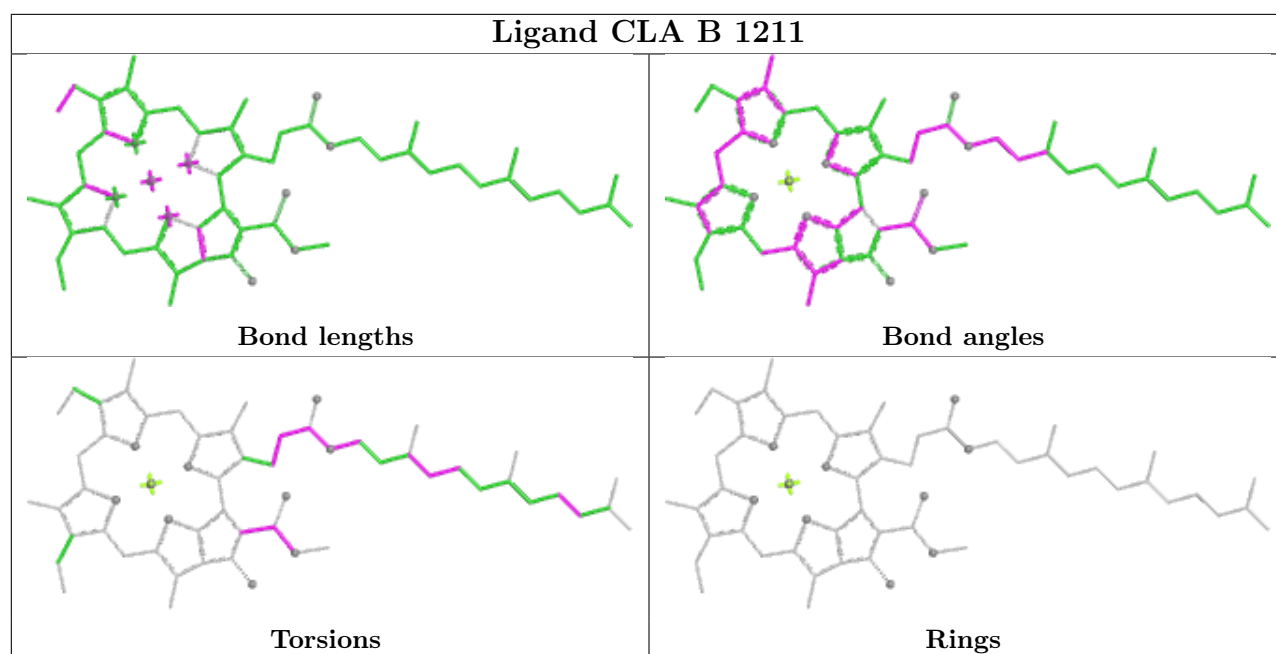


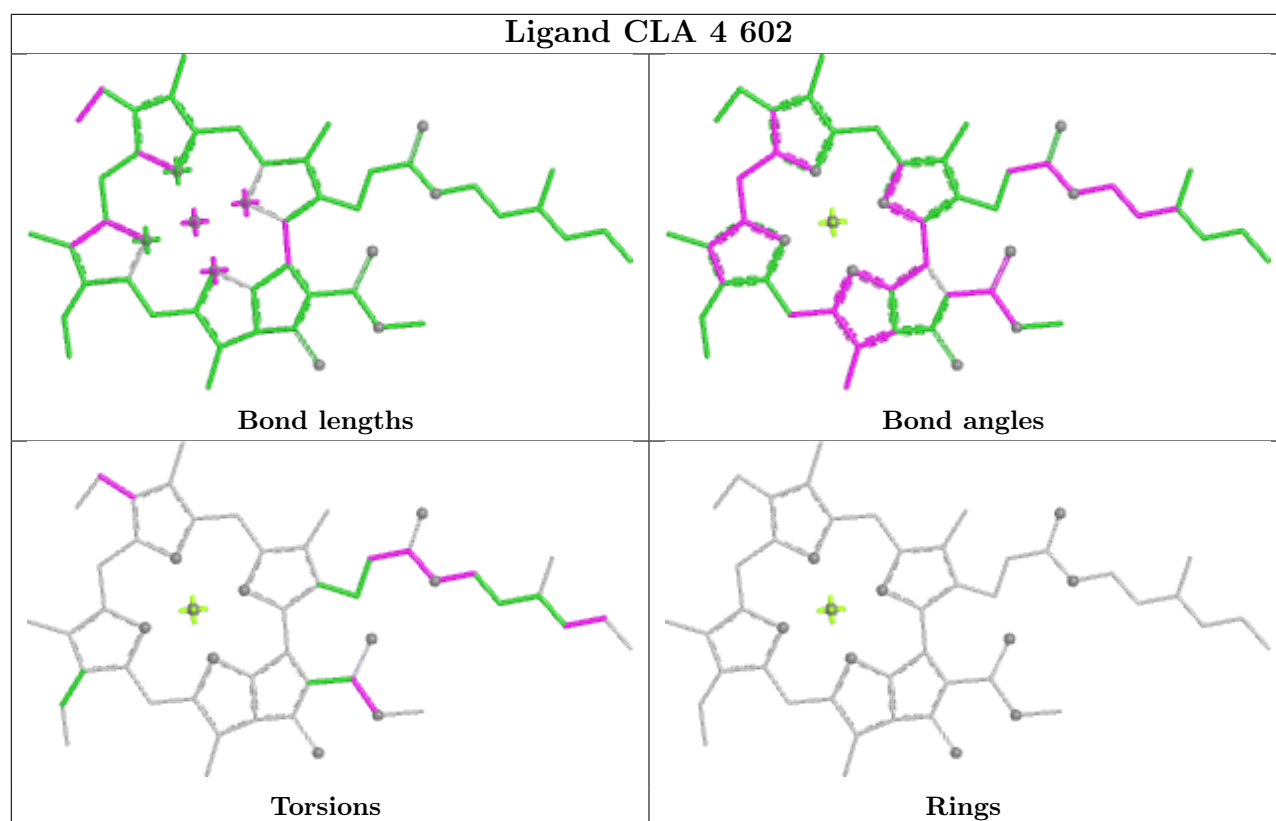
Rings

**Ligand CLA 7 604****Ligand CLA B 1237**

**Ligand CLA 1 608****Ligand CHL 5 610**







## 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.

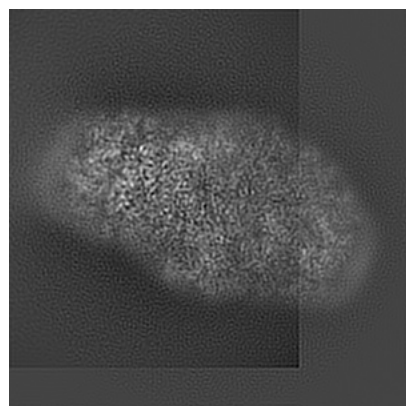
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12180. These allow visual inspection of the internal detail of the map and identification of artifacts.

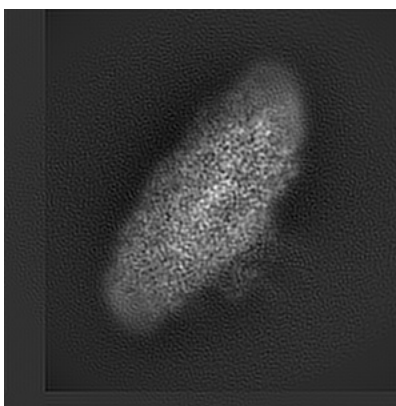
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

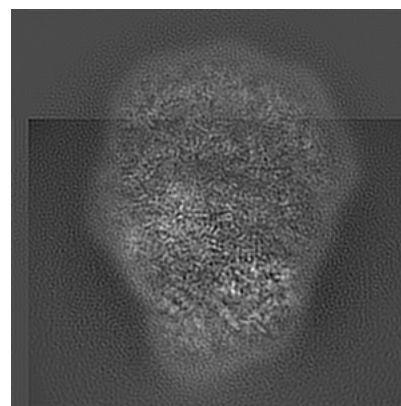
#### 6.1.1 Primary map



X

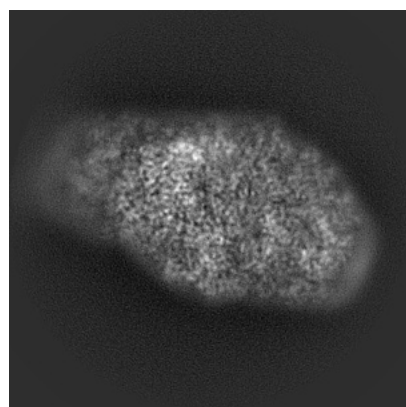


Y

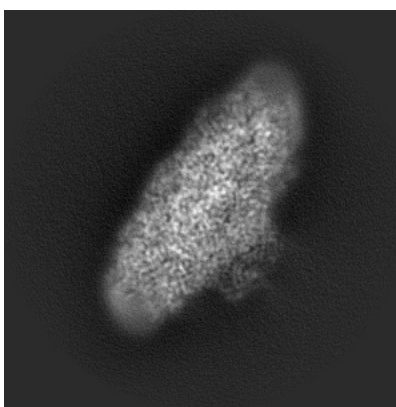


Z

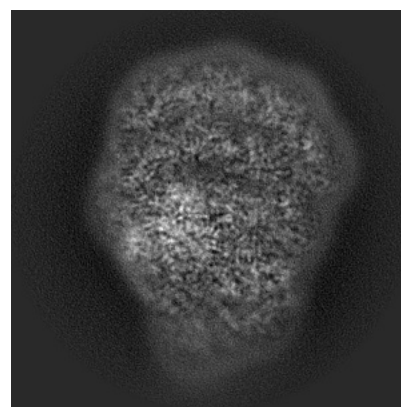
#### 6.1.2 Raw map



X



Y

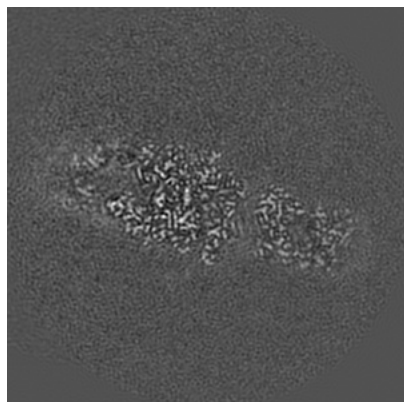


Z

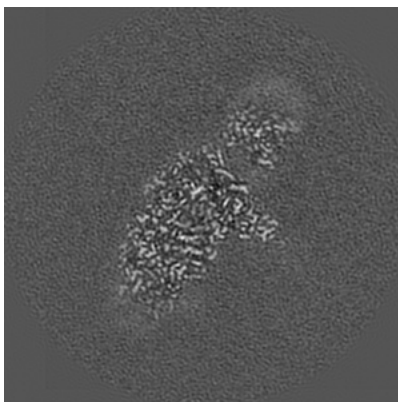
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

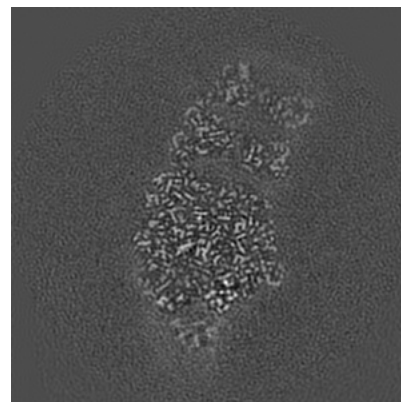
### 6.2.1 Primary map



X Index: 160

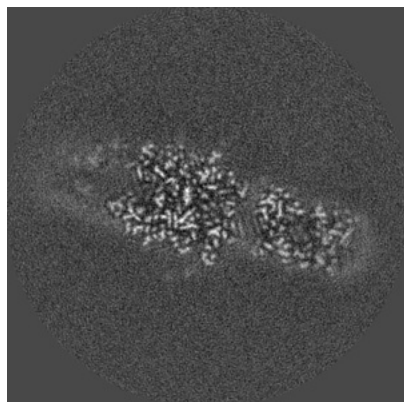


Y Index: 160

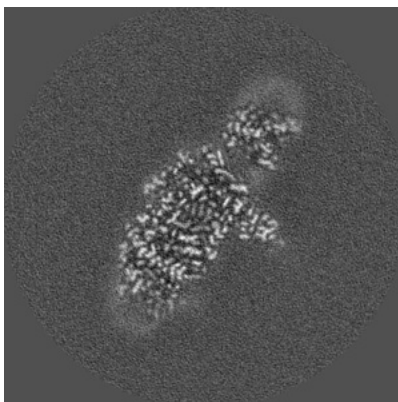


Z Index: 160

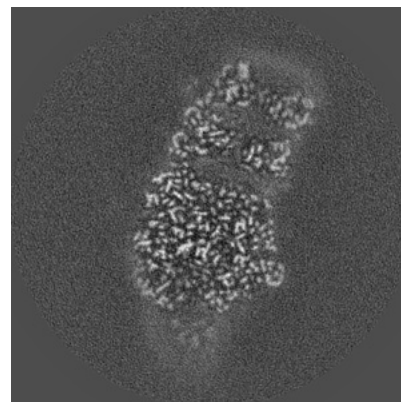
### 6.2.2 Raw map



X Index: 160



Y Index: 160

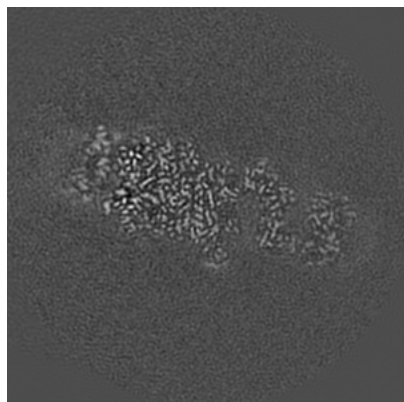


Z Index: 160

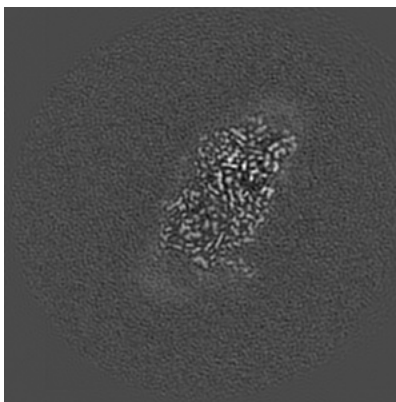
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

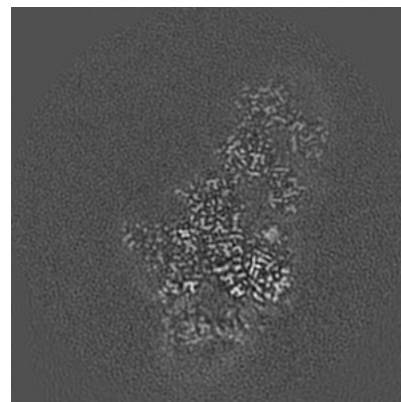
### 6.3.1 Primary map



X Index: 172

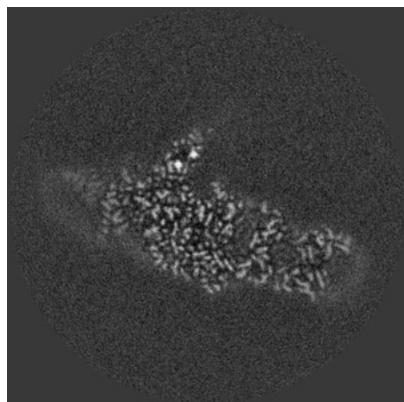


Y Index: 112

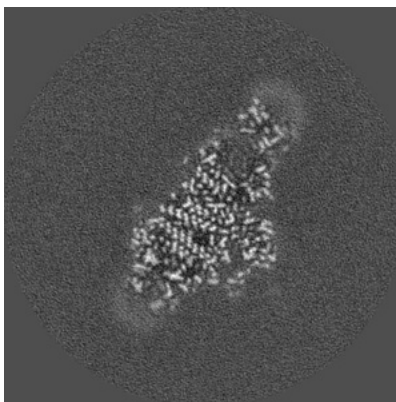


Z Index: 180

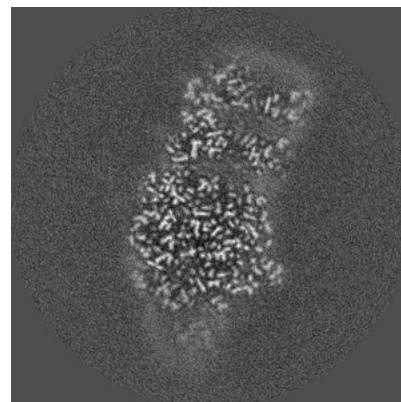
### 6.3.2 Raw map



X Index: 127



Y Index: 145

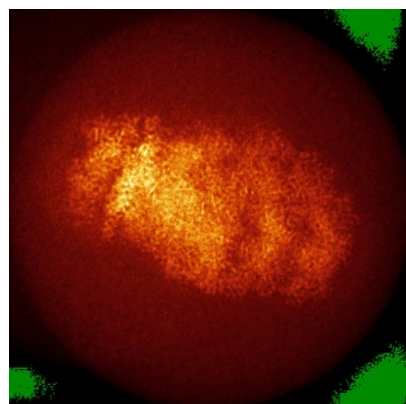


Z Index: 157

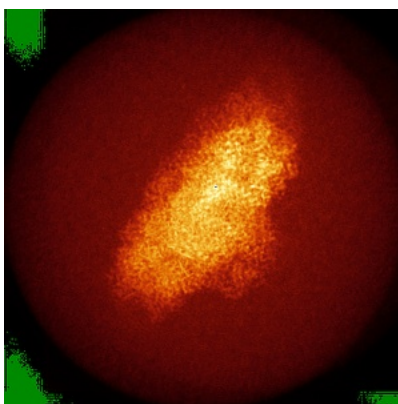
The images above show the largest variance slices of the map in three orthogonal directions.

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

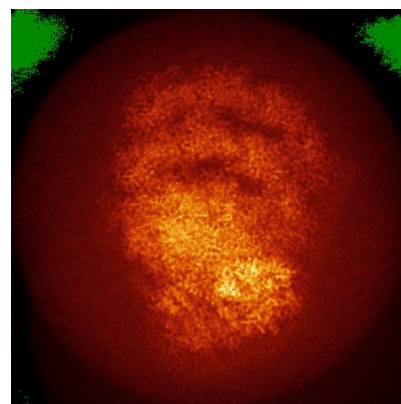
### 6.4.1 Primary map



X

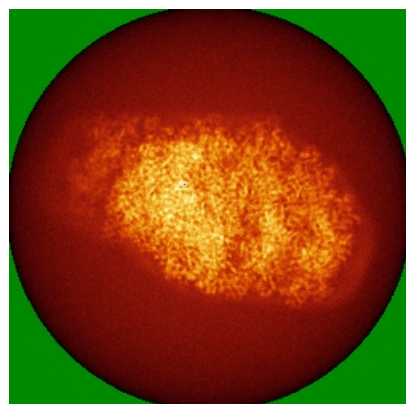


Y

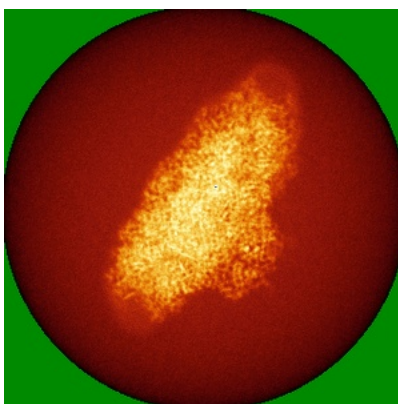


Z

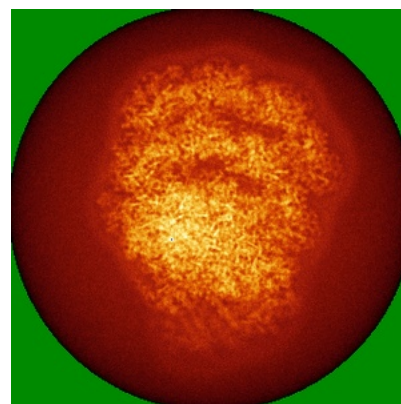
### 6.4.2 Raw map



X



Y

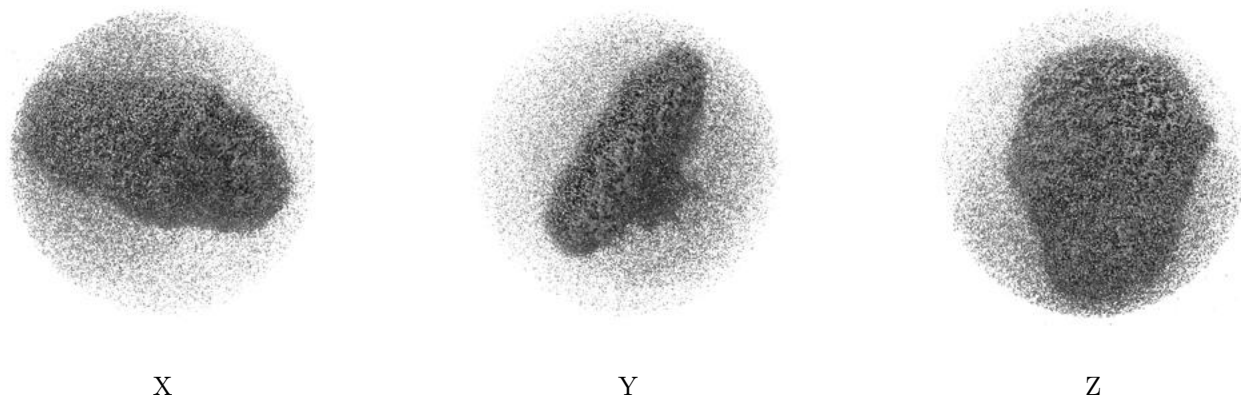


Z

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

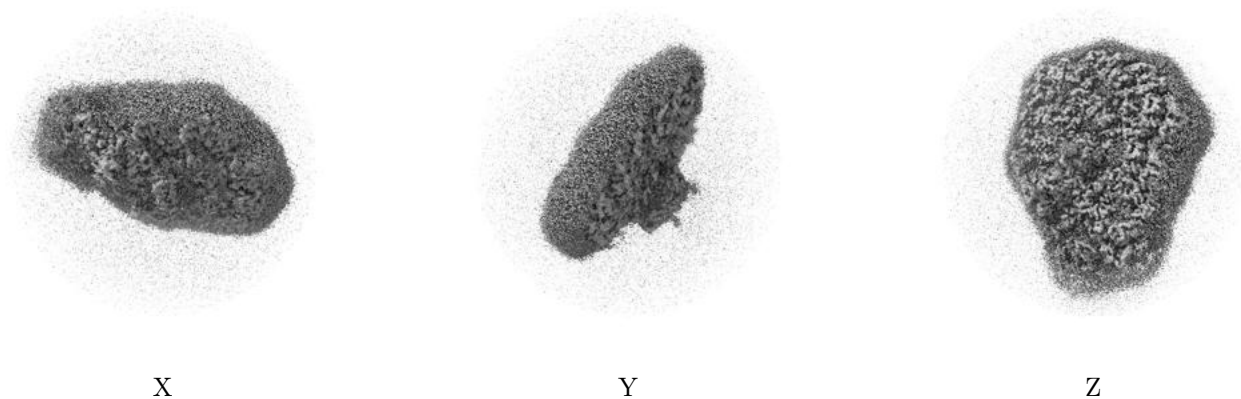
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

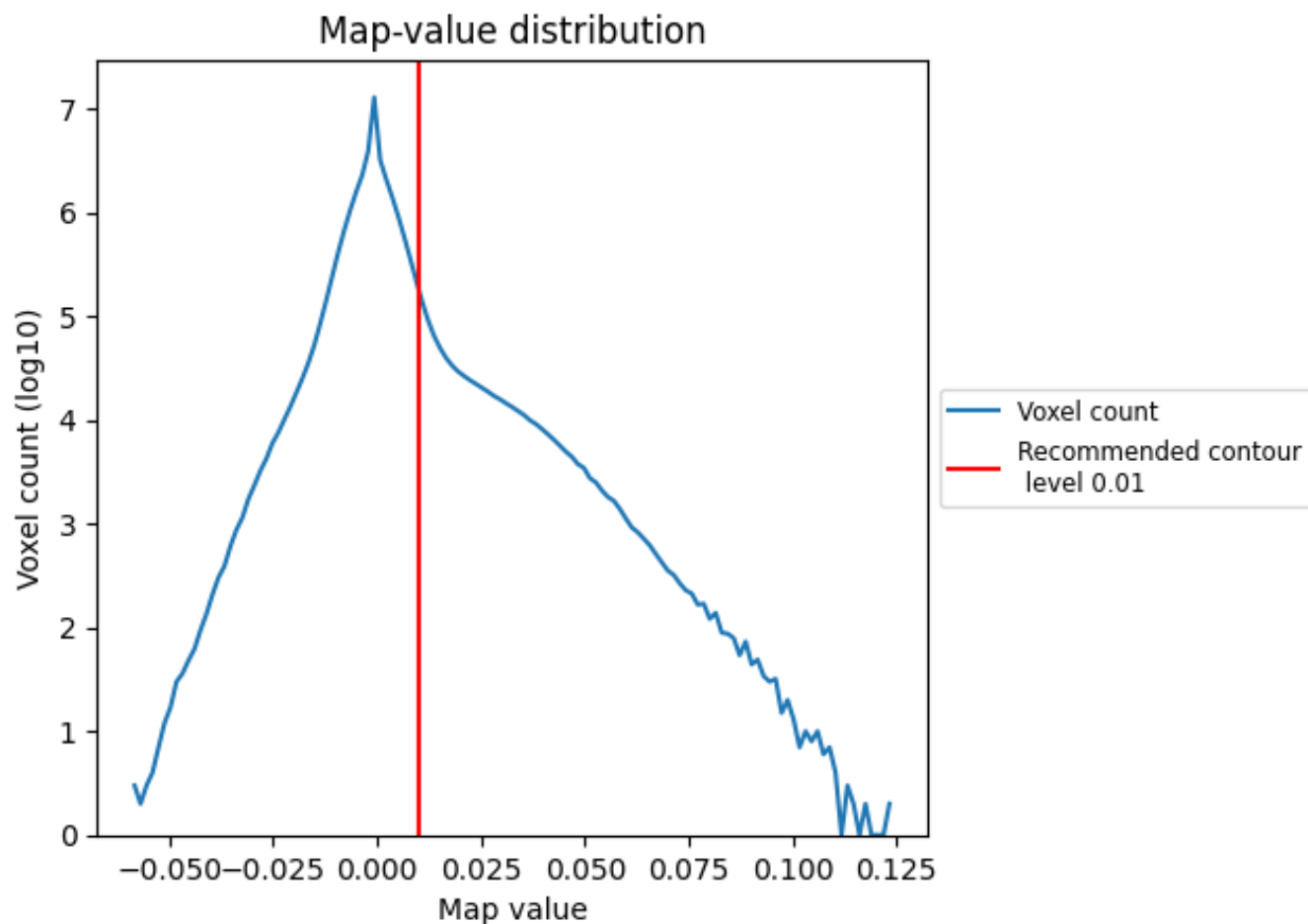
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

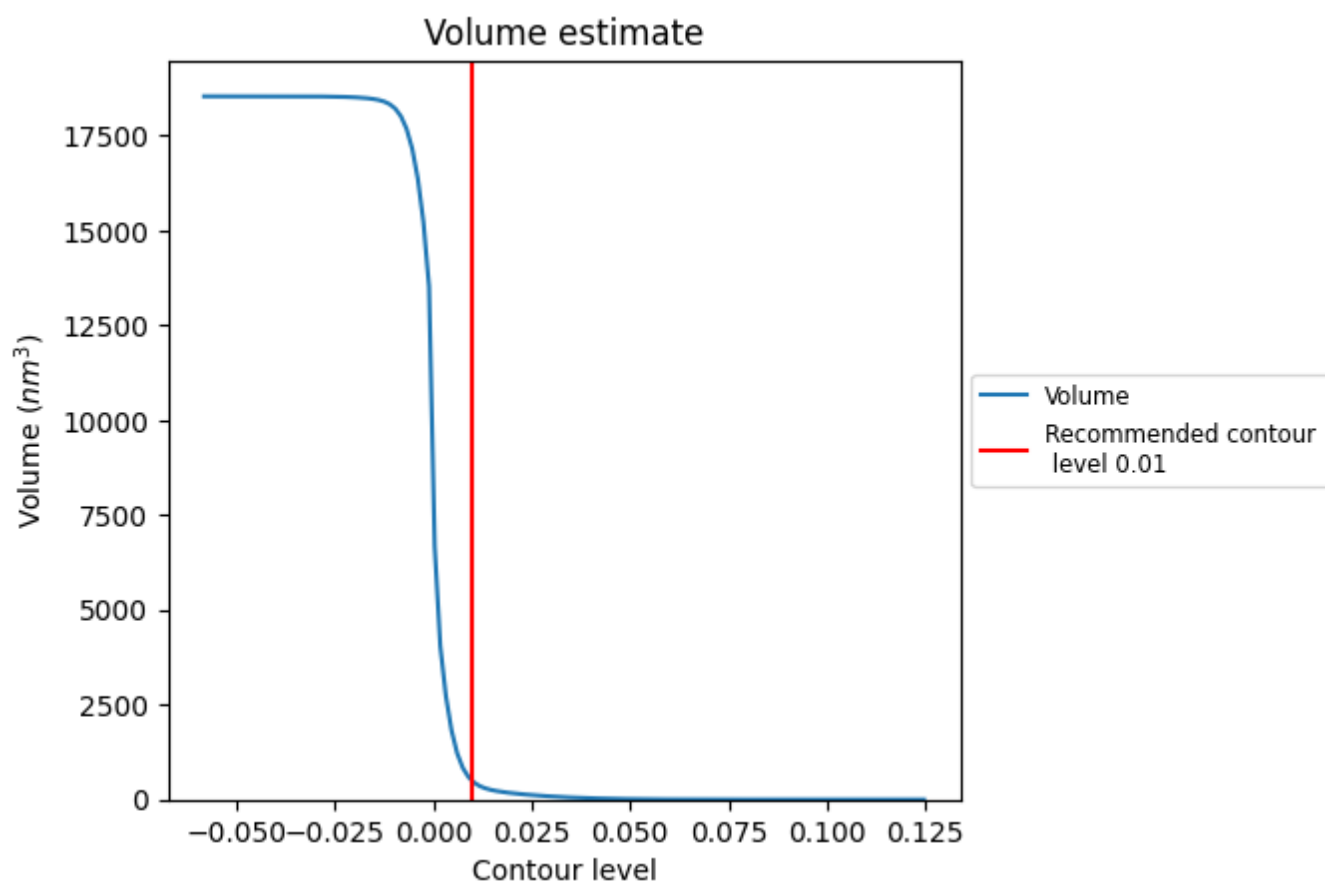
This section contains the results of statistical analysis of the map.

### 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.

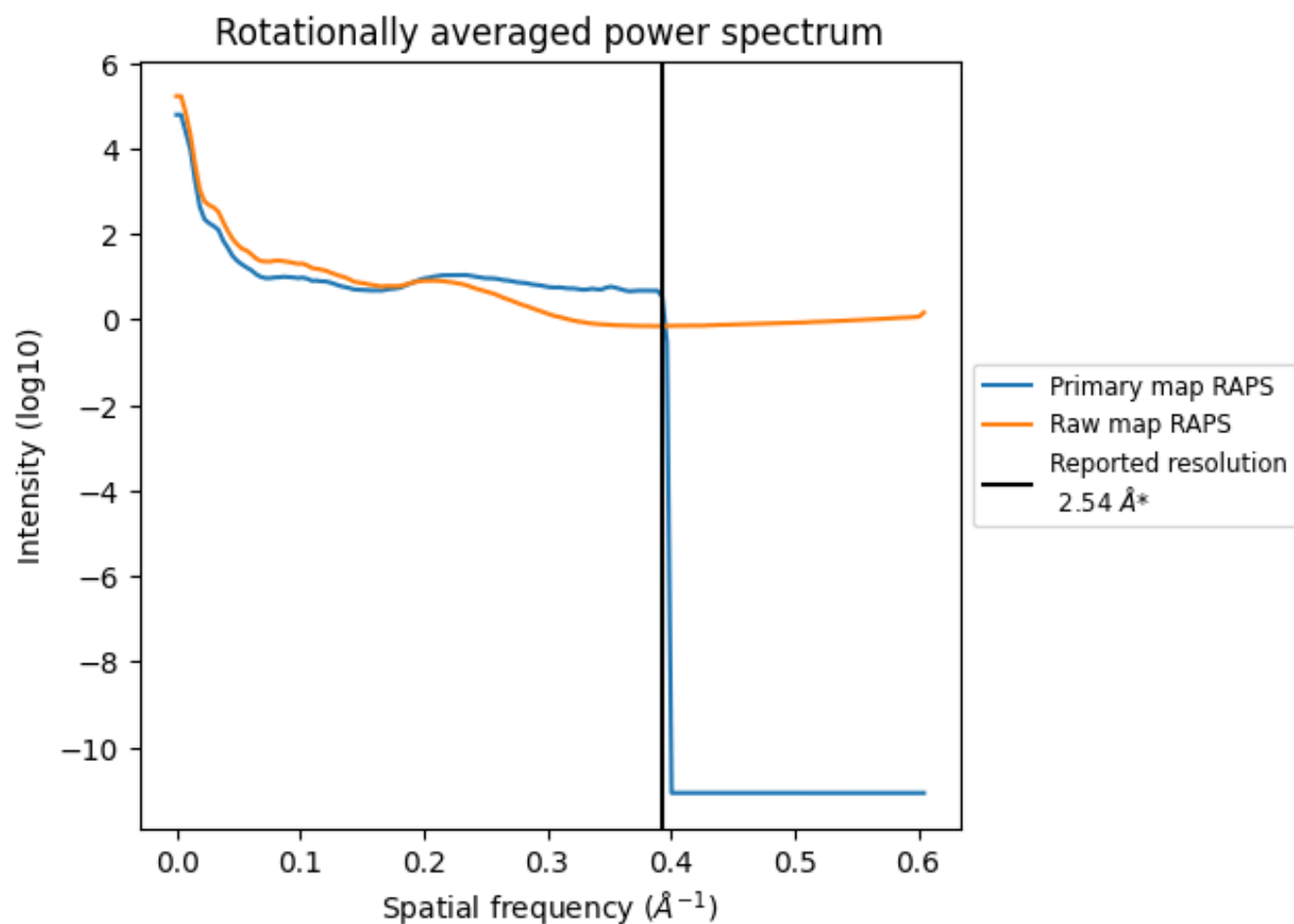
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 483  $\text{nm}^3$ ; this corresponds to an approximate mass of 436 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 ⓘ

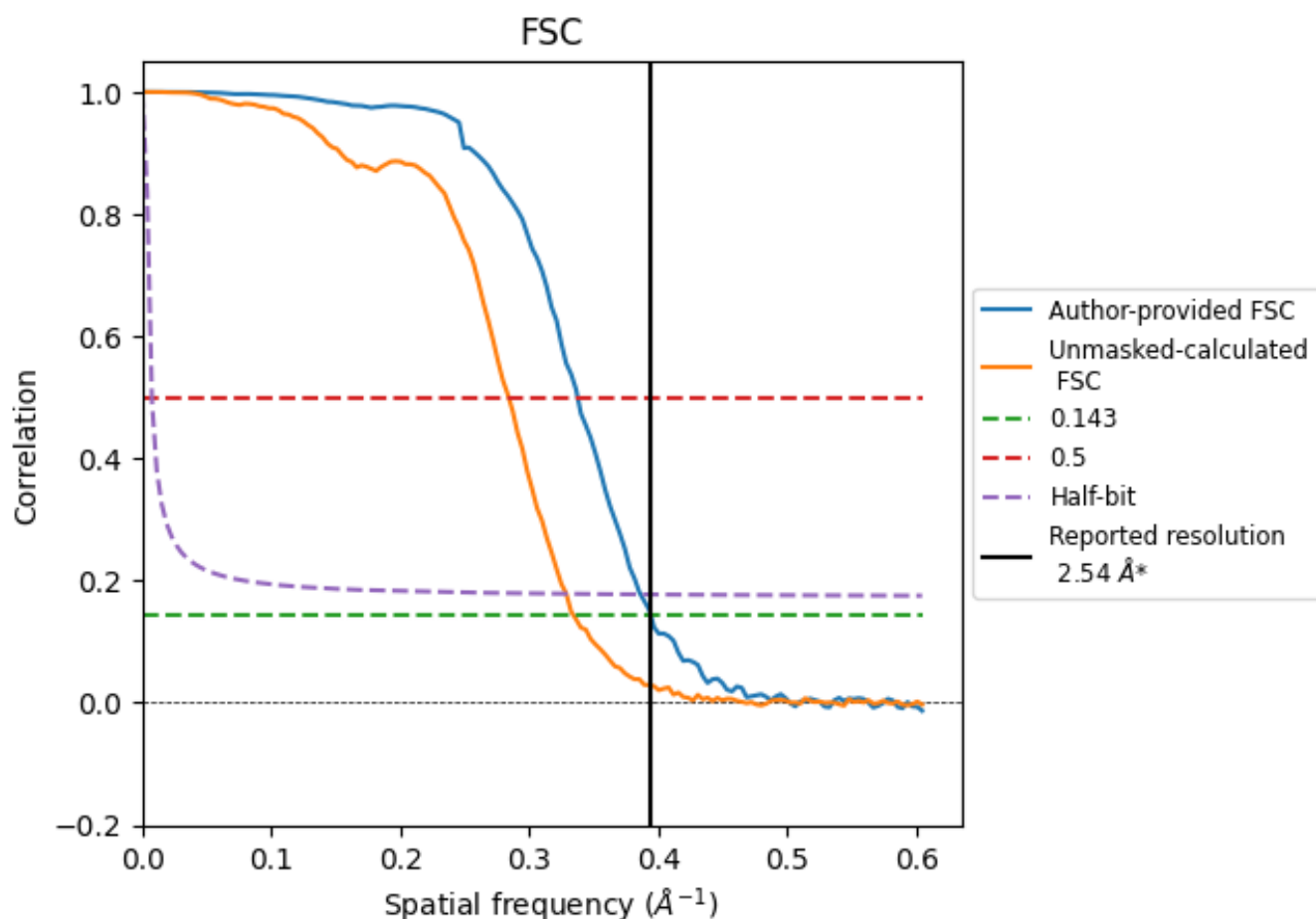


\*Reported resolution corresponds to spatial frequency of 0.394  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.394  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

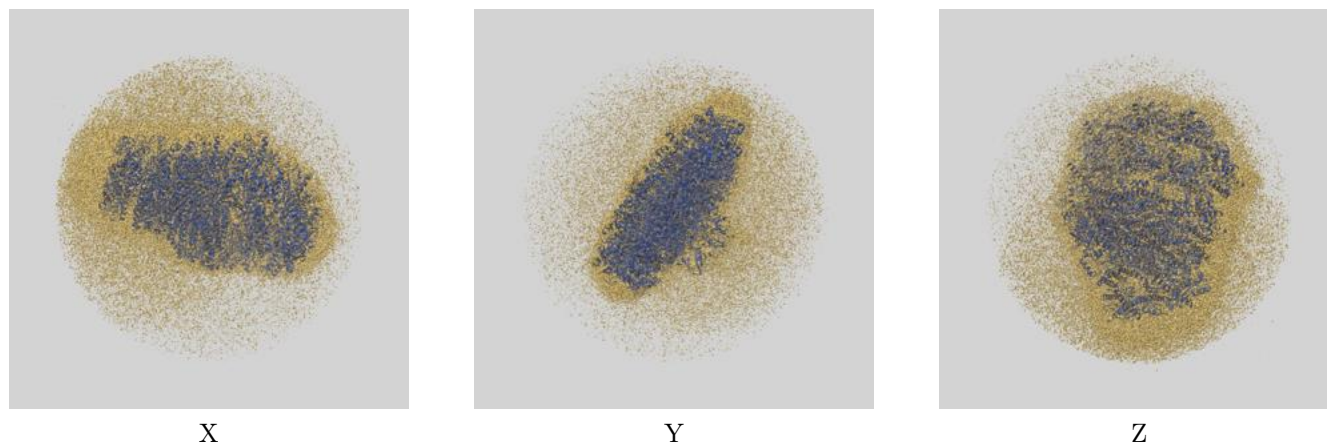
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.54                               | -    | -        |
| Author-provided FSC curve | 2.54                               | 2.96 | 2.59     |
| Unmasked-calculated*      | 2.99                               | 3.52 | 3.04     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.54 by more than 10 %

## 9 Map-model fit [i](#)

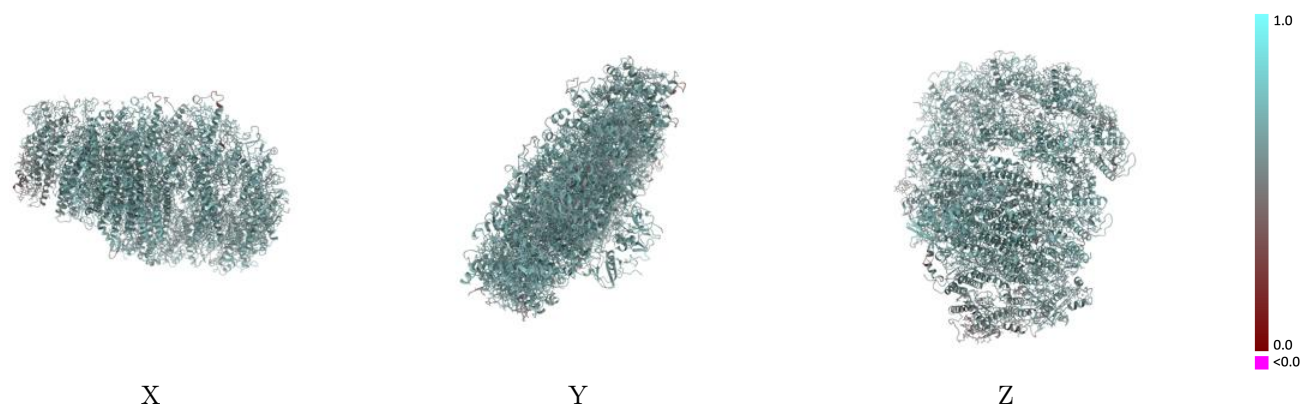
This section contains information regarding the fit between EMDB map EMD-12180 and PDB model 7BGI. Per-residue inclusion information can be found in section [3](#) on page [47](#).

### 9.1 Map-model overlay [i](#)



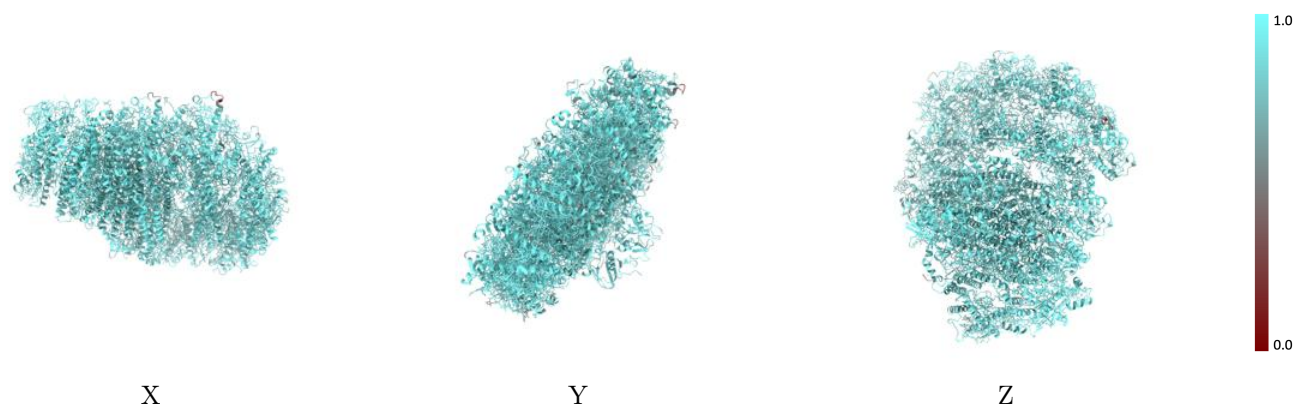
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



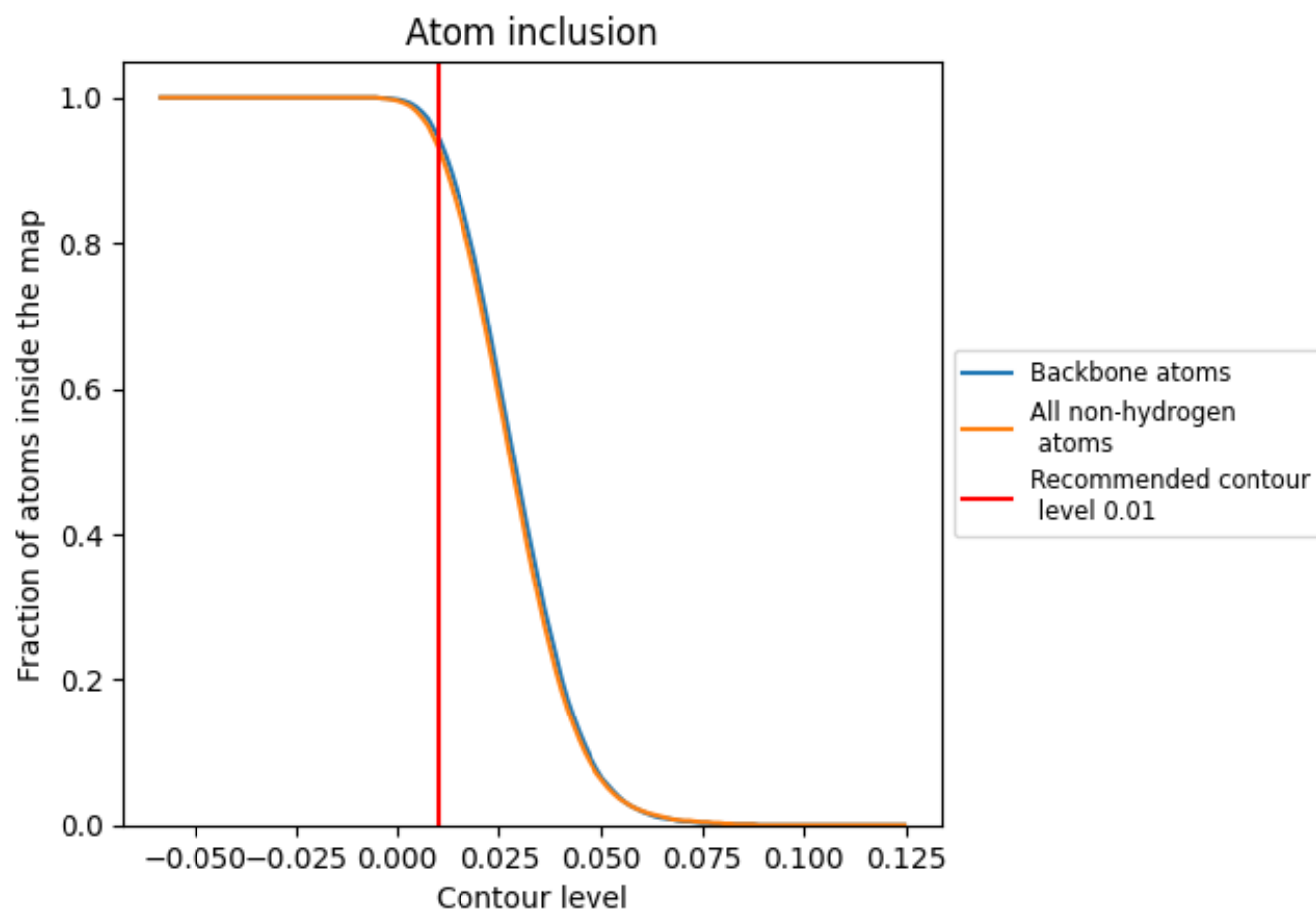
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.9320 | <div><div></div></div> 0.6290 |
| 1     | <div><div></div></div> 0.9110 | <div><div></div></div> 0.6250 |
| 2     | <div><div></div></div> 0.8940 | <div><div></div></div> 0.5190 |
| 3     | <div><div></div></div> 0.9240 | <div><div></div></div> 0.6360 |
| 4     | <div><div></div></div> 0.8850 | <div><div></div></div> 0.6060 |
| 5     | <div><div></div></div> 0.8950 | <div><div></div></div> 0.6180 |
| 6     | <div><div></div></div> 0.9010 | <div><div></div></div> 0.6180 |
| 7     | <div><div></div></div> 0.9310 | <div><div></div></div> 0.6430 |
| 8     | <div><div></div></div> 0.9370 | <div><div></div></div> 0.6450 |
| 9     | <div><div></div></div> 0.9380 | <div><div></div></div> 0.5690 |
| A     | <div><div></div></div> 0.9590 | <div><div></div></div> 0.6640 |
| B     | <div><div></div></div> 0.9710 | <div><div></div></div> 0.6600 |
| C     | <div><div></div></div> 0.9700 | <div><div></div></div> 0.6640 |
| D     | <div><div></div></div> 0.9410 | <div><div></div></div> 0.6380 |
| E     | <div><div></div></div> 0.9530 | <div><div></div></div> 0.6430 |
| F     | <div><div></div></div> 0.9410 | <div><div></div></div> 0.6430 |
| G     | <div><div></div></div> 0.9100 | <div><div></div></div> 0.5900 |
| I     | <div><div></div></div> 0.9750 | <div><div></div></div> 0.6150 |
| J     | <div><div></div></div> 0.9600 | <div><div></div></div> 0.6600 |
| K     | <div><div></div></div> 0.8510 | <div><div></div></div> 0.5850 |
| L     | <div><div></div></div> 0.9030 | <div><div></div></div> 0.5770 |
| Z     | <div><div></div></div> 0.8490 | <div><div></div></div> 0.5870 |

1.0

0.0

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